

### **Linking volatile and non-volatile compounds to sensory profiles and consumer liking of wild edible Nordic mushrooms**

Current information on the links between the chemistry and hedonic liking of edible mushrooms is scarce. In this study, 84 consumers evaluated the appearance, odor, taste, texture and overall liking of samples of Nordic edible wild mushroom species. Subsequently, multivariate models on the effects of non-volatile compounds, odor-contributing volatile compounds, sensory attributes and hedonic likings were created. The non-volatile compounds were measured with quantitative NMR. The five studied mushroom species were different in their sugar and acid contents. Three consumer clusters were found with species\*cluster interactions. Correlations with sensory attributes and chemical components were found, and the multivariate models indicated predictor attributes for each consumer cluster. The results indicate that the sensory properties could be correlated to both volatile and non-volatile compounds, there are consumer clusters with differing likings as regards mushrooms, and these clusters are heterogenic groups with no simple factors such as age explaining their liking scores.

#### **General information**

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Organisations: Materials Science and Environmental Engineering, Turun yliopisto, Tokyo University of Agriculture

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Research output: Contribution to journal > Article > Scientific > peer-review

### **Programmable responsive hydrogels inspired by classical conditioning algorithm**

Living systems have inspired research on non-biological dynamic materials and systems chemistry to mimic specific complex biological functions. Upon pursuing ever more complex life-inspired non-biological systems, mimicking even the most elementary aspects of learning is a grand challenge. We demonstrate a programmable hydrogel-based model system, whose behaviour is inspired by associative learning, i.e., conditioning, which is among the simplest forms of learning. Algorithmically, associative learning minimally requires responsivity to two different stimuli and a memory element. Herein, nanoparticles form the memory element, where a photoacid-driven pH-change leads to their chain-like assembly with a modified spectral behaviour. On associating selected light irradiation with heating, the gel starts to melt upon the irradiation, originally a neutral stimulus. A logic diagram describes such an evolution of the material response. Coupled chemical reactions drive the system out-of-equilibrium, allowing forgetting and memory recovery. The findings encourage to search non-biological materials towards associative and dynamic properties.

#### **General information**

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Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, Aalto University

Contributors: Zhang, H., Zeng, H., Priimägi, A., Ikkala, O.

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Research output: Contribution to journal › Article › Scientific › peer-review

### **Controlled Orientations of Neighboring Tetracene Units by Mixed Self-Assembled Monolayers on Gold Nanoclusters for High-Yield and Long-Lived Triplet Excited States through Singlet Fission**

Although tetracene (Tc) is well-known as a good candidate for singlet fission (SF), the number of high-yield and long-lived triplet excited states through SF is extremely limited because of the relative acceleration of the reverse triplet-triplet annihilation (TTA) considering the energy matching between a singlet and two triplet states. Systematic control of electronic interactions between two neighboring units using conventional covalent linkages and molecular assembly methods to optimize these kinetic processes is quite difficult because of the complicated synthesis and random orientations. In this study, we propose a novel supramolecular strategy utilizing mixed self-assembled monolayers (SAMs) with two different chain lengths. Specifically, mixed Tc-SAMs on gold nanoclusters, which are prepared using Tc-modified heterodisulfides with two different chain lengths, attain high-yield SF ( $\Phi_{SF} \approx 90\%$ ) and individual triplet yields ( $\Phi_T \approx 160\%$ ). The obtained  $\Phi_{SF}$  is the highest value among Tc derivatives in homogeneous solution to the best of our knowledge.

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Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, Keio University, Kobe University

Contributors: Saegusa, T., Sakai, H., Nagashima, H., Kobori, Y., Tkachenko, N. V., Hasobe, T.

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Research output: Contribution to journal › Article › Scientific › peer-review

### **Effects of anode materials on electricity production from xylose and treatability of TMP wastewater in an up-flow microbial fuel cell**

The aim of this study was to determine an optimal anode material for electricity production and COD removal from xylose containing synthetic wastewater in an up-flow microbial fuel cell (MFC), and assess its suitability for treatment of thermomechanical pulping (TMP) wastewater with an enrichment culture at 37 °C. The anode materials tested included carbon-based electrodes (graphite plate, carbon cloth and zeolite coated carbon cloth), metal-based electrodes (tin coated copper) and a metal-carbon assembly (granular activated carbon in stainless steel cage). During continuous operation with xylose, COD removal was 77–86% of which 25–28% was recovered as electricity. The highest power density of 333 ( $\pm 15$ ) mW/m<sup>2</sup> was obtained with the carbon cloth electrode. However, based on an overall analysis including electrode performance, surface area and scalability, the granular activated carbon in stainless steel cage (GAC in SS cage) was chosen to be used as electrode for bioelectrochemical treatment of TMP wastewater. The TMP fed MFC was operated in continuous mode with 1.8 days hydraulic retention time, resulting in 47 ( $\pm 13\%$ ) COD removal of which 1.5% was recovered as electricity with the average power production of 10–15 mW/m<sup>2</sup>. During operation with TMP wastewater, membrane fouling increased the polarization resistance causing a 50% decrease in power production within 30 days. This study shows that MFC pretreatment removes half of the TMP wastewater COD load, reducing the energy required for aerobic treatment.

#### **General information**

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Organisations: Research group: Bio- and Circular Economy, Materials Science and Environmental Engineering, Natl. University of Ireland, Galway, Indian Institute of Technology Hyderabad, Microscopy Center, Kyung Hee University

Contributors: Haavisto, J., Dessi, P., Chatterjee, P., Honkanen, M., Noori, M. T., Kokko, M., Lakaniemi, A. M., Lens, P. N., Puhakka, J. A.

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#### Multiresonant High-Q Plasmonic Metasurfaces

Resonant metasurfaces are devices composed of nanostructured subwavelength scatterers that generate narrow optical resonances, enabling applications in filtering, nonlinear optics, and molecular fingerprinting. It is highly desirable for these applications to incorporate such devices with multiple high-quality-factor resonances; however, it can be challenging to obtain more than a pair of narrow resonances in a single plasmonic surface. Here, we demonstrate a multiresonant metasurface that operates by extending the functionality of surface lattice resonances, which are the collective responses of arrays of metallic nanoparticles. This device features a series of resonances with high-quality factors ( $Q \sim 40$ ), an order of magnitude larger than what is typically achievable with plasmonic nanoparticles, as well as a narrow free spectral range. This design methodology can be used to better tailor the transmission spectrum of resonant metasurfaces and represents an important step toward the miniaturization of optical devices.

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Organisations: Physics, Research group: Nonlinear Optics, Iridian Spectral Technologies, University of Rochester Institute of Optics

Contributors: Reshef, O., Saad-Bin-Alam, M., Huttunen, M. J., Carlow, G., Sullivan, B. T., Ménard, J. M., Dolgaleva, K., Boyd, R. W.

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Research output: Contribution to journal > Article > Scientific > peer-review

## Strategies To Diminish the Emissions of Particles and Secondary Aerosol Formation from Diesel Engines

Particle emissions and secondary aerosol formation from internal combustion engines deteriorate air quality and significantly affect human wellbeing and health. Both the direct particle emissions and the emissions of compounds contributing to secondary aerosol formation depend on choices made in selecting fuels, engine technologies, and exhaust aftertreatment (EAT). Here we study how catalytic EATs, particle filtration, and fuel choices affect these emissions concerning heavy-duty diesel engine. We observed that the most advanced EAT decreased the emissions of fresh exhaust particle mass as much as 98% (from 44.7 to 0.73 mg/kWh) and the formation of aged exhaust particle mass ~100% (from 106.2 to ~0 mg/kWh). The composition of emitted particles depended significantly on the EAT and oxidative aging. While black carbon typically dominated the composition of fresh exhaust particles, aged particles contained more sulfates and organics. The fuel choices had minor effects on the secondary aerosol formation, implicating that, in diesel engines, either the lubricant is a significant source of secondary aerosol precursors or the precursors are formed in the combustion process. Results indicate that the utilization of EAT in diesel engines would produce benefits with respect to exhaust burden on air quality, and thus their utilization should be promoted especially in geographical areas suffering from poor air quality.

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Contributors: Karjalainen, P., Rönkkö, T., Simonen, P., Ntziachristos, L., Juuti, P., Timonen, H., Teinilä, K., Saarikoski, S., Saveljeff, H., Lauren, M., Happonen, M., Matilainen, P., Maunula, T., Nuottimäki, J., Keskinen, J.

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## Porous polybutylene succinate films enabling adhesion of human embryonic stem cell-derived retinal pigment epithelial cells (hESC-RPE)

In the last decade, several studies have shown that polybutylene succinate (PBSu) has a high potential as a biomaterial enabling cell adhesion and growth. In this study, porous PBSu films have been prepared by the breath figure method (BF) and by particulate leaching (PL), and characterized in terms of thickness, surface properties, diffusion capacity and in vitro stability. Because porous films are of high interest for tissue engineering of retinal pigment epithelium (RPE), the initial viability and adhesion of human embryonic stem cell-derived RPE onto the PBSu films was then evaluated. To the best of our knowledge, this is the first study on the adhesion behavior of hESC-RPE onto porous and biodegradable polymer surfaces. The results clearly demonstrated that the two manufacturing methods produced materials with very distinct properties. Films produced by BF expressively demonstrated the highest roughness and surface area, and the lowest water contact angle. These features likely contributed to increase the biocompatibility of the surface, particularly when coated with laminin and collagen IV, as observed by the improved cell viability, cell morphology, adhesion and production of extracellular matrix proteins. Altogether, our results showed not only that PBSu holds high potential in retinal tissue engineering, but also that the physical properties and biocompatibility of the material are highly dependent on the adopted casting method.

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Contributors: Calejo, M. T., Haapala, A., Skottman, H., Kellomäki, M.  
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#### Behavior of the DPH fluorescence probe in membranes perturbed by drugs

1,6-Diphenyl-1,3,5-hexatriene (DPH) is one of the most commonly used fluorescent probes to study dynamical and structural properties of lipid bilayers and cellular membranes via measuring steady-state or time-resolved fluorescence anisotropy. In this study, we present a limitation in the use of DPH to predict the order of lipid acyl chains when the lipid bilayer is doped with itraconazole (ITZ), an antifungal drug. Our steady-state fluorescence anisotropy measurements showed a significant decrease in fluorescence anisotropy of DPH embedded in the ITZ-containing membrane, suggesting a substantial increase in membrane fluidity, which indirectly indicates a decrease in the order of the hydrocarbon chains. This result or its interpretation is in disagreement with the fluorescence recovery after photobleaching measurements and molecular dynamics (MD) simulation data. The results of these experiments and calculations indicate an increase in the hydrocarbon chain order. The MD simulations of the bilayer containing both ITZ and DPH provide explanations for these observations. Apparently, in the presence of the drug, the DPH molecules are pushed deeper into the hydrophobic membrane core below the lipid double bonds, and the probe predominately adopts the orientation of the ITZ molecules that is parallel to the membrane surface, instead of orienting parallel to the lipid acyl chains. For this reason, DPH anisotropy provides information related to the less ordered central region of the membrane rather than reporting the properties of the upper segments of the lipid acyl chains.

#### General information

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Organisations: Physics, Research group: Biological Physics and Soft Matter, Research area: Computational Physics, Uniwersytet Jagiellonski w Krakowie, Max Planck Institute of Colloids and Interfaces, J. Heyrovský Institute of Physical Chemistry  
Contributors: Poojari, C., Wilkosz, N., Lira, R. B., Dimova, R., Jurkiewicz, P., Petka, R., Kepczynski, M., Róg, T.  
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## **Influence of ions to modulate hydrazone and oxime reaction kinetics to obtain dynamically cross-linked hyaluronic acid hydrogels**

Dynamic covalent chemistry forming hydrazone and oxime linkages is attractive due to its simplicity, selectivity and compatibility under aqueous conditions. However, the low reaction rate at physiological pH hampers its use in biomedical applications. Herein, we present different monovalent and bivalent aqueous salt solutions as bio-friendly, non-toxic catalysts which can drive the hydrazone and oxime reactions with excellent efficacy at physiological pH. Direct comparison of hydrazone and oxime reactions using a small molecule model, without any salt catalysis, indicated that oxime formation is 6-times faster than hydrazone formation. Addition of different salts (NaCl, NaBr, KCl, LiCl, LiClO<sub>4</sub>, Na<sub>2</sub>SO<sub>4</sub>, MgCl<sub>2</sub> and CaCl<sub>2</sub>) accelerated the pseudo-first-order reaction kinetics by ~1.2-4.9-fold for acylhydrazone formation and by ~1.5-6.9-fold for oxime formation, in a concentration-dependent manner. We further explored the potential of such catalysts to develop acylhydrazone and oxime cross-linked hyaluronic acid (HA) hydrogels with different physicochemical properties without changing the degree of chemical modification. Analogous to the small molecule model system, the addition of monovalent and divalent salts as catalysts significantly reduced the gelling time. The gelling time for the acylhydrazone cross-linked HA-hydrogel (1.6 wt%) could be reduced from 300 min to 1.2 min by adding 100 mM CaCl<sub>2</sub>, while that for the oxime cross-linked HA-hydrogel (1.2 wt%) could be reduced from 68 min to 1.1 min by adding 50 mM CaCl<sub>2</sub>. This difference in the gelling time also resulted in hydrogels with differential swelling properties as measured after 24 h. Our results are the first to demonstrate the use of salts, for catalyzing hydrogel formation under physiologically relevant conditions.

### **General information**

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Organisations: BioMediTech, Research group: Biomaterials and Tissue Engineering Group, University of Montreal, Uppsala University

Contributors: Wang, S., Nawale, G. N., Oommen, O. P., Hilborn, J., Varghese, O. P.

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Research output: Contribution to journal > Article > Scientific > peer-review

## **Characterizing the micro-impact fatigue behavior of APS and HVOF-sprayed ceramic coatings**

The fatigue life of thermally sprayed Al<sub>2</sub>O<sub>3</sub>- and Cr<sub>2</sub>O<sub>3</sub>-based coatings has been studied under low-energy (0.7–5 mJ) impact conditions. A threshold impact energy and amount of repetitions the coatings can endure with said energy before catastrophic failure was obtained. The catastrophic failure was determined to occur when the fracture mode of the coating switched from brittle cone cracking to quasi-plastic radial cracking. The results are examined relative to the microstructural features along with other properties of the coatings - hardness and cavitation resistance. The experiment provided a new approach for a straightforward comparison of the micro-scale impact fatigue life of thermally sprayed coatings unachievable with previous methods.

### **General information**

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Organisations: Materials Science, Université Bourgogne Franche-Comté - ICB - UTBM - LERMPS

Contributors: Kiiilakoski, J., Langlade, C., Koivuluoto, H., Vuoristo, P.

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Research output: Contribution to journal › Article › Scientific › peer-review

#### Chlorine induced high-temperature corrosion mechanisms in HVOF and HVOF sprayed Cr<sub>3</sub>C<sub>2</sub>-based hardmetal coatings

A novel method that combines thermal analysis and traditional furnace corrosion tests was used to study the corrosion behaviour of thermally sprayed Cr<sub>3</sub>C<sub>2</sub>-based hardmetal coatings at 450 °C and 550 °C under a KCl deposit. This method enabled the identification of the onset temperature of chlorine-induced oxidation to be within 450–500 °C. Two corrosion mechanisms were suggested for these temperatures. At 450 °C, the corrosion rate was slow and mainly controlled by the formation of K<sub>2</sub>CrO<sub>4</sub>. Exposure at 550 °C caused the formation of fine interconnected secondary-carbide precipitates in the metal matrix. Their fast corrosion was identified as the major cause of degradation.

#### General information

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Contributors: Fantozzi, D., Matikainen, V., Uusitalo, M., Koivuluoto, H., Vuoristo, P.

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#### Bibliographical note

EXT="Uusitalo, Mikko"

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Research output: Contribution to journal › Article › Scientific › peer-review

#### Bayesian inversion of a forest reflectance model using Sentinel-2 and Landsat 8 satellite images

The inversion of reflectance models is a generalizable tool to obtain estimates on forest biophysical parameters, such as leaf area index, with theoretically little information need from a study area, instead relying on the knowledge about physical processes in the forest radiation regime. The use of prior information can greatly improve the reflectance model inversion, however, the literature does not yet provide much information on the selection of priors and their influence on the inversion results. In this study, we used a Bayesian approach to invert the PARAS forest reflectance model and retrieve leaf area index from Sentinel-2 MSI and Landsat 8 OLI multispectral satellite images. The PARAS model is based on the theory of spectral invariants, which describes the influence of wavelength-independent parameters on forest radiative transfer. The Bayesian inversion approach is highly flexible, provides uncertainty quantification, and enables the explicit incorporation of prior knowledge into the inversion process. We found that the choice of prior information is crucial in inverting a forest reflectance model to predict leaf area index. Regularizing and informative priors for leaf area index strongly improved the

predictions, relative to an uninformative prior, in that they counteracted the saturation effect of the optical signal occurring at high values for leaf area index. The predictions of leaf area index were more accurate for Landsat 8 than for Sentinel-2, due to potential inconsistencies in the visible bands of Sentinel-2 in our data, and the higher spectral resolution.

#### General information

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Organisations: Computing Sciences, Aalto University, University of Eastern Finland  
Contributors: Schraik, D., Varvia, P., Korhonen, L., Rautiainen, M.  
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Research output: Contribution to journal > Article > Scientific > peer-review

#### Photochemistry of dithiophosphinate $\text{Ni}(\text{S}_2\text{P}(\text{i-Bu})_2)_2$ complex in $\text{CCl}_4$ . Transient species and TD-DFT calculations

Femtosecond spectroscopy and nanosecond laser flash photolysis were used to study the photophysical and photochemical transformations of the bis-diisobutyl-dithiophosphinate Ni(II) complex ( $\text{Ni}(\text{S}_2\text{P}(\text{i-Bu})_2)_2 = \text{Ni}(\text{dtpi})_2$ , where  $\text{dtpi}^- \equiv \text{S}_2\text{P}(\text{i-Bu})_2$ ) in  $\text{CCl}_4$  solutions. The radiation of second harmonic (405 nm) of Ti:Sapphire laser transfers the  $\text{Ni}(\text{dtpi})_2$  complex to an excited  $^1\text{LMCT}$  state. Its decay in  $\text{CCl}_4$  is described by three exponents with time constants 0.58, 2.0 and  $\sim 150$  ps. The first process apparently involves the fast transitions from  $^1\text{LMCT}$  state to  $^3\text{LMCT}$  due to the intersystem crossing (ISC) and then to lower-lying "hot"  $^3\text{LF}$  (Ligand Field) state. The second time constant, most likely, corresponds to the vibrational cooling of this "hot"  $^3\text{LF}$  state. And the third slow process is the transition from  $^3\text{LF}$  state to ground state ( $^1\text{GS}$ ). The quantum yield of photochemical transformation under the 405 irradiation is close to zero, so the study of photochemistry was performed with a nanosecond flash photolysis at 308 nm. In this case an electron transfer from the excited  $\text{Ni}(\text{dtpi})_2$  complex to a solvent molecule leads to the appearance of primary intermediate, the  $[\text{ClNi}(\text{dtpi})(\text{dtpi}^{\cdot\text{rad}})]$  complex, in which a  $\text{dtpi}^{\cdot\text{rad}}$  radical is coordinated with a nickel ion via one sulfur atom. In the fast reaction with  $\text{Ni}(\text{dtpi})_2$ , this complex forms a long-lived dimer  $\text{ClNi}(\text{dtpi})(\text{dtpi}^{\cdot\text{rad}})[\text{Ni}(\text{dtpi})_2]$ . This intermediate for a few hundred microseconds decays in the reaction of recombination with the formation of  $(\text{dtpi})_2$  disulphide and unstable  $\text{ClNi}(\text{dtpi})$  complex. The insoluble  $\text{NiCl}_2$  salt failed in  $\text{CCl}_4$  as the sediment due to the reaction of two  $\text{ClNi}(\text{dtpi})$  complexes. The quantum chemical calculations allowed to determine the geometry of the intermediate complexes arising in the photochemistry of  $\text{Ni}(\text{S}_2\text{P}(\text{i-Bu})_2)_2$  complex.

#### General information

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Organisations: Materials Science and Environmental Engineering, Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Novosibirsk State University, Boreskov Institute of Catalysis SB RAS, Nikolaev Institute of Inorganic Chemistry SB RAS  
Contributors: Solovyev, A. I., Mikheyli, A. V., Plyusnin, V. F., Shubin, A. A., Grivin, V. P., Larionov, S. V., Tkachenko, N. V., Lemmetyinen, H.  
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Source ID: 85067953554

Research output: Contribution to journal › Article › Scientific › peer-review

### **Erosion wear performance of WC-10Co4Cr and Cr<sub>3</sub>C<sub>2</sub>-25NiCr coatings sprayed with high-velocity thermal spray processes**

Thermally sprayed hardmetal coatings are widely used to protect components and surfaces against wear in various applications. Hard and wear resistant coatings increase the component lifetime and can generate significant savings promoting ecological manufacturing. This study focuses on the performance of tungsten carbide (WC-10Co4Cr) and chromium carbide (Cr<sub>3</sub>C<sub>2</sub>-25NiCr) based hardmetal coatings sprayed with gaseous and liquid fuelled high-velocity oxygen-fuel (HVOF) spray processes and a modern high-velocity air-fuel (HVOF) spray process. The coating characterisation revealed reduced carbide dissolution with decreasing process temperature and denser feedstock powder particles. Smaller carbide size in the Cr<sub>3</sub>C<sub>2</sub>-25NiCr material significantly reduced the carbide rebounding leading to higher carbide content in the sprayed coating and improved erosion wear resistance. Most significant improvements were observed in cavitation erosion for HVOF sprayed WC-10Co4Cr coatings (0.4 µm/h) compared to the HVOF sprayed coatings (1.5–3.7 µm/h). The cavitation erosion resistance of the HVOF sprayed coatings was almost at the level of the WC-10Co sintered bulk (0.2 µm/h).

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Tampere University, VZÚ Plzeň - Research and Testing Institute

Contributors: Matikainen, V., Rubio Peregrina, S., Ojala, N., Koivuluoto, H., Schubert, J., Houdková, Vuoristo, P.

Number of pages: 17

Pages: 196-212

Publication date: 25 Jul 2019

Peer-reviewed: Yes

#### **Publication information**

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ISSN (Print): 0257-8972

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Keywords: Cavitation erosion, Coating, Hardmetal, Slurry erosion, Thermal spray

DOIs:

10.1016/j.surfcoat.2019.04.067

#### **Bibliographical note**

INT=msee,"Rubio Peregrina, S."

Source: Scopus

Source ID: 85065223119

Research output: Contribution to journal › Article › Scientific › peer-review

### **Observation of Coexistence of Yu-Shiba-Rusinov States and Spin-Flip Excitations**

We investigate the spectral evolution in different metal phthalocyanine molecules on NbSe<sub>2</sub> surface using scanning tunnelling microscopy (STM) as a function of the coupling with the substrate. For manganese phthalocyanine (MnPc), we demonstrate a smooth spectral crossover from Yu-Shiba-Rusinov (YSR) bound states to spin-flip excitations. This has not been observed previously and it is in contrast to simple theoretical expectations. We corroborate the experimental findings using numerical renormalization group calculations. Our results provide fundamental new insight on the behavior of atomic scale magnetic/SC hybrid systems, which is important, for example, for engineered topological superconductors and spin logic devices.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Aalto University, Jozef Stefan Institute, University of Ljubljana

Contributors: Kezilebieke, S., Žitko, R., Dvorak, M., Ojanen, T., Liljeroth, P.

Number of pages: 6

Pages: 4614-4619

Publication date: 10 Jul 2019

Peer-reviewed: Yes

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ISSN (Print): 1530-6984

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Materials Science(all), Condensed Matter Physics, Mechanical Engineering

Keywords: Magnetic impurity, scanning tunneling microscopy (STM), spin-flip excitation, superconductor, Yu-Shiba-Rusinov state

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Source: Scopus

Source ID: 85069329661

Research output: Contribution to journal > Article > Scientific > peer-review

### FCC-hh: The Hadron Collider: Future Circular Collider Conceptual Design Report Volume 3

In response to the 2013 Update of the European Strategy for Particle Physics (EPPSU), the Future Circular Collider (FCC) study was launched as a world-wide international collaboration hosted by CERN. The FCC study covered an energy-frontier hadron collider (FCC-hh), a highest-luminosity high-energy lepton collider (FCC-ee), the corresponding 100 km tunnel infrastructure, as well as the physics opportunities of these two colliders, and a high-energy LHC, based on FCC-hh technology. This document constitutes the third volume of the FCC Conceptual Design Report, devoted to the hadron collider FCC-hh. It summarizes the FCC-hh physics discovery opportunities, presents the FCC-hh accelerator design, performance reach, and staged operation plan, discusses the underlying technologies, the civil engineering and technical infrastructure, and also sketches a possible implementation. Combining ingredients from the Large Hadron Collider (LHC), the high-luminosity LHC upgrade and adding novel technologies and approaches, the FCC-hh design aims at significantly extending the energy frontier to 100 TeV. Its unprecedented centre-of-mass collision energy will make the FCC-hh a unique instrument to explore physics beyond the Standard Model, offering great direct sensitivity to new physics and discoveries.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Electrical Engineering, CNRS Centre National de la Recherche Scientifique, Istituto Nazionale di Fisica Nucleare Sezione di Bari (INFN BA), Università degli Studi di Bari, Shahid Beheshti University, Bochar Institute of Inorganic Materials (VNIINM), University of Oxford, Royal Holloway University (RHUL), University of Applied Sciences Technikum Wien (UAS TW), TOBB University of Economics and Technology, University of Belgrade, Harvard University, Universidad de Granada, Universitat Politècnica de Valencia, Spain, Paul Scherrer Institut, European Organization for Nuclear Research, Laboratorio Accelatori e Superconduttività Applicata, University Tor Vergata, Kahramanmaraş Sutcu Imam University (KSU), Istituto Nazionale di Fisica Nucleare, Sezione di Catania, Università degli Studi di Catania, University of Manchester, French Atomic Energy Commission (CEA) Saclay, Fermi National Accelerator Laboratory, Istituto Nazionale di Fisica Nucleare, Sezione di Milano, University of Cambridge, University of Birmingham, Eskişehir Technical University (ESTU), Istanbul University, University of California Santa Cruz (UCSC), Linde Kryotechnik AG (Linde), Istituto Nazionale di Fisica Nucleare, Sezione di Firenze, CNR-INO, Università degli Studi di Milano, Massachusetts Institute of Technology, MAN Energy Solutions Schweiz AG (MAN ES), University of Münster, Laboratori Nazionali di Frascati (INFN LNF), Sezione di Padova (INFN PD), Università degli Studi di Padova, Italy, Università di Insubria (UNINSUBRIA)

Contributors: the FCC Collaboration, Abada, A., Abbrescia, M., AbdusSalam, S. S., Abdyukhanov, I., Abelleira Fernandez, J., Abramov, A., Aburua, M., Acar, A. O., Adzic, P. R., Agrawal, P., Aguilar-Saavedra, J. A., Aguilera-Verdugo, J. J., Aiba, M., Aichinger, I., Aielli, G., Akay, A., Akhundov, A., Aksakal, H., Albacete, J. L., Albergo, S., Alekou, A., Aleksa, M., Aleksan, R., Alemany Fernandez, R. M., Alexahin, Y., Alía, R. G., Alioli, S., Alipour Tehrani, N., Allanach, B. C., Allport, P. P., Altinli, M., Altmannshofer, W., Ambrosio, G., Amorim, D., Amstutz, O., Anderlini, L., Andreatza, A., Andreini, M., Andriatis, A., Andris, C., Andronic, A., Angelucci, M., Antinori, F., Antipov, S. A., Antonelli, M., Antonello, M., Lehtinen, T., Penttinen, J. P., Salmi, T., Stenvall, A.

Number of pages: 353  
Pages: 755-1107  
Publication date: 1 Jul 2019  
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Journal: European Physical Journal: Special Topics  
Volume: 228  
Issue number: 4  
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Original language: English  
ASJC Scopus subject areas: Materials Science(all), Physics and Astronomy(all), Physical and Theoretical Chemistry  
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DOIs:  
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<http://urn.fi/URN:NBN:fi:tty-201908282037>  
Source: Scopus  
Source ID: 85068232451  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Pyrolytic behavior of lignocellulosic-based polysaccharides

The thermochemical behavior of cellulose, glucomannan, and xylan was investigated by pyrolysis–gas chromatography–mass spectrometry (Py-GC/MS). In each case, major GC-amenable condensable products were classified into several compound groups, and the formation of these monomer-related fragments from the model substance samples was determined at 500, 600, and 700 °C with a residence time of 5 s and 20 s. The results revealed that despite some general formation trends, no compound group was selectively formed at certain temperatures. Of the 11 product groups, the primary ones, including lactone, furan, and cyclopentenone derivatives, accounted for 72–85% (from cellulose), 86–90% (from glucomannan), and 76–81% (from xylan) of the total amount of pyrolysis products determined. At 500 °C, about half of the major product groups accounted for lactones, such as 3-hydroxy-2-penteno-1,5-lactone and 5H-furan-2-one. It was also confirmed by thermogravimetric analyses that within the temperature range studied, cellulose was thermally more stable than the heterogeneous hemicelluloses. These kinds of data are of importance, for example, with respect to efforts to develop new biorefinery possibilities for renewable resources.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, University of Jyväskylä  
Contributors: Ghalibaf, M., Doddapaneni, T. R. K. C., Alén, R.  
Pages: 121-131  
Publication date: Jul 2019  
Peer-reviewed: Yes  
Early online date: 2018

#### Publication information

Journal: Journal of Thermal Analysis and Calorimetry  
Volume: 137  
Issue number: 1  
ISSN (Print): 1388-6150  
Original language: English  
ASJC Scopus subject areas: Condensed Matter Physics, Physical and Theoretical Chemistry  
Keywords: Cellulose, Condensable products, Glucomannan, Pyrolysis–gas chromatography, Thermogravimetry, Xylan  
DOIs:  
10.1007/s10973-018-7919-y  
Source: Scopus  
Source ID: 85057074557  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Crystalline Wax Esters Regulate the Evaporation Resistance of Tear Film Lipid Layers Associated with Dry Eye Syndrome

Dry eye syndrome (DES), one of the most common ophthalmological diseases, is typically caused by excessive evaporation of tear fluid from the ocular surface. Excessive evaporation is linked to impaired function of the tear film lipid layer (TFLL) that covers the aqueous tear film. The principles of the evaporation resistance of the TFLL have remained unknown, however. We combined atomistic simulations with Brewster angle microscopy and surface potential experiments to explore the organization and evaporation resistance of films composed of wax esters, one of the main components of

the TFLL. The results provide evidence that the evaporation resistance of the TFLL is based on crystalline-state layers of wax esters and that the evaporation rate is determined by defects in the TFLL and its coverage on the ocular surface. On the basis of the results, uncovering the nonequilibrium spreading and crystallization of TFLL films has potential to reveal new means of treating DES.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Helsinki Eye Lab, University of Helsinki, J. Heyrovský Institute of Physical Chemistry, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Computational Physics Laboratory, MEMPHYS-Centre for Biomembrane Physics

Contributors: Paananen, R. O., Javanainen, M., Holopainen, J. M., Vattulainen, I.

Number of pages: 6

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Publication date: 25 Jun 2019

Peer-reviewed: Yes

#### Publication information

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Volume: 10

Issue number: 14

ISSN (Print): 1948-7185

Original language: English

ASJC Scopus subject areas: Materials Science(all), Physical and Theoretical Chemistry

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#### Bibliographical note

EXT="Paananen, Riku O."

Source: Scopus

Source ID: 85069849171

Research output: Contribution to journal > Article > Scientific > peer-review

#### Water-Responsive and Mechanically Adaptive Natural Rubber Composites by in Situ Modification of Mineral Filler Structures

A new biomimetic stimuli-responsive adaptive elastomeric material, whose mechanical properties are altered by a water treatment is reported in this paper. This material is a calcium sulphate ( $\text{CaSO}_4$ ) filled composite with an epoxidized natural rubber (ENR) matrix. By exploiting various phase transformation processes that arise when  $\text{CaSO}_4$  is hydrated, several different crystal structures of  $\text{CaSO}_4 \cdot x\text{H}_2\text{O}$  can be developed in the cross-linked ENR matrix. Significant improvements in the mechanical and thermal properties are then observed in the water-treated composites. When compared with the untreated sample, there is approximately 100% increase in the dynamic modulus. The thermal stability of the composites is also improved by increasing the maximum degradation rate temperature by about 20 °C. This change in behavior results from an in situ development of hydrated crystal structures of the nanosized  $\text{CaSO}_4$  particles in the ENR matrix, which has been verified using Raman spectroscopy, transmission electron microscopy, atomic force microscopy, and X-ray scattering. This work provides a promising and relatively simple pathway for the development of next generation of mechanically adaptive elastomeric materials by an eco-friendly route, which may eventually also be developed into an innovative biodegradable and biocompatible smart polymeric material.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Leibniz-Institut für Polymerforschung Dresden E.V., University of Massachusetts Lowell, Vodafone Department of Mobile Communications Systems, Queen Mary University of London

Contributors: Banerjee, S. S., Hait, S., Natarajan, T. S., Wießner, S., Stöckelhuber, K. W., Jehnichen, D., Janke, A., Fischer, D., Heinrich, G., Busfield, J. J., Das, A.

Number of pages: 8

Pages: 5168-5175

Publication date: 20 Jun 2019

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physical Chemistry B

Volume: 123

Issue number: 24

ISSN (Print): 1520-6106

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry

DOIs:

10.1021/acs.jpccb.9b02125

Source: Scopus

Source ID: 85067653290

Research output: Contribution to journal > Article > Scientific > peer-review

### Epitaxial phases of high Bi content GaSbBi alloys

GaSbBi alloys have recently emerged as attractive materials for mid-infrared optoelectronics owing to strong band gap reduction enabled by Bi incorporation into the GaSb matrix. The fundamental understanding of the epitaxial process required to demonstrate high quality crystals is in an early-developmental phase. From this perspective, we report on the key role played by the Sb/Ga flux ratio in controlling the structural quality and incorporation of high Bi content GaSbBi (up to 14.5%-Bi), revealing three distinct epitaxial phases. The first phase (below stoichiometric Sb/Ga) exhibits Ga-Bi compound droplets, low crystal quality, and reduced Bi content. At the second phase (above stoichiometric Sb/Ga), the crystal exhibits smooth surfaces and excellent crystallinity with efficient Bi incorporation. The last phase corresponds to exceeding a Sb/Ga threshold that leads to reduced Bi incorporation, Bi droplets and degraded crystallinity. This threshold value that defines the optimal growth window is controlled by the temperature as well as the Bi/Ga ratio. Increasing temperature increases the threshold, albeit simultaneously reducing Bi incorporation. Conversely, increasing the Bi/Ga flux ratio increases Bi incorporation, while narrowing down and ultimately closing the window. This study provides a general framework enabling development of high quality GaSbBi heterostructures for emerging mid-infrared optoelectronics.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: ORC

Contributors: Hilska, J., Koivusalo, E., Puustinen, J., Suomalainen, S., Guina, M.

Number of pages: 5

Pages: 67-71

Publication date: 15 Jun 2019

Peer-reviewed: Yes

### Publication information

Journal: Journal of Crystal Growth

Volume: 516

ISSN (Print): 0022-0248

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Inorganic Chemistry, Materials Chemistry

Keywords: A3. Molecular beam epitaxy, B1. Antimonides, B1. Bismuth compounds, B2. Semiconducting III-V materials,

B2. Semiconducting ternary compounds

DOIs:

10.1016/j.jcrysgr.2019.03.028

Source: Scopus

Source ID: 85063780657

Research output: Contribution to journal > Article > Scientific > peer-review

### Tailoring Second-Harmonic Emission from (111)-GaAs Nanoantennas

Second-harmonic generation (SHG) in resonant dielectric Mie-scattering nanoparticles has been hailed as a powerful platform for nonlinear light sources. While bulk-SHG is suppressed in elemental semiconductors, for example, silicon and germanium due to their centrosymmetry, the group of zincblende III-V compound semiconductors, especially (100)-grown AlGaAs and GaAs, have recently been presented as promising alternatives. However, major obstacles to push the technology toward practical applications are the limited control over directionality of the SH emission and especially zero forward/backward radiation, resulting from the peculiar nature of the second-order nonlinear susceptibility of this otherwise highly promising group of semiconductors. Furthermore, the generated SH signal for (100)-GaAs nanoparticles depends strongly on the polarization of the pump. In this work, we provide both theoretically and experimentally a solution to these problems by presenting the first SHG nanoantennas made from (111)-GaAs embedded in a low index material. These nanoantennas show superior forward directionality compared to their (100)-counterparts. Most importantly, based on the special symmetry of the crystalline structure, it is possible to manipulate the SHG radiation pattern of the nanoantennas by changing the pump polarization without affecting the linear properties and the total nonlinear conversion efficiency, hence paving the way for efficient and flexible nonlinear beam-shaping devices.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Nonlinear Optics, Physics, Australian National University, Friedrich-Schiller-University Jena, School of Engineering and Information Technology, University of New South Wales (UNSW) Australia, Russian Academy of Sciences

Contributors: Sautter, J. D., Xu, L., Miroshnichenko, A. E., Lysevych, M., Volkovskaya, I., Smirnova, D. A., Camacho-Morales, R., Zangeneh Kamali, K., Karouta, F., Vora, K., Tan, H. H., Kauranen, M., Staude, I., Jagadish, C., Neshev, D. N., Rahmani, M.

Number of pages: 7

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Publication date: 12 Jun 2019

Peer-reviewed: Yes

### Publication information

Journal: Nano Letters

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ISSN (Print): 1530-6984

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Materials Science(all), Condensed Matter Physics, Mechanical Engineering

Keywords: Dielectric nanoantennas, directional emission, III-V semiconductors, Mie resonance, multipolar interference, second harmonic generation

DOIs:

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Source: Scopus

Source ID: 85067057047

Research output: Contribution to journal > Article > Scientific > peer-review

### The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers

Understanding the molecular mechanisms governing nanoparticle–membrane interactions is of prime importance for drug delivery and biomedical applications. Neutron reflectometry (NR) experiments are combined with atomistic and coarse-grained molecular dynamics (MD) simulations to study the interaction between cationic gold nanoparticles (AuNPs) and model lipid membranes composed of a mixture of zwitterionic di-stearoyl-phosphatidylcholine (DSPC) and anionic di-stearoyl-phosphatidylglycerol (DSPG). MD simulations show that the interaction between AuNPs and a pure DSPC lipid bilayer is modulated by a free energy barrier. This can be overcome by increasing temperature, which promotes an irreversible AuNP incorporation into the lipid bilayer. NR experiments confirm the encapsulation of the AuNPs within the lipid bilayer at temperatures around 55 °C. In contrast, the AuNP adsorption is weak and impaired by heating for a DSPC–DSPG (3:1) lipid bilayer. These results demonstrate that both the lipid charge and the temperature play pivotal roles in AuNP–membrane interactions. Furthermore, NR experiments indicate that the (negative) DSPG lipids are associated with lipid extraction upon AuNP adsorption, which is confirmed by coarse-grained MD simulations as a lipid-crawling effect driving further AuNP aggregation. Overall, the obtained detailed molecular view of the interaction mechanisms sheds light on AuNP incorporation and membrane destabilization.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Biological Physics and Soft Matter, Research area: Computational Physics, Physics, Computational Physics Laboratory, University of Helsinki, Politecnico di Milano, Institut Laue-Langevin, Max Planck Institute of Colloids and Interfaces, MEMPHYS–Center for Biomembrane Physics, Norwegian Univ. of Sci. and Technol., G2Elab/Institut Néel

Contributors: Lolicato, F., Joly, L., Martinez-Seara, H., Fragneto, G., Scoppola, E., Baldelli Bombelli, F., Vattulainen, I., Akola, J., Maccarini, M.

Publication date: 7 Jun 2019

Peer-reviewed: Yes

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Journal: Small

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Issue number: 23

Article number: 1805046

ISSN (Print): 1613-6810

Original language: English

ASJC Scopus subject areas: Biotechnology, Biomaterials, Chemistry(all), Materials Science(all)

Keywords: gold nanoparticles, lipid membranes, molecular dynamics simulations, nanotoxicity, neutron reflectometry

Electronic versions:

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### Bibliographical note

EXT="Martinez-Seara, Hector"

Source: Scopus

Source ID: 85064688737

Research output: Contribution to journal > Article > Scientific > peer-review

### Analytical Expressions for Spring Constants of Capillary Bridges and Snap-in Forces of Hydrophobic Surfaces

When a force probe with a small liquid drop adhered to its tip makes contact with a substrate of interest, the normal force right after contact is called the snap-in force. This snap-in force is related to the advancing contact angle or the contact radius at the substrate. Measuring snap-in forces has been proposed as an alternative to measure the advancing contact angles of surfaces. The snap-in occurs when the distance between the probe surface and the substrate is  $h_S$ , which is amenable to geometry, assuming the drop was a spherical cap before snap-in. Equilibrium is reached at a distance  $h_E < h_S$ . At equilibrium, the normal force  $F = 0$ , and the capillary bridge is a spherical segment, amenable again to geometry. For a small normal displacement  $\Delta h = h - h_E$ , the normal force can be approximated with  $F \approx -k_1 \Delta h$  or  $F \approx -k_1 \Delta h - k_2 \Delta h^2$ , where  $k_1 = -\partial F / \partial h$  and  $k_2 = -1/2 \cdot \partial^2 F / \partial h^2$  are the effective linear and quadratic spring constants of the bridge, respectively. Analytical expressions for  $k_{1,2}$  are found using Kenmotsu's parameterization. Fixed contact angle and fixed contact radius conditions give different forms of  $k_{1,2}$ . The expressions for  $k_1$  found here are simpler, yet equivalent to the earlier derivation by Kusumaatmaja and Lipowsky (2010). Approximate snap-in forces are obtained by setting  $\Delta h = h_S - h_E$ . These approximate analytical snap-in forces agree with the experimental data from Liimatainen et al. (2017) and a numerical method based on solving the shape of the interface. In particular, the approximations are most accurate for super liquid-repellent surfaces. For such surfaces, readers may find this new analytical method more convenient than solving the shape of the interface numerically.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: BioMediTech

Contributors: Sariola, V.

Number of pages: 7

Pages: 7129-7135

Publication date: 4 Jun 2019

Peer-reviewed: Yes

### Publication information

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Issue number: 22

ISSN (Print): 0743-7463

Original language: English

ASJC Scopus subject areas: Materials Science(all), Condensed Matter Physics, Surfaces and Interfaces, Spectroscopy, Electrochemistry

Electronic versions:

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<http://urn.fi/URN:NBN:fi:tty-201906171893>

Source: Scopus

Source ID: 85066806357

Research output: Contribution to journal > Article > Scientific > peer-review

### Correlation of Surface Morphology and Interfacial Adhesive Behavior between Cellulose Surfaces: Quantitative Measurements in Peak-Force Mode with the Colloidal Probe Technique

A better understanding of cellulose-cellulose interactions is needed in applications such as paper making and all-cellulose composites. To date, cellulose-cellulose studies have been chemistry-oriented. In these studies, the sample surfaces have been modified with different chemicals and then tested under an atomic force microscope (AFM) using a colloidal probe (CP). Studies of cellulose-cellulose interaction based on sample morphology and mechanical properties have been rare as

a result of the complex surface structure and the soft texture of the cellulose. The current surface interaction models, such as the Johnson-Kendall-Roberts (JKR) model in which the studied bodies are assumed to have smooth surfaces, can no longer fully reveal the interfacial behavior between two cellulose surfaces. Therefore, we propose a new type of contact model for rough-rough interaction by dividing the surface contacts into primary and secondary levels. The main idea of the new model is to take into account local individual contact details between rough surfaces. The model considers the effect of the surface topography by including the asperities and valleys on a cellulose sphere used as the colloidal probe in imaging the topography of a cellulose membrane (CM). In addition, the correlation between the surface morphology and adhesion is studied. To verify the importance of including the effect of the surface roughness in contact analysis and validate our hypothesis on the correlation between the surface morphology and adhesion, an extensive set of experiments was performed. In the experiments, a combination of the AFM peak-force mode (PFM) and the CP technique was employed to acquire a massive amount of information on cellulose-cellulose interactions by measuring the adhesion among six CSs of different sizes and a CM.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Micro and Nanosystems Research Group, BioMediTech, Harbin Institute of Technology, Tokyo University of Science

Contributors: Lai, Y., Zhang, H., Sugano, Y., Xie, H., Kallio, P.

Number of pages: 10

Pages: 7312-7321

Publication date: 4 Jun 2019

Peer-reviewed: Yes

#### **Publication information**

Journal: Langmuir

Volume: 35

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ISSN (Print): 0743-7463

Original language: English

ASJC Scopus subject areas: Materials Science(all), Condensed Matter Physics, Surfaces and Interfaces, Spectroscopy, Electrochemistry

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Source: Scopus

Source ID: 85066731882

Research output: Contribution to journal > Article > Scientific > peer-review

#### **Methods for simultaneous robot-world-hand-eye calibration: A comparative study**

In this paper, we propose two novel methods for robot-world-hand-eye calibration and provide a comparative analysis against six state-of-the-art methods. We examine the calibration problem from two alternative geometrical interpretations, called 'hand-eye' and 'robot-world-hand-eye', respectively. The study analyses the effects of specifying the objective function as pose error or reprojection error minimization problem. We provide three real and three simulated datasets with rendered images as part of the study. In addition, we propose a robotic arm error modeling approach to be used along with the simulated datasets for generating a realistic response. The tests on simulated data are performed in both ideal cases and with pseudo-realistic robotic arm pose and visual noise. Our methods show significant improvement and robustness on many metrics in various scenarios compared to state-of-the-art methods.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computing Sciences, Remote Handling Project Team

Contributors: Ali, I., Suominen, O., Gotchev, A., Morales, E. R.

Publication date: 2 Jun 2019

Peer-reviewed: Yes

#### **Publication information**

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Volume: 19

Issue number: 12

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ISSN (Print): 1424-8220

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Atomic and Molecular Physics, and Optics, Biochemistry, Instrumentation, Electrical and Electronic Engineering

Keywords: Hand-eye calibration, Optimization, Robot-world-hand-eye calibration

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Source: Scopus

Source ID: 85068904338

Research output: Contribution to journal > Article > Scientific > peer-review

### **Bioimpedance Sensor Array for Long-Term Monitoring of Wound Healing from Beneath the Primary Dressings and Controlled Formation of H<sub>2</sub>O<sub>2</sub> Using Low-Intensity Direct Current**

Chronic wounds impose a significant financial burden for the healthcare system. Currently, assessment and monitoring of hard-to-heal wounds are often based on visual means and measuring the size of the wound. The primary wound dressings must be removed before assessment can be done. We have developed a quasi-monopolar bioimpedance-measurement-based method and a measurement system to determine the status of wound healing. The objective of this study was to demonstrate that with an appropriate setup, long-term monitoring of wound healing from beneath the primary dressings is feasible. The developed multielectrode sensor array was applied on the wound area and left under the primary dressings for 142 h. The impedance of the wounds and the surrounding intact skin area was measured regularly during the study at 150 Hz, 300 Hz, 1 kHz, and 5 kHz frequencies. At the end of the follow-up period, the wound impedance had reached the impedance of the intact skin at the higher frequencies and increased significantly at the lowest frequencies. The measurement frequency affected the measurement sensitivity in wound monitoring. The skin impedance remained stable over the measurement period. The sensor array also enabled the administration of periodical low-intensity direct current (LIDC) stimulation in order to create an antimicrobial environment across the wound area via the controlled formation of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>).

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: BioMediTech, Turku University Hospital, Kaarinantie 700, Åbo Akademi University

Contributors: Kekonen, A., Bergelin, M., Johansson, M., Kumar Joon, N., Bobacka, J., Viik, J.

Publication date: 31 May 2019

Peer-reviewed: Yes

#### **Publication information**

Journal: Sensors

Volume: 19

Issue number: 11

ISSN (Print): 1424-8220

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Atomic and Molecular Physics, and Optics, Biochemistry, Instrumentation, Electrical and Electronic Engineering

Keywords: beneath the dressings, bioimpedance, hydrogen peroxide, long-term monitoring, low-intensity direct current, multielectrode, quasi-monopolar, sensor array, wound dressing, wound monitoring, wound stimulation

Electronic versions:

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DOIs:

10.3390/s19112505

URLs:

<http://urn.fi/URN:NBN:fi:tty-201906241904>

Source: Scopus

Source ID: 85067176313

Research output: Contribution to journal > Article > Scientific > peer-review

### **Reaction between Peroxy and Alkoxy Radicals Can Form Stable Adducts**

Peroxy (RO<sub>2</sub>) and alkoxy (RO) radicals are prototypical intermediates in any hydrocarbon oxidation. In this work, we use computational methods to (1) study the mechanism and kinetics of the RO<sub>2</sub> + OH reaction for previously unexplored "R" structures (R = CH(O)CH<sub>2</sub> and R = CH<sub>3</sub>C(O)) and (2) investigate a hitherto unaccounted channel of molecular growth, R'O<sub>2</sub> + RO. On the singlet surface, these reactions rapidly form ROOOH and R'OOOR adducts, respectively. The former

decomposes to  $\text{RO} + \text{HO}_2$  and  $\text{R(O)OH} + \text{O}_2$  products, while the main decomposition channel for the latter is back to the reactant radicals. Decomposition rates of  $\text{R'OOOR}$  adducts varied between 103 and  $0.015 \text{ s}^{-1}$  at 298 K and 1 atm. The most long-lived  $\text{R'OOOR}$  adducts likely account for some fraction of the elemental compositions detected in the atmosphere that are commonly assigned to stable covalently bound dimers.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Physics, University of Helsinki  
Contributors: Iyer, S., Rissanen, M. P., Kurtén, T.  
Number of pages: 7  
Pages: 2051-2057  
Publication date: 2 May 2019  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Letters  
Volume: 10  
Issue number: 9  
ISSN (Print): 1948-7185  
Original language: English  
ASJC Scopus subject areas: Materials Science(all), Physical and Theoretical Chemistry  
Electronic versions:  
acs.jpcllett.9b00405  
DOIs:  
10.1021/acs.jpcllett.9b00405  
URLs:  
<http://urn.fi/URN:NBN:fi:tty-201906261912>  
Source: Scopus  
Source ID: 85064871304  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Energy-dependent diffusion in a soft periodic Lorentz gas

The periodic Lorentz gas is a paradigmatic model to examine how macroscopic transport emerges from microscopic chaos. It consists of a triangular lattice of circular hard scatterers with a moving point particle. Recently this system became relevant as a model for electronic transport in low-dimensional nanosystems such as molecular graphene. However, to more realistically mimic such dynamics, the hard Lorentz gas scatterers should be replaced by soft potentials. Here we study diffusion in a soft Lorentz gas with Fermi potentials under variation of the total energy of the moving particle. Our goal is to understand the diffusion coefficient as a function of the energy. In our numerical simulations we identify three different dynamical regimes: (i) the onset of diffusion at small energies; (ii) a transition where for the first time a particle reaches the top of the potential, characterized by the diffusion coefficient abruptly dropping to zero; and (iii) diffusion at high energies, where the diffusion coefficient increases according to a power law in the energy. All these different regimes are understood analytically in terms of simple random walk approximations.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Research area: Computational Physics, Research group: Quantum Control and Dynamics, Physics, School of Mathematical Sciences, Technische Universität Berlin, Universität zu Köln, Computational Physics Laboratory  
Contributors: Gil-Gallegos, S., Klages, R., Solanpää, J., Räsänen, E.  
Number of pages: 18  
Pages: 143-160  
Publication date: 1 May 2019  
Peer-reviewed: Yes

#### Publication information

Journal: European Physical Journal: Special Topics  
Volume: 228  
Issue number: 1  
ISSN (Print): 1951-6355  
Original language: English  
ASJC Scopus subject areas: Materials Science(all), Physics and Astronomy(all), Physical and Theoretical Chemistry  
DOIs:  
10.1140/epjst/e2019-800136-8

Source: Scopus

Source ID: 85066258822

Research output: Contribution to journal › Article › Scientific › peer-review

### **Moiré superlattices and 2D electronic properties of graphite/MoS<sub>2</sub> heterostructures**

Heterostructures of graphite/MoS<sub>2</sub> display a wide range of lattice registry due to rotational alignment and/or lattice mismatch. Using high resolution scanning tunneling microscopy and spectroscopy (STM/STS) we investigated electronic properties of these heterostructures and observed changes in the bandgap as a function of the twist angle between the layers. Green's function based electronic structure calculations were carried out in order to shed light on the mechanism underlying the observed bandgap changes. Indirect coupling between the p<sub>z</sub> orbitals of the substrate Carbon atoms and the d<sub>z<sup>2</sup></sub> orbitals of the MoS<sub>2</sub> layers (mediated by the p<sub>z</sub> orbitals of the bottom S layers) is found to be responsible for changes in the valence-band edge. Simple stacking of van der Waals materials with diverse properties have the potential to enable the fabrication of novel materials and device structures with tailored electronic properties.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Temple University, Russian Academy of Sciences, Northeastern University, National Tsing-Hua University, Institute of Physics Academia Sinica Taiwan, National University of Singapore

Contributors: Trainer, D. J., Putilov, A. V., Wang, B., Lane, C., Saari, T., Chang, T. R., Jeng, H. T., Lin, H., Xi, X., Nieminen, J., Bansil, A., Iavarone, M.

Pages: 325-330

Publication date: May 2019

Peer-reviewed: Yes

Early online date: 2017

#### **Publication information**

Journal: Journal of Physics and Chemistry of Solids

Volume: 128

ISSN (Print): 0022-3697

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics

DOIs:

10.1016/j.jpcs.2017.10.034

Source: Scopus

Source ID: 85036647170

Research output: Contribution to journal › Article › Scientific › peer-review

### **Spin filtering in silicene by edges and chemically or electrically induced interfaces**

Silicene is a graphene-like material with relatively strong spin-orbit coupling exhibiting gapless topologically protected edge states. In addition, it has a buckled structure, and hence, it stands as a feasible candidate for spintronic applications, where spin-polarized channels could be controlled with external electric fields realized with voltage gates attached to a silicene sheet. Breaking the periodicity in 2D-materials with spin-orbit coupling produces one-dimensional edge and interface nanostructures that may give rise to an intrinsic locking of spin-polarization to electron momentum. We consider field induced and chemical ways to create interfaces to give way to spin polarized states for both zigzag and armchair alignments. While the spin polarization of a field induced interface channel can be feasibly tuned, a chemical interface is less flexibly tunable. However, controlling Fermi-level, e.g. with a gate voltage, might serve as a spin valve along the interface.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Northeastern University

Contributors: Saari, T., Nieminen, J.

Pages: 316-324

Publication date: May 2019

Peer-reviewed: Yes

Early online date: 2018

#### **Publication information**

Journal: Journal of Physics and Chemistry of Solids

Volume: 128

ISSN (Print): 0022-3697

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics

Keywords: Electronic structure, Green's function techniques, Interfaces, Silicene, Spin-orbit coupling

DOIs:

10.1016/j.jpccs.2017.12.037

Source: Scopus

Source ID: 85040567725

Research output: Contribution to journal › Article › Scientific › peer-review

### Mass balance control of crushing circuits

This paper describes a novel circuit-wide control scheme that addresses the challenging problem of mass balance control of crushing circuits. The control objective is to ensure 100% utilization at the circuit bottleneck and hence push the realized performance towards the theoretical maximum. The present control problem is challenging due to long transport delays, complex circuit layout, under-actuated process, several uncontrolled disturbance flows, varying number of active equipment, varying downstream demand, and changing bottleneck location. The proposed mass balance control scheme involves feeding the circuit according to actual demand and realized circuit throughput, whilst maintaining the amount of material accumulated into the circuit and ensuring the physical integrity of the circuit. Therefore, the circuit feeding is based on the realized processing capacity, rather than an individual bin level or an operator decision. To ensure the efficient use of available surge capacity, a limiting control structure is proposed to simultaneously realize the in-circuit multi-objective limit violation control and loose bin level control strategy. The proposed scheme offers a simple solution for the otherwise complex control problem, which can be easily and efficiently implemented using classic control methods. The paper details an entire design procedure, from the fundamental theory, through dynamic modeling and controller tuning, to the complete circuit control system design and implementation. The proposed scheme is evaluated under extensive full-scale and simulated experiments at various production scenarios and equipment combinations. The rigorous control experiments revealed that the proposed scheme delivered the desired behavior in every possible scenario. This enables the circuit to reach its true potential.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Automation Technology and Mechanical Engineering, Research group: Automation and Systems Theory, Chalmers University of Technology, University of Queensland

Contributors: Itävuori, P., Hulthén, E., Yahyaei, M., Vilkkö, M.

Number of pages: 11

Pages: 37-47

Publication date: May 2019

Peer-reviewed: Yes

### Publication information

Journal: Minerals Engineering

Volume: 135

ISSN (Print): 0892-6875

Original language: English

ASJC Scopus subject areas: Control and Systems Engineering, Chemistry(all), Geotechnical Engineering and Engineering Geology, Mechanical Engineering

Keywords: Crushing, Dynamic modeling, Limiting control, Mass balance control, Sensor fusion

DOIs:

10.1016/j.mineng.2019.02.033

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Source: Scopus

Source ID: 85062035841

Research output: Contribution to journal › Article › Scientific › peer-review

### Complex Behavior of Phosphatidylcholine-Phosphatidic Acid Bilayers and Monolayers: Effect of Acyl Chain Unsaturation

Phosphatidic acids (PAs) have many biological functions in biomembranes, e.g., they are involved in the proliferation, differentiation, and transformation of cells. Despite decades of research, the molecular understanding of how PAs affect the properties of biomembranes remains elusive. In this study, we explored the properties of lipid bilayers and monolayers composed of PAs and phosphatidylcholines (PCs) with various acyl chains. For this purpose, the Langmuir monolayer technique and atomistic molecular dynamics (MD) simulations were used to study the miscibility of PA and PC lipids and the molecular organization of mixed bilayers. The monolayer experiments demonstrated that the miscibility of membrane components strongly depends on the structure of the hydrocarbon chains and thus on the overall lipid shape. Interactions between PA and PC molecules vary from repulsive, for systems containing lipids with saturated and unsaturated acyl tails (strongly positive values of the excess free energy of mixing), to attractive, for systems in which all lipid tails are saturated (negative values of the excess free energy of mixing). The MD simulations provided atomistic insight into polar interactions (formation of hydrogen bonds and charge pairs) in PC-PA systems. H-bonding between PA monoanions and PCs in mixed bilayers is infrequent, and the lipid molecules interact mainly via electrostatic interactions. However, the number of charge

pairs significantly decreases with the number of unsaturated lipid chains in the PA-PC system. The PA dianions weakly interact with the zwitterionic lipids, but their headgroups are more hydrated as compared to the monoanionic form. The acyl chains in all PC-PA bilayers are more ordered compared to single-component PC systems. In addition, depending on the combination of lipids, we observed a deeper location of the PA phosphate groups compared to the PC phosphate groups, which can alter the presentation of PAs for the peripheral membrane proteins, affecting their accessibility for binding. ©

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: Biological Physics and Soft Matter, Research area: Computational Physics, University of Helsinki, Uniwersytet Jagiellonski w Krakowie

Contributors: Kulig, W., Korolainen, H., Zatorska, M., Kwolek, U., Wydro, P., Kepczynski, M., Róg, T.

Number of pages: 13

Pages: 5944-5956

Publication date: 30 Apr 2019

Peer-reviewed: Yes

#### Publication information

Journal: Langmuir

Volume: 35

Issue number: 17

ISSN (Print): 0743-7463

Original language: English

ASJC Scopus subject areas: Materials Science(all), Condensed Matter Physics, Surfaces and Interfaces, Spectroscopy, Electrochemistry

DOIs:

10.1021/acs.langmuir.9b00381

Source: Scopus

Source ID: 85065022226

Research output: Contribution to journal > Article > Scientific > peer-review

#### Analysis of GaAsBi growth regimes in high resolution with respect to As/Ga ratio using stationary MBE growth

The control of Bi incorporation and material properties in III-V-Bi alloys has proved challenging due to their high sensitivity to the epitaxial growth parameters. Here, we present a methodology for determining the variation in the Ga, As, and Bi fluxes and the temperature across a stationary substrate in molecular beam epitaxy. By correlating the flux distributions with material properties, we identify distinct regimes for epitaxy of GaAsBi. In particular, we devise a detailed image of the interplay between Bi incorporation and structural properties of a bulk GaAs<sub>0.96</sub>Bi<sub>0.04</sub> layer grown on GaAs(1 0 0) with respect to the As/Ga ratio. The influence of As/Ga is analyzed with high resolution over the important stoichiometric range (i.e. As/Ga = 0.6–1.6). Growth outside the near-stoichiometric As/Ga regime leads to decreased Bi incorporation, decreased structural quality and the formation of Ga, Ga/Bi or Bi droplets. On the other hand, growth at As/Ga = 1.00–1.17 leads to maximized material quality. For this regime, the surface roughness is further optimized by fine-tuning the As/Ga ratio to suppress surface mounding to a value of 0.5 nm. The results reveal the extreme sensitivity of GaAsBi growth to small variations in the As/Ga ratio, and demonstrate the applicability of stationary growth in studying these effects.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: ORC

Contributors: Puustinen, J., Hilska, J., Guina, M.

Number of pages: 9

Pages: 33-41

Publication date: 1 Apr 2019

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Crystal Growth

Volume: 511

ISSN (Print): 0022-0248

Original language: English

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Keywords: A3. Molecular beam epitaxy, B1. Bismuth compounds, B2. Semiconducting III-V materials, B2. Semiconducting ternary compounds

DOIs:

10.1016/j.jcrysgro.2019.01.010

Source: Scopus

Source ID: 85060893423

Research output: Contribution to journal > Article > Scientific > peer-review

### **Hydrolysis and drug release from poly(ethylene glycol)-modified lactone polymers with open porosity**

The ability to release active agents from a porous scaffold structure in situ enables the simultaneous structural support for the cells proliferating and differentiating towards tissue as well as the stimulation of tissue regeneration. Due to the great potentiality of such approach, drug-releasing scaffolds were fabricated from hydrolytically degradable polymers. Three copolymers of poly(ethylene glycol),  $\epsilon$ -caprolactone, L- and D,L-lactide were synthesized and blended with bone-growth inducing active agents, dexamethasone (DM) and 2-phospho-L-ascorbic acid trisodium salt (AS). Porous scaffolds were prepared by means of super-critical carbon dioxide foaming. In the final scaffold structures, the particle size, location and the water solubility of the drug affected the release kinetics. As the large and water soluble AS particles were more exposed to the buffer solution compared to small DM particles, the AS release was burst-like whereas DM showed a long-term release. The material structure had a significant effect on the release kinetics as the porous scaffolds released active agents faster compared to the solid cylinders. Furthermore, this study showed the strong effect of polymer degradation and wettability on the release, which were more determinative than the pore architecture.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: BioMediTech, Aalto University, Orton Orthopaedic Hospital

Contributors: Asikainen, S., Paakinaho, K., Kyhkynen, A. K., Hannula, M., Malin, M., Ahola, N., Kellomäki, M., Seppälä, J.

Number of pages: 11

Pages: 165-175

Publication date: 1 Apr 2019

Peer-reviewed: Yes

#### **Publication information**

Journal: European Polymer Journal

Volume: 113

ISSN (Print): 0014-3057

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Organic Chemistry, Polymers and Plastics, Materials Chemistry

Keywords: 2-Phospho-L-ascorbic acid trisodium salt, Bulk degradation, Dexamethasone, Drug release, Hydrolytic degradation, Supercritical carbon dioxide foaming

DOIs:

10.1016/j.eurpolymj.2019.01.056

Source: Scopus

Source ID: 85060767586

Research output: Contribution to journal > Article > Scientific > peer-review

### **Positioning information privacy in intelligent transportation systems: An overview and future perspective**

Today, the Intelligent Transportation Systems (ITS) are already in deep integration phase all over the world. One of the most significant enablers for ITS are vehicle positioning and tracking techniques. Worldwide integration of ITS employing Dedicated Short Range Communications (DSRC) and European standard for vehicular communication, known as ETSI ITS-G5, brings a variety of options to improve the positioning in areas where GPS connectivity is lacking precision. Utilization of the ready infrastructure, next-generation cellular 5G networks, and surrounding electronic devices together with conventional positioning techniques could become the solution to improve the overall ITS operation in vehicle-to-everything (V2X) communication scenario. Nonetheless, effective and secure communication protocols between the vehicle and roadside units should be both analyzed and improved in terms of potential attacks on the transmitted positioning-related data. In particular, said information might be misused or stolen at the infrastructure side conventionally assumed to be trusted. In this paper, we first survey different methods of vehicle positioning, which is followed by an overview of potential attacks on ITS systems. Next, we propose potential improvements allowing mutual authentication between the vehicle and infrastructure aiming at improving positioning data privacy. Finally, we propose a vision on the development and standardization aspects of such systems.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Electrical Engineering, St. Petersburg State University of Aerospace Instrumentation, ITMO University, Brno University of Technology

Contributors: Ometov, A., Bezzateev, S., Davydov, V., Shchesniak, A., Masek, P., Lohan, E. S., Koucheryavy, Y.

Publication date: 1 Apr 2019

Peer-reviewed: Yes

## Publication information

Journal: Sensors

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Article number: 1603

ISSN (Print): 1424-8220

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Atomic and Molecular Physics, and Optics, Biochemistry, Instrumentation, Electrical and Electronic Engineering

Keywords: Authentication, Data privacy, GDPR, Intelligent transportation systems, Positioning

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Source: Scopus

Source ID: 85064829981

Research output: Contribution to journal › Article › Scientific › peer-review

## Alpha radiation-induced luminescence by am-241 in aqueous nitric acid solution

When exposed to air, alpha particles cause the production of light by exciting the molecules surrounding them. This light, the radioluminescence, is indicative of the presence of alpha radiation, thus allowing for the optical sensing of alpha radiation from distances larger than the few centimeters an alpha particle can travel in air. While the mechanics of radioluminescence in air and other gas compositions is relatively well understood, the same cannot be said about the radioluminescence properties of liquids. Better understanding of the radioluminescence properties of liquids is essential to design methods for the detection of radioactively contaminated liquids by optical means. In this article, we provide radioluminescence images of Am-241 dissolved in aqueous nitric acid ( $\text{HNO}_3$ ) solution and present the recorded radioluminescence spectrum with a maximum between and, and a steep decrease at the short wavelength side of the maximum. The shape of the spectrum resembles a luminescence process rather than Cerenkov light, bremsstrahlung, or other mechanisms with broadband emission. We show that the amount of light produced is about 150 times smaller compared to that of the same amount of Am-241 in air. The light production in the liquid is evenly distributed throughout the sample volume with a slight increase on the surface of the liquid. The radioluminescence intensity is shown to scale linearly with the Am-241 concentration and not be affected by the  $\text{HNO}_3$  concentration.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, University of Helsinki, European Commission Joint Research Centre

Contributors: Kerst, T., Malmbeck, R., Ial Banik, N. L., Toivonen, J.

Publication date: 1 Apr 2019

Peer-reviewed: Yes

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Journal: Sensors (Switzerland)

Volume: 19

Issue number: 7

Article number: 1602

ISSN (Print): 1424-8220

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Atomic and Molecular Physics, and Optics, Biochemistry, Instrumentation, Electrical and Electronic Engineering

Keywords: Alpha radiation, Americium, Liquid phase luminescence, Radioluminescence

Electronic versions:

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URLs:

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Source: Scopus

Source ID: 85064822061

Research output: Contribution to journal › Article › Scientific › peer-review

### **A Pentacene-based Nanotube Displaying Enriched Electrochemical and Photochemical Activities**

Unlike previously well-studied, acyclic pentacene oligomers, the first synthesis of a cyclic pentacene trimer with a fixed tubular conformation is reported. A short-step synthesis starting from common pentacenequinone yielded the target molecule with a 1.5 nanometer length and a subnanometer pore. Steady-state spectroscopic analyses revealed that the close proximity of the non-conjugated, three pentacene chromophores allows the nanotube to display stepwise electrochemical/chemical oxidation characteristics. Furthermore, time-resolved transient absorption measurements elucidated the generation of an excited triplet state of the nanotube, with high quantum yield reaching about 180 % through intramolecular singlet fission and a very long triplet lifetime.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Tokyo Institute of Technology, University of Yamanashi, Keio University

Contributors: Kuroda, K., Yazaki, K., Tanaka, Y., Akita, M., Sakai, H., Hasobe, T., Tkachenko, N. V., Yoshizawa, M.

Pages: 1115-1119

Publication date: Jan 2019

Peer-reviewed: Yes

Early online date: 2018

#### **Publication information**

Journal: Angewandte Chemie - International Edition

Volume: 58

Issue number: 4

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Original language: English

ASJC Scopus subject areas: Catalysis, Chemistry(all)

Keywords: macrocycles, nanotubes, pentacene, singlet fission, triplet states

DOIs:

10.1002/anie.201812976

Source: Scopus

Source ID: 85059193866

Research output: Contribution to journal > Article > Scientific > peer-review

### **Charge carrier dynamics in tantalum oxide overlayered and tantalum doped hematite photoanodes**

We employ atomic layer deposition to prepare 50 nm thick hematite photoanodes followed by passivating them with a 0.5 nm thick Ta<sub>2</sub>O<sub>5</sub>-overlayer and compare them with samples uniformly doped with the same amount of tantalum. We observe a three-fold improvement in photocurrent with the same onset voltage using Ta-overlayer hematite photoanodes, while electrochemical impedance spectroscopy under visible light irradiation shows a decreased amount of surface states under water splitting conditions. The Ta-doped samples have an even higher increase in photocurrent along with a 0.15 V cathodic shift in the onset voltage and decreased resistivity. However, the surface state capacitance for the Ta-doped sample is twice that of the reference photoanode, which implies a larger amount of surface hole accumulation. We further utilize transient absorption spectroscopy in the sub-millisecond to second timescale under operating conditions to show that electron trapping in both Ta<sub>2</sub>O<sub>5</sub>-passivated and Ta-doped samples is markedly reduced. Ultrafast transient absorption spectroscopy in the sub-picosecond to nanosecond timescale shows faster charge carrier dynamics and reduced recombination in the Ta-doped hematite photoanode resulting in the increased photoelectrochemical performance when compared with the Ta<sub>2</sub>O<sub>5</sub>-overlayer sample. Our results show that passivation does not affect the poor charge carrier dynamics intrinsic to hematite based photoanodes. The Ta-doping strategy results in more efficient electron extraction, solving the electron trapping issue and leading to increased performance over the surface passivation strategy.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Chemistry & Advanced Materials, Materials Science and Environmental Engineering, Physics, Research group: Surface Science

Contributors: Ruoko, T., Hiltunen, A., Iivonen, T., Ulkuniemi, R., Lahtonen, K., Ali-Löytty, H., Mizohata, K., Valden, M., Leskelä, M., Tkachenko, N. V.

Number of pages: 10

Pages: 3206-3215

Publication date: Jan 2019

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Materials Chemistry A

Volume: 7

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ISSN (Print): 2050-7488

Original language: English

ASJC Scopus subject areas: Chemistry(all), Renewable Energy, Sustainability and the Environment, Materials Science(all)

Electronic versions:

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### **Bibliographical note**

INT=phys,"Ulkuniemi, Riina"

Source: Scopus

Source ID: 85061474749

Research output: Contribution to journal › Article › Scientific › peer-review

### **O<sub>2</sub>-requiring molecular reporters of gene expression for anaerobic microorganisms**

Many genetic reporter systems require molecular oxygen; therefore, the use of reporter genes to study molecular mechanisms in anaerobic microorganisms has been hampered by the lack of convenient reporting systems. We describe reporter gene whole cell-based biosensor systems based on luciferase genes and the associated oxygen-requiring enzymes. By using two different oxygen-dependent reporters, insect and bacterial luciferases, and two bacterial hosts, Gram (+) *Bifidobacterium longum* and Gram (-) *Escherichia coli*, we show that the enzymes can be used in gene expression studies of anaerobic bacteria. *E. coli*, a facultative anaerobe, was grown both in aerobic and anaerobic conditions with an arabinose-inducible expression system. We show that a short treatment time of few minutes in ambient atmosphere is sufficient to detect light emission from living cells that is directly proportional to the number of cells and to the inducer concentration. The induction levels were the same in both the aerobically and anaerobically cultured cells. Similar results were obtained in the case of *B. longum* cultured in anaerobic conditions.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Università degli Studi di Milano

Contributors: Guglielmetti, S., Santala, V., Mangayil, R., Ciranna, A., Karp, M. T.

Number of pages: 6

Pages: 1-6

Publication date: 2019

Peer-reviewed: Yes

Early online date: 20 Sep 2018

### **Publication information**

Journal: Biosensors and Bioelectronics

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Original language: English

ASJC Scopus subject areas: Biotechnology, Biophysics, Biomedical Engineering, Electrochemistry

Keywords: Bioluminescence, Gram (+), Gram (-), Luciferase, Arabinose induction

Electronic versions:

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DOIs:

10.1016/j.bios.2018.09.066

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<http://urn.fi/URN:NBN:fi:tty-201901181115>

Source: Scopus

Source ID: 85053858794

Research output: Contribution to journal › Article › Scientific › peer-review

### **An automated algorithm for reliable equation of state fitting of magnetic systems**

In computational physics and materials science ground-state properties are often extracted from an equation of state fit to energy-volume data. Magnetic systems often have multiple magnetic phases present in the energy-volume data, which poses a challenge for the fitting approach because the results are sensitive to the selection of included fitting points. This is because practically all popular equation of state fitting functions, such as Murnaghan and Birch-Murnaghan, assume just one phase and therefore cannot correctly fit magnetic energy-volume data that contains multiple phases. When fitting

magnetic energy-volume data it is therefore important to select the range of fitting points in such a way that only points from the one relevant phase are included. We present a simple algorithm that makes the point selection automatically. Selecting fitting points automatically removes human bias and should also be useful for large-scale projects where selecting all fitting points by hand is not feasible.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research area: Computational Physics, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Uppsala University, Department of Physics and Astronomy, University of Turku, Royal Institute of Technology

Contributors: Levämäki, H., Tian, L., Vitos, L., Ropo, M.

Number of pages: 8

Pages: 121-128

Publication date: 2019

Peer-reviewed: Yes

#### Publication information

Journal: Computational Materials Science

Volume: 156

ISSN (Print): 0927-0256

Original language: English

ASJC Scopus subject areas: Computer Science(all), Chemistry(all), Materials Science(all), Mechanics of Materials, Physics and Astronomy(all), Computational Mathematics

Keywords: EOS, Equation of state fitting

DOIs:

10.1016/j.commatsci.2018.09.026

Source: Scopus

Source ID: 85053772857

Research output: Contribution to journal > Article > Scientific > peer-review

#### Low-dimensional formamidinium lead perovskite architectures via controllable solvent intercalation

We report the formation of a new class of solvent-intercalated two-dimensional (SI-2D) formamidinium lead halide perovskites. They can be mixed with three-dimensional (3D) stoichiometric perovskites by controlling the ratio of the precursor solutions. The composite leads to greatly improved photoluminescence quantum yield (PLQY) over the 3D compound. The enhanced PLQY is attributed to a type-I band alignment between the 3D and SI-2D, as revealed by first-principles calculations, which results in confined excitons with enhanced radiative recombination. The films exhibited excellent thermal and air stability retaining PLQY > 20% over 2 months in ambient conditions. Assemblies of halide perovskites with mixed dimensionality offer a pathway to enhance optoelectronic performance and device lifetimes.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Korea Advanced Institute of Science and Technology (KAIST), Yonsei University

Contributors: Shin, M., Kim, J., Jung, Y. K., Ruoko, T., Priimagi, A., Walsh, A., Shin, B.

Number of pages: 7

Pages: 3945-3951

Publication date: 2019

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Materials Chemistry C

Volume: 7

Issue number: 13

ISSN (Print): 2050-7534

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Chemistry

DOIs:

10.1039/c9tc00379g

Source: Scopus

Source ID: 85064717293

Research output: Contribution to journal > Article > Scientific > peer-review

## **Tuning of nonlinear absorption in highly luminescent CdSe based quantum dots with core-shell and core/multi-shell architectures**

We present our effort on an efficient way of tuning the nonlinear absorption mechanisms in ultra-small CdSe based quantum dots by implementing core-shell and core/multi-shell architectures. Depending on the size, architecture and composition of the QDs, these materials exhibited resonant and near-resonant nonlinear optical absorption properties such as saturable (SA) and reverse saturable (RSA) absorption for 5 ns pulses of 532 nm. These QDs exhibited a non-monotonic dependence of the effective two-photon absorption coefficient ( $\beta$ ) under nanosecond excitation with a maximum value for a thinner shell. We obtained a nonlinear absorption enhancement of an order of magnitude by adopting the core-shell architecture compared to their individual counterparts. Interestingly, CdSe QDs exhibit SA and/or RSA depending on their size and show a switching over from SA to RSA as the input intensity increases. We explained the enhanced nonlinear absorption in core-shell QDs compared to their individual counterparts in view of enhanced local fields associated with the core-shell structure. Thus, the present nanostructured materials are excellent candidates as saturable absorbers and optical limiters.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, University of Johannesburg, Mahatma Gandhi University, Qatar University, Laboratory of Photonics, University of Concepcion

Contributors: Bhagyaraj, S., Perumbilavil, S., Udayabashkar, R., Mangalaraja, R. V., Thomas, S., Kalarikkal, N., Oluwafemi, O. S.

Number of pages: 11

Pages: 11424-11434

Publication date: 2019

Peer-reviewed: Yes

### **Publication information**

Journal: Physical Chemistry Chemical Physics

Volume: 21

Issue number: 21

ISSN (Print): 1463-9076

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1039/c9cp00476a

Source: Scopus

Source ID: 85066623857

Research output: Contribution to journal > Article > Scientific > peer-review

## **Multiphoton Excitation of CsPbBr<sub>3</sub> Perovskite Quantum Dots (PQDs): How Many Electrons Can One PQD Donate to Multiple Molecular Acceptors?**

Metastable multiexcitonic states (MESs) of semiconductor quantum dots can be involved in multielectron transfer reactions, which opens new perspectives in nanomaterials-based optoelectronic applications. Herein, we demonstrate the generation of a MES in CsPbBr<sub>3</sub> perovskite quantum dots (PQDs) and its dissociation dynamics through multiple electron transfers to molecular electron acceptors, anthraquinones (AQs), bound to the PQD surface by a carboxylic anchor. As many as 14 excitons are produced at an excitation density of roughly 220  $\mu\text{J cm}^{-2}$  without detectable PQD degradation. Addition of AQ results in the formation of PQD-AQ hybrids with excess of AQs (PQD:AQ  $\approx$  1:20), which opens the possibility of multielectron transfer acts from MES to AQs. We found that the electron transfer saturates after roughly five transfer acts and that the first electron transfer (ET) time constant is as short as 1 ps. However, each ET increases the Coulomb potential barrier for the next ET, which decreases the rate of ET, resulting in a saturation after five ETs.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Bio- and Circular Economy, Materials Science and Environmental Engineering

Contributors: Mandal, S., Tkachenko, N. V.

Number of pages: 7

Pages: 2775-2781

Publication date: 2019

Peer-reviewed: Yes

### **Publication information**

Journal: Journal of Physical Chemistry Letters

ISSN (Print): 1948-7185

Original language: English

ASJC Scopus subject areas: Materials Science(all), Physical and Theoretical Chemistry

Electronic versions:

acs.jpcclett.9b01045

DOIs:

10.1021/acs.jpcclett.9b01045

URLs:

<http://urn.fi/URN:NBN:fi:tty-201906281918>

Source: Scopus

Source ID: 85066897133

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Spodumene tailings for porcelain and structural materials: Effect of temperature (1050–1200°C) on the sintering and properties**

The use of industrial by-products as substitute to conventional natural resources in ceramic production is of interest from an environment preservation and solid wastes management. This paper deals with the recycling of tailings from spodumene concentration during lithium production (Quartz Feldspar Sand; QFS), for the production of porcelain and structural materials. The QFS obtained from spodumene processing consisted mainly of quartz, albite, microcline with traces of muscovite. Mixtures of QFS and standard porcelain ingredients were sintered at 1050–1200 °C at 50 °C intervals and their properties were compared with a conventional porcelain composition prepared under the same conditions. Phase composition was assessed by XRD analysis using Rietveld refinement. Tests such as water absorption, apparent density, sintering shrinkage, compressive and flexural strength were used for physical comparison. The results showed that higher densification was achieved at 1200 °C, with a drastic reduction of water absorption below 1%. A compressive strength of 40 MPa was obtained at 1050 °C in the composition made of 50 wt% QFS and 50 wt% kaolin, increasing to 85 MPa at 1100 °C. The strength increase was attributed to better glassy phase formation and mullite growth. The QFS was found to contain no hazardous elements and showed promising sintering results, indicating its high suitability to substitute conventional resources in the production of ceramic materials.

#### **General information**

Publication status: Accepted/In press

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Univ of Oulu

Contributors: Lemougna, P. N., Yliniemi, J., Ismailov, A., Levänen, E., Tanskanen, P., Kinnunen, P., Roning, J., Illikainen, M.

Publication date: 2019

Peer-reviewed: Yes

#### **Publication information**

Journal: Minerals Engineering

Article number: 105843

ISSN (Print): 0892-6875

Original language: English

ASJC Scopus subject areas: Control and Systems Engineering, Chemistry(all), Geotechnical Engineering and Engineering Geology, Mechanical Engineering

Keywords: Feldspars, Mine tailings, Porcelain, Quartz, Structural applications

DOIs:

10.1016/j.mineng.2019.105843

Source: Scopus

Source ID: 85067234637

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Volatile fatty acid adsorption on anion exchange resins: kinetics and selective recovery of acetic acid**

The removal of volatile fatty acids was examined through adsorption on anion exchange resins in batch systems. During the initial screening step, granular activated carbon and 11 anion exchange resins were tested and the resins Amberlite IRA-67 and Dowex optipore L-493 were chosen for further investigation. The adsorption kinetics and diffusion mechanism and adsorption isotherms of the two resins for VFA were evaluated. Based on the selective adsorption capacity of the resins, a sequential batch process was tested to achieve separation of acetic acid from the VFA mixture and selective recoveries > 85% acetic acid and ~ 75% propionic acid was achieved.

#### **General information**

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education, Institute for Water Education

Contributors: Eregowda, T., Rene, E. R., Rintala, J., Lens, P. N.

Publication date: 2019

Peer-reviewed: Yes

### Publication information

Journal: Separation Science and Technology (Philadelphia)

ISSN (Print): 0149-6395

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all), Process Chemistry and Technology, Filtration and Separation

Keywords: anion-exchange resins, Brunauer-Emmett-Teller model, selective recovery, Volatile fatty acids

DOIs:

10.1080/01496395.2019.1600553

Source: Scopus

Source ID: 85065190589

Research output: Contribution to journal > Article > Scientific > peer-review

### Possible strategy to use differential mobility spectrometry in real time applications

Differential Mobility Spectrometry (DMS), also called as FAIMS is a variation of atmospheric pressure ion mobility measurement techniques and is capable of providing information about the electric field - mobility dependence of ions. In this method, a combined electric field is used. This field consists of asymmetric oscillating electric field of high intensity and low static field component. Analytical information in DMS is 2-dimensional dependence of ionic current on oscillating field amplitude and the value of static field intensity. The measurement of DMS signal for whole ranges of both variables is time consuming and also generates lot of data. It is a disadvantage of DMS method, which limits the use of this otherwise powerful technology in real time applications that require a response time of few seconds. This paper presents a way to limit measurement time by heuristic knowledge of the properties of the data space and another method based on the concept of Shannon Entropy to find operating parameters satisfying both separation and signal to noise ratio requirements.

### General information

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

Organisations: BioMediTech, Tampere University Hospital, Military University of Technology, Department of Surgery, Tampere University of Applied Sciences, LappeenrantaLahti University of Technology LUT

Contributors: Anttalainen, O., Puton, J., Kontunen, A., Karjalainen, M., Kumpulainen, P., Oksala, N., Safaei, Z., Roine, A.

Publication date: 2019

Peer-reviewed: Yes

### Publication information

Journal: International Journal for Ion Mobility Spectrometry

ISSN (Print): 1435-6163

Original language: English

ASJC Scopus subject areas: Spectroscopy

Keywords: Differential mobility spectrometry, DMS, FAIMS, Shannon entropy

Electronic versions:

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DOIs:

10.1007/s12127-019-00251-1

URLs:

<http://urn.fi/URN:NBN:fi:tty-201907081950>

Source: Scopus

Source ID: 85067989586

Research output: Contribution to journal > Article > Scientific > peer-review

### Synthesis of 6,12-disubstituted methanodibenzo[b,f][1,5]dioxocins: Pyrrolidine catalyzed self-condensation of 2'-Hydroxyacetophenones

The preparation of unprecedented 6,12-disubstituted methanodibenzo[b,f][1,5]dioxocins from pyrrolidine catalyzed self-condensation of 2'-hydroxyacetophenones is herein described. This method provides easy access to this highly bridged complex core, resulting in construction of two C-O and two C-C bonds, a methylene bridge and two quaternary centers in a single step. The intricate methanodibenzo[b,f][1,5]dioxocin compounds were obtained in up to moderate yields after optimization of the reaction conditions concerning solvent, reaction times and the use of additives. Several halide substituted methanodibenzo[b,f][1,5]dioxocins could be prepared from correspondent 2'-hydroxyacetophenones.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Faculdade de Farmacia da Universidade de Lisboa, University of Jyväskylä  
Contributors: Assoah, B., Riihonen, V., Vale, J. R., Valkonen, A., Candeias, N. R.  
Publication date: 2019  
Peer-reviewed: Yes

#### Publication information

Journal: Molecules

Volume: 24

Issue number: 13

Article number: 2405

ISSN (Print): 1420-3049

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Chemistry (miscellaneous), Molecular Medicine, Pharmaceutical Science, Drug Discovery, Physical and Theoretical Chemistry, Organic Chemistry

Keywords: 1,5-dioxocin, 20-hydroxyacetophenone, Enamine, Self-condensation

Electronic versions:

molecules-24-02405

DOIs:

10.3390/molecules24132405

URLs:

<http://urn.fi/URN:NBN:fi:ty-201908282044>

#### Bibliographical note

EXT="Valkonen, Arto"

INT=msee,"Riihonen, Vesa"

INT=msee,"Vale, João R."

Source: Scopus

Source ID: 85068362408

Research output: Contribution to journal > Article > Scientific > peer-review

#### Metabolic profiling of water-soluble compounds from the extracts of dark septate endophytic fungi (DSE) isolated from scots pine (*Pinus sylvestris* L.) seedlings using UPLC–orbitrap–MS

Endophytes are microorganisms living inside plant hosts and are known to be beneficial for the host plant vitality. In this study, we isolated three endophytic fungus species from the roots of Scots pine seedlings growing on Finnish drained peatland setting. The isolated fungi belonged to dark septate endophytes (DSE). The metabolic profiles of the hot water extracts of the fungi were investigated using Ultrahigh Performance Liquid Chromatography with Diode Array Detection and Electron Spray Ionization source Mass Spectrometry with Orbitrap analyzer (UPLC–DAD–ESI–MS–Orbitrap). Out of 318 metabolites, we were able to identify 220, of which a majority was amino acids and peptides. Additionally, opine amino acids, amino acid quinones, Amadori compounds, cholines, nucleobases, nucleosides, nucleotides, siderophores, sugars, sugar alcohols and disaccharides were found, as well as other previously reported metabolites from plants or endophytes. Some differences of the metabolic profiles, regarding the amount and identity of the found metabolites, were observed even though the fungi were isolated from the same host. Many of the discovered metabolites have been described possessing biological activities and properties, which may make a favorable contribution to the host plant nutrient availability or abiotic and biotic stress tolerance.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Bio- and Circular Economy, Natural Resources Institute Finland (Luke), Turku University of Applied Science, University of Helsinki, School of Chemical Engineering, Aalto University

Contributors: Tienaho, J., Karonen, M., Muilu–Mäkelä, R., Wähälä, K., Denegri, E. L., Franzén, R., Karp, M., Santala, V., Sarjala, T.

Publication date: 2019

Peer-reviewed: Yes

#### Publication information

Journal: Molecules

Volume: 24

Issue number: 12

Article number: 2330

ISSN (Print): 1420-3049

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Chemistry (miscellaneous), Molecular Medicine, Pharmaceutical Science, Drug Discovery, Physical and Theoretical Chemistry, Organic Chemistry

Keywords: Acephala applanata, Coniochaeta mutabilis, Endophytes, Endophytic fungi, Humicolopsis cephalosporioides, Metabolites, Peptides, Phialocephala fortinii, Scots pine, UPLC-MS

Electronic versions:

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DOIs:

10.3390/molecules24122330

URLs:

<http://urn.fi/URN:NBN:fi:tty-201908282045>

### Bibliographical note

EXT="Franzén, Robert"

Source: Scopus

Source ID: 85068104207

Research output: Contribution to journal > Article > Scientific > peer-review

### Exclusive occurrence of photoinduced energy transfer and switching of its direction by rectangular $\pi$ -extension of nanographenes

As structure defined cutouts of the graphene lattice, nanographene molecules have gained plenty of attention because of their high potential for versatile applications in organic electronics and energy conversion devices and as ideal model systems for the better understanding of intrinsic structure-property correlations of graphenes. In this study, well-defined nanographenes with  $sp^2$  carbon networks of different sizes, hexa-peri-hexabenzocoronene (HBC) and its rectangularly  $\pi$ -extended version, a short graphene nanoribbon (GNR), have been covalently functionalized with photoactive porphyrin molecules. On the basis of their spectroscopic studies, the photodynamics of the porphyrin-linked nanographenes was found to be influenced substantially by the size of the nanographenes. Photoexcitation of the porphyrin-HBC linked system led to exclusive energy transfer (EnT) from the first singlet excited state ( $S_1$ ) of the nanographene to the porphyrin, whereas opposite selective EnT occurred from the first and second singlet excited states ( $S_1$  and  $S_2$ ) of the porphyrin to the nanographene in the porphyrin-GNR linked system. In particular, ultrafast efficient EnTs from both the  $S_2$  and  $S_1$  states of the porphyrin to GNR mimic the corresponding ultrafast EnTs from the  $S_2$  and  $S_1$  states of carotenoids to chlorophylls in light-harvesting systems of natural photosynthesis. Such unique photophysical properties will be useful for the rational design of carbon-based photofunctional nanomaterials for optoelectronics and solar energy conversion devices.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, Kyoto University, Institute for Integrated Cell-Material Sciences

Contributors: Umeyama, T., Hanaoka, T., Yamada, H., Namura, Y., Mizuno, S., Ohara, T., Baek, J., Park, J., Takano, Y., Stranius, K., Tkachenko, N. V., Imahori, H.

Number of pages: 9

Pages: 6642-6650

Publication date: 2019

Peer-reviewed: Yes

### Publication information

Journal: Chemical Science

Volume: 10

Issue number: 27

ISSN (Print): 2041-6520

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Electronic versions:

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DOIs:

10.1039/c9sc01538h

URLs:

<http://urn.fi/URN:NBN:fi:tty-201909042060>

Source: Scopus

Source ID: 85068830304

Research output: Contribution to journal > Article > Scientific > peer-review

### The maximum Hosoya index of unicyclic graphs with diameter at most four

The Hosoya index of a graph is defined by the total number of the matchings of the graph. In this paper, we determine the maximum Hosoya index of unicyclic graphs with  $n$  vertices and diameter 3 or 4. Our results somewhat answer a question

proposed by Wagner and Gutman in 2010 for unicyclic graphs with small diameter.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computing Sciences, Research group: Computational Medicine and Statistical Learning Laboratory (CMSL), Central South University China, Shandong Normal University, University of Applied Sciences Upper Austria, School of Management, Department of Biomedical Computer Science and Mechatronics UMIT, Nankai University

Contributors: Liu, W., Ban, J., Feng, L., Cheng, T., Emmert-Streib, F., Dehmer, M.

Publication date: 2019

Peer-reviewed: Yes

#### Publication information

Journal: Symmetry

Volume: 11

Issue number: 8

Article number: 1034

ISSN (Print): 2073-8994

Original language: English

ASJC Scopus subject areas: Computer Science (miscellaneous), Chemistry (miscellaneous), Mathematics(all), Physics and Astronomy (miscellaneous)

Keywords: Diameter, Hosoya index, Unicyclic graphs

Electronic versions:

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DOIs:

[10.3390/sym11081034](https://doi.org/10.3390/sym11081034)

URLs:

<http://urn.fi/URN:NBN:fi:tty-201909122088>

Source: Scopus

Source ID: 85070495373

Research output: Contribution to journal > Article > Scientific > peer-review

#### The Hosoya entropy of graphs revisited

In this paper we extend earlier results on Hosoya entropy (H-entropy) of graphs, and establish connections between H-entropy and automorphisms of graphs. In particular, we determine the H-entropy of graphs whose automorphism group has exactly two orbits, and characterize some classes of graphs with zero H-entropy.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Computational Medicine and Statistical Learning Laboratory (CMSL), Computing Sciences, Shahid Rajaei Teacher Training University, University of Applied Sciences Upper Austria, School of Management, Hall in Tyrol, Nankai University, The City College of New York (CUNY), Aalto University, Peking University

Contributors: Ghorbani, M., Dehmer, M., Mowshowitz, A., Tao, J., Emmert-Streib, F.

Publication date: 2019

Peer-reviewed: Yes

#### Publication information

Journal: Symmetry

Volume: 11

Issue number: 8

Article number: 1013

ISSN (Print): 2073-8994

Original language: English

ASJC Scopus subject areas: Computer Science (miscellaneous), Chemistry (miscellaneous), Mathematics(all), Physics and Astronomy (miscellaneous)

Keywords: Automorphism of graphs, Graph entropy, Graph products

Electronic versions:

[symmetry-11-01013-v2](#)

DOIs:

[10.3390/sym11081013](https://doi.org/10.3390/sym11081013)

URLs:

<http://urn.fi/URN:NBN:fi:tty-201909122089>

Source: Scopus



Source ID: 85070525428

Research output: Contribution to journal > Article > Scientific > peer-review

### **Temperature scanning stress relaxation behavior of water responsive and mechanically adaptive elastomer nanocomposites**

The decrease of stress at constant strain, that is, the stress relaxation process as a function of temperature, is a central mechanical characteristics of elastomer nanocomposites for their potential applications. However, in the conventional stress relaxation test, the relaxation behavior is usually determined as a function of time at constant temperature. The present work reports the temperature scanning stress relaxation (TSSR) characteristics of a new kind of mechanically adaptive elastomer nanocomposite by monitoring the nonisothermal relaxation behavior as a function of temperature. This kind of adaptive elastomer nanocomposite was prepared by introducing calcium sulfate ( $\text{CaSO}_4$ ), as the water-responsive phase into the hydrophilic elastomer matrix. The influence of water-induced structural changes on TSSR behavior was investigated. Water treatment had a strong effect on the shape of the relaxation spectrum of the nanocomposite. It was revealed that the in situ development of hydrated nano-rod crystal structures of  $\text{CaSO}_4$  in the elastomer matrix was responsible for the changes in the mechanical relaxation behavior of the composites. Atomic force microscopy was used to verify this nano-rod crystal morphology in the elastomer matrix. The mechanism of water-induced mechanical reinforcement of the composite was explored from dynamic mechanical analysis of the material and correlated with its stress relaxation behavior.

#### **General information**

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Leibniz-Institut für Polymerforschung Dresden E.V., University of Massachusetts Lowell, Vodafone Department of Mobile Communications Systems

Contributors: Banerjee, S. S., Natarajan, T. S., Subramani B., E., Wießner, S., Janke, A., Heinrich, G., Das, A.

Publication date: 2019

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Applied Polymer Science

Article number: 48344

ISSN (Print): 0021-8995

Original language: English

ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry

Keywords: adaptive elastomer nanocomposite, calcium sulphate, mechanical reinforcement, morphology, temperature scanning stress relaxation

DOIs:

10.1002/app.48344

Source: Scopus

Source ID: 85070677934

Research output: Contribution to journal > Article > Scientific > peer-review

### **Reversible photodoping of TiO<sub>2</sub> nanoparticles**

Observations on strong photochromic effect of crystalline TiO<sub>2</sub> quantum dots (mean size  $\approx$  4 nm) are presented. The synthesized quantum dots consist of irregularly shaped anatase TiO<sub>2</sub> nanoparticles (NPs) and are dispersed in butanol (8 % by mass). Obtained NPs exhibit a dramatic photo-response to UV light, enabling effective transmittance modulation of in a broad wavelength range extending from visible to near-infrared region, and even the thermal black body radiation regime beyond 10  $\mu\text{m}$ . The exceptional photo-response is attributed to hole-scavenging by butanol, TiO<sub>2</sub> self-reduction, injection of electrons to the conduction band, and consequent localized surface plasmon resonances in NPs. Observed optical effect is reversible and the initial high transmittance state can be restored simply by exposing the NPs to air. Applied NP synthesis route is economic and can be easily scaled for applications such as smart window technologies.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Research group: Surface Science, Univ Tartu, University of Tartu, University of Tartu Institute of Physics, Inst Phys, University of Tartu

Contributors: Joost, U., Sutka, A., Oja, M., Smits, K., Doebelin, N., Loot, A., Järvekülg, M., Hirsimäki, M., Valden, M., Nommiste, E.

Pages: 8968-8974

Publication date: 26 Dec 2018

Peer-reviewed: Yes

Early online date: 10 Dec 2018

#### **Publication information**

Journal: Chemistry of Materials

Volume: 30

Issue number: 24

ISSN (Print): 0897-4756

Ratings:

Scopus rating (2018): CiteScore 9.92 SJR 4.224 SNIP 1.769

Original language: English

ASJC Scopus subject areas: Inorganic Chemistry, Materials Chemistry, Surfaces and Interfaces, Electronic, Optical and Magnetic Materials, Condensed Matter Physics

Keywords: tio2, nano, nanoparticle, photochromic, anatase, light, photonics, functional

DOIs:

10.1021/acs.chemmater.8b04813

URLs:

<http://urn.fi/URN:NBN:fi:ty-201812142858>. Embargo ends: 10/12/19

### Bibliographical note

INT=fot,"Joost, Urmas"

Research output: Contribution to journal > Article > Scientific > peer-review

### Less Is More: Enhancement of Second-Harmonic Generation from Metasurfaces by Reduced Nanoparticle Density

We investigate optical second-harmonic generation (SHG) from metasurfaces where noncentrosymmetric V-shaped gold nanoparticles are ordered into regular array configurations. In contrast to expectations, a substantial enhancement of the SHG signal is observed when the number density of the particles in the array is reduced. More specifically, by halving the number density, we obtain over 5-fold enhancement in SHG intensity. This striking result is attributed to favorable interparticle interactions mediated by the lattice, where surface-lattice resonances lead to spectral narrowing of the plasmon resonances. Importantly, however, the results cannot be explained by the improved quality of the plasmon resonance alone. Instead, the lattice interactions also lead to further enhancement of the local fields at the particles. The experimental observations agree very well with results obtained from numerical simulations including lattice interactions.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Institute of Physics, Nicolaus Copernicus University, University of Eastern Finland, CRPP

Contributors: Czaplicki, R., Kiviniemi, A., Huttunen, M. J., Zang, X., Stolt, T., Vartiainen, I., Butet, J., Kuittinen, M., Martin, O. J., Kauranen, M.

Number of pages: 6

Pages: 7709-7714

Publication date: 12 Dec 2018

Peer-reviewed: Yes

### Publication information

Journal: Nano Letters

Volume: 18

Issue number: 12

ISSN (Print): 1530-6984

Ratings:

Scopus rating (2018): CiteScore 12.71 SJR 6.211 SNIP 2.396

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Materials Science(all), Condensed Matter Physics, Mechanical Engineering

Keywords: interparticle interactions, Metal nanoparticles, nonlinear optics, plasmonic resonances, second-harmonic generation, surface-lattice resonances

DOIs:

10.1021/acs.nanolett.8b03378

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1808.06439

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<https://arxiv.org/abs/1808.06439> (ArXiv version)

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Source ID: 85058303843

Research output: Contribution to journal > Article > Scientific > peer-review

### Experimental moment resistance of rectangular hollow section T joints

Resistance is the main property of tubular joints. The determination of the joint resistance from the experimental load-deformation curve always represents a challenging task. Currently there are two main methods to find the experimental resistance, which are called plastic and ultimate resistance. However, there is no single opinion on which one should be commonly used. Based on the experimental results, this paper directly compares the two existed approaches. The study is restricted to welded square hollow section T joints under in-plane bending moment. The paper considers only the joints with  $\beta < 0.85$ , i.e. when the behaviour of the joint is governed by chord face failure. The results show that plastic resistance leads to more conservative results than ultimate resistance, providing thus safer results. However, attention should be also paid to the difference between the labour intensity of the presented methods.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Civil Engineering  
Contributors: Garifullin, M.  
Publication date: 5 Dec 2018  
Peer-reviewed: Yes

#### Publication information

Journal: MATEC Web of Conferences  
Volume: 245  
Article number: 08003  
ISSN (Print): 2274-7214  
Ratings:  
Scopus rating (2018): CiteScore 0.42 SJR 0.169 SNIP 0.548  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Engineering(all)  
Electronic versions:  
matecconf\_eece2018\_08003  
DOIs:  
10.1051/matecconf/201824508003  
URLs:  
<http://urn.fi/URN:NBN:fi:ty-201901091034>  
Source: Scopus  
Source ID: 85058463414  
Research output: Contribution to journal > Conference article > Scientific > peer-review

### Structural basis of actin monomer re-charging by cyclase-Associated protein

Actin polymerization powers key cellular processes, including motility, morphogenesis, and endocytosis. The actin turnover cycle depends critically on "re-charging" of ADP-Actin monomers with ATP, but whether this reaction requires dedicated proteins in cells, and the underlying mechanism, have remained elusive. Here we report that nucleotide exchange catalyzed by the ubiquitous cytoskeletal regulator cyclase-Associated protein (CAP) is critical for actin-based processes in vivo. We determine the structure of the CAP-Actin complex, which reveals that nucleotide exchange occurs in a compact, sandwich-like complex formed between the dimeric actin-binding domain of CAP and two ADP-Actin monomers. In the crystal structure, the C-Terminal tail of CAP associates with the nucleotide-sensing region of actin, and this interaction is required for rapid re-charging of actin by both yeast and mammalian CAPs. These data uncover the conserved structural basis and biological role of protein-catalyzed re-charging of actin monomers.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Physics, University of Helsinki Institute of Biotechnology, Brandeis University  
Contributors: Kotila, T., Kogan, K., Enkavi, G., Guo, S., Vattulainen, I., Goode, B. L., Lappalainen, P.  
Publication date: 1 Dec 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Nature Communications  
Volume: 9  
Issue number: 1  
Article number: 1892  
ISSN (Print): 2041-1723  
Ratings:  
Scopus rating (2018): CiteScore 12.19 SJR 5.992 SNIP 2.805

Original language: English

ASJC Scopus subject areas: Chemistry(all), Biochemistry, Genetics and Molecular Biology(all), Physics and Astronomy(all)

Electronic versions:

s41467-018-04231-7

DOIs:

10.1038/s41467-018-04231-7

Source: Scopus

Source ID: 85047005231

Research output: Contribution to journal > Article > Scientific > peer-review

### Beaming random lasers with soliton control

Random lasers are resonator-less light sources where feedback stems from recurrent scattering at the expense of spatial profile and directionality. Suitably-doped nematic liquid crystals can random lase when optically pumped near resonance(s); moreover, through molecular reorientation within the transparency region, they support self-guided optical spatial solitons, i.e., light-induced waveguides. Here, we synergistically combine solitons and collinear pumping in weakly scattering dye-doped nematic liquid crystals, whereby random lasing and self-confinement concur to beaming the emission, with several improved features: all-optical switching driven by a low-power input, laser directionality and smooth output profile with high-conversion efficiency, externally controlled angular steering. Such effects make soliton-assisted random lasers an outstanding route towards application-oriented random lasers.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Research group: Nonlinear Optics, University "Roma Tre", University of Southampton, Case Western Reserve University, CNR-NANOTEC & University of Calabria, Institute for Complex Systems

Contributors: Perumbilavil, S., Piccardi, A., Barboza, R., Buchnev, O., Kauranen, M., Strangi, G., Assanto, G.

Number of pages: 7

Publication date: 1 Dec 2018

Peer-reviewed: Yes

### Publication information

Journal: Nature Communications

Volume: 9

Issue number: 1

Article number: 3863

ISSN (Print): 2041-1723

Ratings:

Scopus rating (2018): CiteScore 12.19 SJR 5.992 SNIP 2.805

Original language: English

ASJC Scopus subject areas: Chemistry(all), Biochemistry, Genetics and Molecular Biology(all), Physics and Astronomy(all)

Electronic versions:

s41467-018-06170-9

DOIs:

10.1038/s41467-018-06170-9

URLs:

<http://urn.fi/URN:NBN:fi:tty-201810262477>

Source: Scopus

Source ID: 85053667214

Research output: Contribution to journal > Article > Scientific > peer-review

### Machine learning plastic deformation of crystals

Plastic deformation of micron-scale crystalline solids exhibits stress-strain curves with significant sample-to-sample variations. It is a pertinent question if this variability is purely random or to some extent predictable. Here we show, by employing machine learning techniques such as regression neural networks and support vector machines that deformation predictability evolves with strain and crystal size. Using data from discrete dislocations dynamics simulations, the machine learning models are trained to infer the mapping from features of the pre-existing dislocation configuration to the stress-strain curves. The predictability vs strain relation is non-monotonic and exhibits a system size effect: larger systems are more predictable. Stochastic deformation avalanches give rise to fundamental limits of deformation predictability for intermediate strains. However, the large-strain deformation dynamics of the samples can be predicted surprisingly well.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Physics, Aalto University, Department of Applied Physics  
Contributors: Salmenjoki, H., Alava, M. J., Laurson, L.  
Publication date: 1 Dec 2018  
Peer-reviewed: Yes

### Publication information

Journal: Nature Communications  
Volume: 9  
Issue number: 1  
Article number: 5307  
ISSN (Print): 2041-1723  
Ratings:  
Scopus rating (2018): CiteScore 12.19 SJR 5.992 SNIP 2.805  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Biochemistry, Genetics and Molecular Biology(all), Physics and Astronomy(all)  
Electronic versions:  
s41467-018-07737-2  
DOIs:  
10.1038/s41467-018-07737-2  
URLs:  
<http://urn.fi/URN:NBN:fi:ty-201901091035>  
Source: Scopus  
Source ID: 85058601336  
Research output: Contribution to journal › Article › Scientific › peer-review

### Bi-directional cell-pericellular matrix interactions direct stem cell fate

Modifiable hydrogels have revealed tremendous insight into how physical characteristics of cells' 3D environment drive stem cell lineage specification. However, in native tissues, cells do not passively receive signals from their niche. Instead they actively probe and modify their pericellular space to suit their needs, yet the dynamics of cells' reciprocal interactions with their pericellular environment when encapsulated within hydrogels remains relatively unexplored. Here, we show that human bone marrow stromal cells (hMSC) encapsulated within hyaluronic acid-based hydrogels modify their surroundings by synthesizing, secreting and arranging proteins pericellularly or by degrading the hydrogel. hMSC's interactions with this local environment have a role in regulating hMSC fate, with a secreted proteinaceous pericellular matrix associated with adipogenesis, and degradation with osteogenesis. Our observations suggest that hMSC participate in a bi-directional interplay between the properties of their 3D milieu and their own secreted pericellular matrix, and that this combination of interactions drives fate.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Research group: Biomaterials and Tissue Engineering Group, Faculty of Biomedical Sciences and Engineering, King's College London, The Francis Crick Institute, UCL Eastman Dental Institute, Imperial College, London, 24.8.2012, University College London, Uppsala University, University of Toronto, Canada  
Contributors: Ferreira, S. A., Motwani, M. S., Faull, P. A., Seymour, A. J., Yu, T. T., Enayati, M., Taheem, D. K., Salzlechner, C., Haghighi, T., Kania, E. M., Oommen, O. P., Ahmed, T., Loaiza, S., Parzych, K., Dazzi, F., Varghese, O. P., Festy, F., Grigoriadis, A. E., Auner, H. W., Snijders, A. P., Bozec, L., Gentleman, E.  
Number of pages: 12  
Publication date: Dec 2018  
Peer-reviewed: Yes

### Publication information

Journal: Nature Communications  
Volume: 9  
Issue number: 1  
Article number: 4049  
ISSN (Print): 2041-1723  
Ratings:  
Scopus rating (2018): CiteScore 12.19 SJR 5.992 SNIP 2.805  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Biochemistry, Genetics and Molecular Biology(all), Physics and Astronomy(all)

Electronic versions:

s41467-018-06183-4

DOIs:

10.1038/s41467-018-06183-4

URLs:

<http://urn.fi/URN:NBN:fi:tty-201811012525>

Source: Scopus

Source ID: 85054315213

Research output: Contribution to journal > Article > Scientific > peer-review

### **Aminobenzylated 4-Nitrophenols as Antibacterial Agents Obtained from 5-Nitrosalicylaldehyde through a Petasis Borono-Mannich Reaction**

Multidrug-resistant bacteria are one of the current biggest threats to public health and are responsible for most nosocomial infections. Herein, we report the efficient and facile synthesis of antibacterial agents aminoalkylphenols, derived from 5-nitrosalicylaldehyde and prepared through a Petasis borono-Mannich multicomponent reaction. Minimum inhibitory concentrations (MICs) as low as 1.23  $\mu\text{M}$  for a chlorine derivative were determined for multidrug-resistant Gram-positive bacteria, namely, *Staphylococcus aureus* and *Enterococcus faecalis*, two of the main pathogens responsible for infections in a hospital environment. The most promising antibacterial agents were further tested against eight strains of four Gram-positive species in order to elucidate their antibacterial broadness. In vitro cytotoxicity assays of the most active aminoalkylphenol revealed considerably lower toxicity against mammalian cells, as concentrations one order of magnitude higher than the determined MICs were required to induce human keratinocyte cell death. The phenol moiety was verified to be important in deeming the antibacterial properties of the analyzed compounds, although no correlation between such properties and their antioxidant activity was observed. A density functional theory computational study substantiated the ability of aminoalkylphenols to serve as precursors of ortho-quinone methides.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, CBIOS-Universidade Lusófona Research Center for Biosciences and Health Technologies, National Institute of Health, Faculdade de Farmacia da Universidade de Lisboa

Contributors: Rimpiläinen, T., Andrade, J., Nunes, A., Ntungwe, E., Fernandes, A. S., Vale, J. R., Rodrigues, J., Gomes, J. P., Rijo, P., Candeias, N. R.

Number of pages: 12

Pages: 16191-16202

Publication date: 29 Nov 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: ACS Omega

Volume: 3

Issue number: 11

ISSN (Print): 2470-1343

Ratings:

Scopus rating (2018): CiteScore 2.54 SJR 0.754 SNIP 0.673

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

Electronic versions:

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DOIs:

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URLs:

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Source: Scopus

Source ID: 85057603661

Research output: Contribution to journal > Article > Scientific > peer-review

### **Machine learning analysis of extreme events in optical fibre modulation instability**

A central research area in nonlinear science is the study of instabilities that drive extreme events. Unfortunately, techniques for measuring such phenomena often provide only partial characterisation. For example, real-time studies of instabilities in nonlinear optics frequently use only spectral data, limiting knowledge of associated temporal properties. Here, we show how machine learning can overcome this restriction to study time-domain properties of optical fibre modulation instability based only on spectral intensity measurements. Specifically, a supervised neural network is trained to correlate the spectral and temporal properties of modulation instability using simulations, and then applied to analyse

high dynamic range experimental spectra to yield the probability distribution for the highest temporal peaks in the instability field. We also use unsupervised learning to classify noisy modulation instability spectra into subsets associated with distinct temporal dynamic structures. These results open novel perspectives in all systems exhibiting instability where direct time-domain observations are difficult.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Photonics, UMR 6174  
Contributors: Närhi, M., Salmela, L., Toivonen, J., Billet, C., Dudley, J. M., Genty, G.  
Number of pages: 1  
Publication date: 22 Nov 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Nature Communications  
Volume: 9  
Issue number: 1  
ISSN (Print): 2041-1723  
Ratings:  
Scopus rating (2018): CiteScore 12.19 SJR 5.992 SNIP 2.805  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Biochemistry, Genetics and Molecular Biology(all), Physics and Astronomy(all)  
Electronic versions:  
s41467-018-07355-y  
DOIs:  
10.1038/s41467-018-07355-y  
URLs:  
<http://urn.fi/URN:NBN:fi:tty-201901071017>  
Source: Scopus  
Source ID: 85057100886  
Research output: Contribution to journal > Article > Scientific > peer-review

#### High Nitrogen Removal in a Constructed Wetland Receiving Treated Wastewater in a Cold Climate

Constructed wetlands provide cost-efficient nutrient removal, with minimal input of human labor and energy, and their number is globally increasing. However, in northern latitudes, wetlands are rarely utilized, because their nutrient removal efficiency has been questioned due to the cold climate. Here, we studied nutrient retention and nitrogen removal in a boreal constructed wetland (4-ha) receiving treated nitrogen-rich wastewater. On a yearly basis, most of the inorganic nutrients were retained by the wetland. The highest retention efficiency was found during the ice-free period, being 79% for ammonium-nitrogen (NH<sub>4</sub><sup>+</sup>-N), 71% for nitrate-nitrogen (NO<sub>3</sub><sup>-</sup>-N), and 88% for phosphate-phosphorus (PO<sub>4</sub><sup>3-</sup>-P). Wetland also acted as a buffer zone during the disturbed nitrification process of the wastewater treatment plant. Denitrification varied between 106 and 252 mg N m<sup>-2</sup> d<sup>-1</sup> during the ice-free period. During the ice-cover period, total gaseous nitrogen removal was 147 mg N m<sup>-2</sup> d<sup>-1</sup>, from which 66% was removed as N<sub>2</sub>, 28.5% as N<sub>2</sub>O through denitrification, and 5.5% as N<sub>2</sub> through anammox. Nearly 2600 kg N y<sup>-1</sup> was estimated to be removed through microbial gaseous N-production which equaled 72% of NO<sub>3</sub><sup>-</sup>-N and 60% of TN yearly retention in the wetland. The wetland retained nutrients even in winter, when good oxygen conditions prevailed under ice. The results suggest that constructed wetlands are an efficient option for wastewater nitrogen removal and nutrient retention also in cold climates.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, University of Helsinki, Jyväskylän yliopisto, University of Eastern Finland  
Contributors: Uusheimo, S., Huotari, J., Tulonen, T., Aalto, S. L., Rissanen, A. J., Arvola, L.  
Number of pages: 8  
Pages: 13343-13350  
Publication date: 20 Nov 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Environmental science & technology  
Volume: 52  
Issue number: 22  
ISSN (Print): 0013-936X

Ratings:

Scopus rating (2018): CiteScore 7.38 SJR 2.514 SNIP 1.959

Original language: English

ASJC Scopus subject areas: Chemistry(all), Environmental Chemistry

DOIs:

10.1021/acs.est.8b03032

Source: Scopus

Source ID: 85056728368

Research output: Contribution to journal > Article > Scientific > peer-review

### High-Yield Generation of Triplet Excited States by an Efficient Sequential Photoinduced Process from Energy Transfer to Singlet Fission in Pentacene-Modified CdSe/ZnS Quantum Dots

Singlet fission (SF) is expected to improve photoenergy conversion systems by generating two electrons from one photon. Pentacenes meet the energy-level matching condition between a singlet and two triplet states:  $[E(S_1) \geq 2E(T_1)]$ . However, the molar absorption coefficients of pentacenes in the approximately 400–500 nm region are limited, whereas quantum dots, such as CdSe/ZnS (QD), possess high fluorescence quantum yields and particle-size-dependent fluorescence wavelengths. Thus, a combination of QD (D) and pentacene (A) provides a system of both an enhanced light-harvesting efficiency throughout the solar spectrum and an efficient conversion of the harvested light into the triplet states by SF. Based on these points, m-phenylene-bridged triisopropylsilane (TIPS)-pentacene dimer-functionalized QD (denoted as m-(Pc)<sub>2</sub>-QD) was synthesized to examine the sequential photoinduced process from energy transfer to SF. In femtosecond transient absorption measurements, initial energy transfer from QD to pentacene (quantum yield: 87 %) and subsequent SF were efficiently observed. The quantum yield of triplet states of pentacene units ( $\Phi_T$ ) based on the excitation of QD attained is  $160 \pm 6.7$  %.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Keio University

Contributors: Sakai, H., Inaya, R., Tkachenko, N. V., Hasobe, T.

Number of pages: 10

Pages: 17062-17071

Publication date: 16 Nov 2018

Peer-reviewed: Yes

#### Publication information

Journal: Chemistry - A European Journal

Volume: 24

Issue number: 64

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2018): CiteScore 4.77 SJR 1.842 SNIP 0.972

Original language: English

ASJC Scopus subject areas: Catalysis, Organic Chemistry

Keywords: energy transfer, pentacene, quantum dot, sequential photophysical process, singlet fission

DOIs:

10.1002/chem.201803257

Source: Scopus

Source ID: 85055548433

Research output: Contribution to journal > Article > Scientific > peer-review

### M2M Communication Assessment in Energy-Harvesting and Wake-Up Radio Assisted Scenarios Using Practical Components

Techniques for wireless energy harvesting (WEH) are emerging as a fascinating set of solutions to extend the lifetime of energy-constrained wireless networks, and are commonly regarded as a key functional technique for almost perpetual communications. For example, with WEH technology, wireless devices are able to harvest energy from different light sources or Radio Frequency (RF) signals broadcast by ambient or dedicated wireless transmitters to support their operation and communications capabilities. WEH technology will have increasingly wider range of use in upcoming applications such as wireless sensor networks, Machine-to-Machine (M2M) communications, and the Internet of Things. In this paper, the usability and fundamental limits of joint RF and solar cell or photovoltaic harvesting based M2M communication systems are studied and presented. The derived theoretical bounds are in essence based on the Shannon capacity theorem, combined with selected propagation loss models, assumed additional link nonidealities, diversity processing, as well as the given energy harvesting and storage capabilities. Fundamental performance limits and available capacity of the communicating link are derived and analyzed, together with extensive numerical results evaluated in different practical scenarios, including realistic implementation losses and state-of-the-art printed supercapacitor performance figures with voltage doubler-based voltage regulator. In particular, low power sensor type communication



applications using passive and semi-passive wake-up radio (WuR) are addressed in the study. The presented analysis principles and results establish clear feasibility regions and performance bounds for wireless energy harvesting based low rate M2M communications in the future IoT networks.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Electronics and Communications Engineering, Nano Communication Centre, Department of Electrical and Computer Engineering, Ohio State University

Contributors: Rinne, J., Keskinen, J., Berger, P. R., Lupo, D., Valkama, M.

Publication date: 16 Nov 2018

Peer-reviewed: Yes

#### Publication information

Journal: Sensors (Basel, Switzerland)

Volume: 18

Issue number: 11

ISSN (Print): 1424-8220

Ratings:

Scopus rating (2018): CiteScore 3.72 SJR 0.592 SNIP 1.576

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Atomic and Molecular Physics, and Optics, Biochemistry, Instrumentation, Electrical and Electronic Engineering

Keywords: diversity system, M2M communications, perpetual communications, propagation loss, Shannon limit, supercapacitor, wake-up radio, wireless energy harvesting

Electronic versions:

sensors-18-03992-v2

DOIs:

10.3390/s18113992

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201901071020>

Source: Scopus

Source ID: 85056711381

Research output: Contribution to journal > Article > Scientific > peer-review

#### Molecular-Scale Ligand Effects in Small Gold-Thiolate Nanoclusters

Because of the small size and large surface area of thiolate-protected Au nanoclusters (NCs), the protecting ligands are expected to play a substantial role in modulating the structure and properties, particularly in the solution phase. However, little is known on how thiolate ligands explicitly modulate the structural properties of the NCs at atomic level, even though this information is critical for predicting the performance of Au NCs in application settings including as a catalyst interacting with small molecules and as a sensor interacting with biomolecular systems. Here, we report a combined experimental and theoretical study, using synchrotron X-ray spectroscopy and quantum mechanics/molecular mechanics simulations, that investigates how the protecting ligands impact the structure and properties of small  $\text{Au}_{18}(\text{SR})_{14}$  NCs. Two representative ligand types, smaller aliphatic cyclohexanethiolate and larger hydrophilic glutathione, are selected, and their structures are followed experimentally in both solid and solution phases. It was found that cyclohexanethiolate ligands are significantly perturbed by toluene solvent molecules, resulting in structural changes that cause disorder on the surface of  $\text{Au}_{18}(\text{SR})_{14}$  NCs. In particular, large surface cavities in the ligand shell are created by interactions between toluene and cyclohexanethiolate. The appearance of these small molecule-accessible sites on the NC surface demonstrates the ability of Au NCs to act as a catalyst for organic phase reactions. In contrast, glutathione ligands encapsulate the Au NC core via intermolecular interactions, minimizing structural changes caused by interactions with water molecules. The much better protection from glutathione ligands imparts a rigidified surface and ligand structure, making the NCs desirable for biomedical applications due to the high stability and also offering a structural-based explanation for the enhanced photoluminescence often reported for glutathione-protected Au NCs.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Dalhousie University, Universitat Autònoma de Barcelona, Spain, Catalan Institute for Research and Advanced Studies (ICREA), Carnegie Mellon University, National University of Singapore, Norwegian Univ. of Sci. and Technol.

Contributors: Chevrier, D. M., Raich, L., Rovira, C., Das, A., Luo, Z., Yao, Q., Chatt, A., Xie, J., Jin, R., Akola, J., Zhang, P.

Number of pages: 7

Pages: 15430-15436

Publication date: 14 Nov 2018

Peer-reviewed: Yes

### Publication information

Journal: Journal of the American Chemical Society

Volume: 140

Issue number: 45

ISSN (Print): 0002-7863

Ratings:

Scopus rating (2018): CiteScore 14.75 SJR 7.468 SNIP 2.634

Original language: English

ASJC Scopus subject areas: Catalysis, Chemistry(all), Biochemistry, Colloid and Surface Chemistry

DOIs:

10.1021/jacs.8b09440

Source: Scopus

Source ID: 85056236370

Research output: Contribution to journal > Article > Scientific > peer-review

### Biological treatment of selenium-laden wastewater containing nitrate and sulfate in an upflow anaerobic sludge bed reactor at pH 5.0

This study investigated the removal of selenate ( $\text{SeO}_4^{2-}$ ), sulfate ( $\text{SO}_4^{2-}$ ) and nitrate ( $\text{NO}_3^-$ ) at different influent pH values ranging from 7.0 to 5.0 and 20 °C in an upflow anaerobic sludge blanket (UASB) reactor using lactate as an electron donor. At pH 5.0, the UASB reactor showed a 20–30% decrease in reactor performance compared to operation at pH 5.5 to 7.0, reaching removal efficiencies of 79%, 15%, 43% and 61% for  $\text{NO}_3^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{Se}_{\text{total}}$  and  $\text{Se}_{\text{diss}}$ , respectively. However, the reactor stability was an issue upon lowering the pH to 5.0 and further experiments are recommended. The sludge formed during low pH operation had a fluffy, floc-like appearance with filamentous structure, possibly due to the low polysaccharide (PS) to protein (PN) ratio (0.01 PS/PN) in the soluble extracellular polymeric substances (EPS) matrix of the biomass. Scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX) analysis of the sludge confirmed Se oxyanion reduction and deposition of  $\text{Se}_0$  particles inside the biomass. Microbial community analysis using Illumina MiSeq sequencing revealed that the families of Campylobacteraceae and Desulfomicrobiaceae were the dominant phylotypes throughout the reactor operation at approximately 23% and 10% relative abundance, respectively. Furthermore, approximately 10% relative abundance of both Geobacteraceae and Spirochaetaceae was observed in the granular sludge during the pH 5.0 operation. Overall, this study demonstrated the feasibility of UASB operation at pH values ranging from 7.0 to 5.0 for removing Se and other oxyanions from wastewaters.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Bhabha Atomic Research Centre, Montana State University (MSU), Hydraulic and Environmental Engineering (IHE) Inst. for Water Education

Contributors: Tan, L. C., Nancharaiah, Y. V., Lu, S., van Hullebusch, E. D., Gerlach, R., Lens, P. N.

Number of pages: 10

Pages: 684-693

Publication date: 1 Nov 2018

Peer-reviewed: Yes

### Publication information

Journal: Chemosphere

Volume: 211

ISSN (Print): 0045-6535

Ratings:

Scopus rating (2018): CiteScore 5.34 SJR 1.448 SNIP 1.54

Original language: English

ASJC Scopus subject areas: Environmental Engineering, Environmental Chemistry, Chemistry(all), Pollution, Health, Toxicology and Mutagenesis

Keywords: Acid mine drainage, Anaerobic granular sludge, Microbial diversity, Selenate bioreduction, UASB reactor

DOIs:

10.1016/j.chemosphere.2018.07.079

Source: Scopus

Source ID: 85053212365

Research output: Contribution to journal > Article > Scientific > peer-review

### Tribocorrosion behaviour of aluminium bronze in 3.5 wt.% NaCl solution

Tribocorrosion behaviour of aluminium bronze CuAl10Fe5Ni5 in 3.5 wt.% NaCl solution was investigated in a pin-on-disc facility containing an electrochemical cell. Oxidising capacity and contact pressure to alumina counterbody were varied. Pure corrosion occurred as selective dissolution of  $\alpha$  phase included in the eutectoid structure. Contact to counterbody introduced plastic deformation, extrusion of the material and abrasive wear. Wear-corrosion interactions varied between the two contact pressures, with lower material losses appearing at the higher pressure. The significant acceleration of

material degradation by the interactions was not clearly reflected to kinetics or thermodynamics of corrosion. These results are presented and discussed here.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, VTT Technical Research Centre of Finland

Contributors: Huttunen-Saarivirta, E., Isotahdon, E., Metsäjoki, J., Salminen, T., Carpén, L., Ronkainen, H.

Number of pages: 17

Pages: 207-223

Publication date: 1 Nov 2018

Peer-reviewed: Yes

#### Publication information

Journal: Corrosion Science

Volume: 144

ISSN (Print): 0010-938X

Ratings:

Scopus rating (2018): CiteScore 6.76 SJR 2.131 SNIP 2.595

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all), Materials Science(all)

Keywords: Corrosion, Plastic deformation, Selective dissolution, Tribocorrosion, Wear

DOIs:

10.1016/j.corsci.2018.08.058

#### Bibliographical note

EXT="Huttunen-Saarivirta, E."

EXT="Isotahdon, E."

EXT="Metsäjoki, J."

Source: Scopus

Source ID: 85053038794

Research output: Contribution to journal > Article > Scientific > peer-review

#### Computation of Dynamic Polarizabilities and van der Waals Coefficients from Path-Integral Monte Carlo

We demonstrate computation of total dynamic multipole polarizabilities using path-integral Monte Carlo method (PIMC). The PIMC approach enables accurate thermal and nonadiabatic mixing of electronic, rotational, and vibrational degrees of freedom. Therefore, we can study the thermal effects, or lack thereof, in the full multipole spectra of the chosen one- and two-electron systems: H, Ps, He, Ps<sub>2</sub>, H<sub>2</sub>, and HD<sup>+</sup>. We first compute multipole-multipole correlation functions up to octupole order in imaginary time. The real-domain spectral function is then obtained by analytical continuation with the maximum entropy method. In general, sharpness of the active spectra is limited, but the obtained off-resonant polarizabilities are in good agreement with the existing literature. Several weak and strong thermal effects are observed. Furthermore, the polarizabilities of Ps<sub>2</sub> and some higher multipole and higher frequency data have not been published before. In addition, we compute isotropic dispersion coefficients C<sub>6</sub>, C<sub>8</sub>, and C<sub>10</sub> between pairs of species using the simplified Casimir-Polder formulas.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: Electronic Structure Theory, Research area: Computational Physics

Contributors: Tiihonen, J., Kylänpää, I., Rantala, T. T.

Number of pages: 14

Pages: 5750-5763

Publication date: 2 Oct 2018

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chemical Theory and Computation

Volume: 14

ISSN (Print): 1549-9618

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Scopus rating (2018): CiteScore 5.7 SJR 2.236 SNIP 1.562

Original language: English

ASJC Scopus subject areas: Computer Science Applications, Physical and Theoretical Chemistry

Electronic versions:

dynamicpolarizability\_achemso. Embargo ended: 2/10/19

DOIs:

10.1021/acs.jctc.8b00859

URLs:

<http://urn.fi/URN:NBN:fi:ty-201811162595>. Embargo ended: 2/10/19

Source: Scopus

Source ID: 85055154322

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Quantification of bio-anode capacitance in bioelectrochemical systems using Electrochemical Impedance Spectroscopy**

Understanding the electrochemical properties of bio-anodes is essential to improve performance of bioelectrochemical systems. Electrochemical Impedance Spectroscopy (EIS) is often used to study these properties in detail. Analysis of the EIS response, however, is challenging due to the interfering effect of the large capacitance of typically used graphite and carbon-based electrodes. In this study, we used flat electrodes made of conductive Fluorine-doped Tin Oxide (FTO) as anode, and monitored bio-anode performance. We show that with this configuration, it is possible to accurately separate the distinct contributions to the electrical response of the bio-anodes: charge transfer, biofilm and diffusion resistances, and biofilm capacitance. We observed that the capacitance of the biofilm increased from  $2 \mu\text{F cm}^{-2}$  to  $450 \mu\text{F cm}^{-2}$  during biofilm growth, showing a relationship with current and total produced charge. These results suggest that biofilm capacitance is a measure for the amount of active biomass in bioelectrochemical systems. At the end of the experiment, the biofilm was harvested from the FTO electrode and an average yield of  $0.55 \text{ g COD biomass/mol e}^{-}$  was determined.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Wageningen University and Research Centre, Wetsus, Centre for Sustainable Water Technology, Universitat Jaume I

Contributors: Heijne, A. T., Liu, D., Sulonen, M., Sleutels, T., Fabregat-Santiago, F.

Number of pages: 6

Pages: 533-538

Publication date: 1 Oct 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Power Sources

Volume: 400

ISSN (Print): 0378-7753

Ratings:

Scopus rating (2018): CiteScore 7.19 SJR 1.947 SNIP 1.433

Original language: English

ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Energy Engineering and Power Technology, Physical and Theoretical Chemistry, Electrical and Electronic Engineering

Keywords: BES, Bioanode, Biomass yield, Capacitance, Electrochemical Impedance Spectroscopy, MET, Microbial fuel cell

Electronic versions:

1-s2.0-S0378775318308620-main

DOIs:

10.1016/j.jpowsour.2018.08.003

URLs:

<http://urn.fi/URN:NBN:fi:ty-201809212323>

Source: Scopus

Source ID: 85052096235

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Mechanical, thermal, and burning properties of viscose fabric composites: Influence of epoxy resin modification**

The influence of epoxy resin modification by 3-aminopropyltriethoxysilane (APTES) on various properties of warp knitted viscose fabric is reported in this study. Dynamic mechanical, impact resistance, flexural, thermal properties, and burning behavior of the epoxy/viscose fabric composites are studied with respect to varying content of silane coupling agent. The results obtained for APTES-modified epoxy resin based composites reinforced with unmodified viscose fabric composites are compared to unmodified epoxy resin based composites reinforced with APTES-modified viscose fabric. The dynamic mechanical behavior of the APTES-modified resin based composites indicates improved interfacial adhesion. The composites prepared from modified epoxy resin exhibited a twofold increase in impact resistance. The improved adhesion between the fiber and modified resin was also visible from the scanning electron microscope analysis of the impact fracture surface. There was less influence of resin modification on the flexural properties of the composites. The 5% APTES modification induced early degradation of composites compared to all other composites. The burning rate of all the composites under study is rated to be satisfactory for use in automotive interior applications.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Centria University of Applied Sciences, University of Borås, Yanbu Industrial College, Jozef Stefan Institute, Swedish Centre for Resource Recovery

Contributors: Rajan, R., Rainosalu, E., Ramamoorthy, S. K., Thomas, S. P., Zavašnik, J., Vuorinen, J., Skrifvars, M.

Publication date: 20 Sep 2018

Peer-reviewed: Yes

### Publication information

Journal: Journal of Applied Polymer Science

Volume: 135

Issue number: 36

Article number: 46673

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2018): CiteScore 2.25 SJR 0.554 SNIP 0.814

Original language: English

ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry

Keywords: cellulose and other wood products, functionalization of polymers, mechanical properties, thermal properties, thermosets

DOIs:

10.1002/app.46673

### Bibliographical note

EXT="Skrifvars, Mikael"

Source: Scopus

Source ID: 85049105961

Research output: Contribution to journal > Article > Scientific > peer-review

### Electro-concentration for chemical-free nitrogen capture as solid ammonium bicarbonate

Source-separated urine is a promising stream for nutrient capture using electrochemical technologies. It contains the majority of macronutrients present in municipal wastewater in a concentrated, high ionic conductivity liquid and in N:P:K ratios suitable for agricultural application. The purpose of this study was to recover nutrients from urine, and particularly nitrogen as a solid without any chemical addition. Simulated source-separated urine was concentrated using a three-compartment electrochemical system, applying a range of current densities and feed compositions. Electro-concentration into a liquid concentrate reached maximum recovery of 72:61:79% for N:P:K, respectively, from a synthetic feed simulating ureolysed and digested urine, with a specific electrical energy consumption of 47 MJ/kg N and current efficiency of 67% for ammonium. Cooling the concentrate to  $-18\text{ }^{\circ}\text{C}$  resulted in solid ammonium bicarbonate crystal formation in samples with high ammonium bicarbonate ionic product and high relative ammonium bicarbonate ionic strength. Precipitation started to occur when ammonium bicarbonate ionic product was higher than  $2.25\text{ M}^2$  and ammonium bicarbonate accounted for more than 62% of the total ionic strength of the feed. The maximum observed nitrogen recovery into solid ammonium bicarbonate reached 17% using a current density of  $100\text{ A m}^{-2}$ . Based on these results, electro-concentration is a promising technology for urine nutrient capture. However, capture as solid ammonium bicarbonate is feasible only if higher recovery efficiencies are achieved by removing competing ions.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, University of Queensland

Contributors: Jermakka, J., Thompson Brewster, E., Ledezma, P., Freguia, S.

Number of pages: 8

Pages: 48-55

Publication date: 12 Sep 2018

Peer-reviewed: Yes

Early online date: 2018

### Publication information

Journal: Separation and Purification Technology

Volume: 203

ISSN (Print): 1383-5866

Ratings:

Scopus rating (2018): CiteScore 5.05 SJR 1.158 SNIP 1.458

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Filtration and Separation

Keywords: Ammonium bicarbonate precipitation, Electro-concentration, Nutrient recovery, Urine

DOIs:

10.1016/j.seppur.2018.04.023

Source: Scopus

Source ID: 85045218335

Research output: Contribution to journal › Article › Scientific › peer-review

### **A compact olfactometer for IMS measurements and testing human perception**

Production of easily controllable and measurable odor stimuli is needed when studying human olfaction, olfaction-related physiology and psychological reactions to odors. Controlled odor producing instruments are called olfactometers. For testing and calibrating new olfactometers or sensor arrays, a reliable input signal has to be produced to verify their accurate functionality. A common input signal in various olfactometers has been the use of volatile organic compounds (VOCs) in gaseous form. We present a compact olfactometer able to produce controlled continuous odor stimuli from three individual channels. For measuring the output gas flow, we used a ChemPro 100i (EnviroNics, Finland) device that is based on aspiration ion mobility spectrometry (aIMS). IMS is a robust and sensitive method for measuring VOCs and is used especially in detecting toxic industrial chemicals and chemical warfare agents, but the technology is also suitable for other olfactory-related applications. The olfactometer was used to produce synthetic jasmine scent using three main odor components from jasmine oil and all the components were diluted using propylene glycol. The dilutions were supplied to the system using programmable syringe pumps, which guided the dilutions to individual evaporation units. We conducted experiments to verify the functionality of our olfactometer. Analysis of the ChemPro100i data showed that olfactometer can use different odor components to produce continuous, stable output flows with controlled concentrations.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Micro and Nanosystems Research Group, Research group: Sensor Technology and Biomeasurements (STB)

Contributors: Nieminen, V., Karjalainen, M., Salminen, K., Rantala, J., Kontunen, A., Isokoski, P., Müller, P., Kallio, P., Surakka, V., Lekkala, J.

Number of pages: 10

Pages: 71-80

Publication date: Sep 2018

Peer-reviewed: Yes

Early online date: 21 Jun 2018

#### **Publication information**

Journal: International Journal for Ion Mobility Spectrometry

Volume: 21

Issue number: 3

ISSN (Print): 1435-6163

Ratings:

Scopus rating (2018): CiteScore 1.74 SJR 0.712 SNIP 0.756

Original language: English

ASJC Scopus subject areas: Spectroscopy

Keywords: Human perception, Ion mobility spectrometry, Odor, Olfactometer

Electronic versions:

Nieminen\_et\_al--A\_compact\_olfactometer\_for\_IMS

DOIs:

10.1007/s12127-018-0235-1

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201909233449>

#### **Bibliographical note**

INT=tut-bmt,"Nieminen, Ville"

Source: Scopus

Source ID: 85048753843

Research output: Contribution to journal › Article › Scientific › peer-review

### **Effects of pyrolysis temperature on the hydrologically relevant porosity of willow biochar**

Biochar pore space consists of porosity of multiple length scales. In direct water holding applications like water storage for plant water uptake, the main interest is in micrometre-range porosity since these pores are able to store water that is easily available for plants. Gas adsorption measurements which are commonly used to characterize the physical pore structure of biochars are not able to quantify this pore-size range. While pyrogenetic porosity (i.e. pores formed during pyrolysis process) tends to increase with elevated process temperature, it is uncertain whether this change affects the pore space capable to store plant available water. In this study, we characterized biochar porosity with x-ray tomography

which provides quantitative information on the micrometer-range porosity. We imaged willow dried at 60 °C and biochar samples pyrolysed in three different temperatures (peak temperatures 308, 384, 489 °C, heating rate 2 °C min<sup>-1</sup>). Samples were carefully prepared and traced through the experiments, which allowed investigation of porosity development in micrometre size range. Pore space was quantified with image analysis of x-ray tomography images and, in addition, nanoscale porosity was examined with helium ion microscopy. The image analysis results show that initial pore structure of the raw material determines the properties of micrometre-range porosity in the studied temperature range. Thus, considering the pore-size regime relevant to the storage of plant available water, pyrolysis temperature in the studied range does not provide means to optimize the biochar structure. However, these findings do not rule out that process temperature may affect the water retention properties of biochars by modifying the chemical properties of the pore surfaces.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Natural Resources Institute Finland (Luke), Jyväskylän yliopisto, Foshan University, Zhejiang A & F University

Contributors: Hyvältuoma, J., Hannula, M., Arstila, K., Wang, H., Kulju, S., Rasa, K.

Publication date: Sep 2018

Peer-reviewed: Yes

Early online date: 2018

#### Publication information

Journal: Journal of Analytical and Applied Pyrolysis

Volume: 134

ISSN (Print): 0165-2370

Ratings:

Scopus rating (2018): CiteScore 4.05 SJR 1.11 SNIP 1.256

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

Keywords: Biochar, Image analysis, Porosity, Slow pyrolysis, X-ray tomography

DOIs:

10.1016/j.jaap.2018.07.011

#### Bibliographical note

EXT="Kulju, Sampo"

Source: Scopus

Source ID: 85050304071

Research output: Contribution to journal > Article > Scientific > peer-review

#### Photoinduced Energy Transfer in ZnCdSeS Quantum Dot-Phthalocyanines Hybrids

In this article, interaction between ZnCdSeS quantum dot (QD) and phthalocyanines with variable linker has been reported. Steady-state and time-resolved spectroscopic investigation reveals that only photoinduced energy transfer occurs from QD to phthalocyanines. To evaluate quantitatively the energy transfer, the Poisson statistics of QD-dye complex formation was used in the analysis of steady-state and time-resolved emission quenching, which allows to estimate the energy transfer rate constant for an ideal one-to-one complex. The measured rate constants are compared to the rates evaluated based on the classic Förster theory, which shows roughly 1 nm discrepancy in the energy transfer distance estimation, or one order in magnitude discrepancy in the transfer rate constants.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Universidad Autónoma de Madrid, Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Mersin University

Contributors: Mandal, S., Garcia Iglesias, M., Ince, M., Torres, T., Tkachenko, N. V.

Number of pages: 10

Pages: 10048-10057

Publication date: 31 Aug 2018

Peer-reviewed: Yes

#### Publication information

Journal: ACS Omega

Volume: 3

Issue number: 8

ISSN (Print): 2470-1343

Ratings:

Scopus rating (2018): CiteScore 2.54 SJR 0.754 SNIP 0.673  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)  
Electronic versions:  
acsomega.8b01623  
DOIs:  
10.1021/acsomega.8b01623  
URLs:  
<http://urn.fi/URN:NBN:fi:tty-201810012343>  
Source: Scopus  
Source ID: 85052704543  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Selenate removal in biofilm systems: Effect of nitrate and sulfate on selenium removal efficiency, biofilm structure and microbial community**

**BACKGROUND:** Selenium (Se) discharged into natural waterbodies can accumulate over time and have negative impacts on the environment. Se-laden wastewater streams can be treated using biological processes. However, the presence of other electron acceptors in wastewater, such as nitrate ( $\text{NO}_3^-$ ) and sulfate ( $\text{SO}_4^{2-}$ ), can influence selenate ( $\text{SeO}_4^{2-}$ ) reduction and impact the efficiency of biological treatment systems. **RESULTS:**  $\text{SeO}_4^{2-}$  removal by biofilms formed from an anaerobic sludge inoculum was investigated in the presence of  $\text{NO}_3^-$  and  $\text{SO}_4^{2-}$  using drip flow reactors operated continuously for 10 days at pH 7.0 and 30°C. The highest total Se (~60%) and  $\text{SeO}_4^{2-}$  (~80%) removal efficiencies were observed when the artificial wastewater contained  $\text{SO}_4^{2-}$ . A maximum amount of  $68 \mu\text{mol Se cm}^{-2}$  was recovered from the biofilm matrix in  $\text{SO}_4^{2-}$ + $\text{SeO}_4^{2-}$  exposed biofilms and biofilm mass was 2.7-fold increased for biofilms grown in the presence of  $\text{SO}_4^{2-}$ . When  $\text{SeO}_4^{2-}$  was the only electron acceptor, biofilms were thin and compact. In the simultaneous presence of  $\text{NO}_3^-$  or  $\text{SO}_4^{2-}$ , biofilms were thicker (> 0.6 mm), less compact and exhibited gas pockets. **CONCLUSION:** The presence of  $\text{SO}_4^{2-}$  had a beneficial effect on biofilm growth and the  $\text{SeO}_4^{2-}$  removal efficiency, while the presence of  $\text{NO}_3^-$  did not have a significant effect on  $\text{SeO}_4^{2-}$  removal by the biofilms.

#### **General information**

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Chemistry and Bioengineering, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education, Montana State University (MSU), Bhabha Atomic Research Centre, UPEM  
Contributors: Tan, L. C., Espinosa-Ortiz, E. J., Nancharaiyah, Y. V., van Hullebusch, E. D., Gerlach, R., Lens, P. N.  
Pages: 2380-2389  
Publication date: Aug 2018  
Peer-reviewed: Yes  
Early online date: 1 Jan 2018

#### **Publication information**

Journal: Journal of Chemical Technology and Biotechnology  
Volume: 93  
Issue number: 8  
ISSN (Print): 0268-2575  
Ratings:

Scopus rating (2018): CiteScore 2.88 SJR 0.715 SNIP 0.883  
Original language: English  
ASJC Scopus subject areas: Biotechnology, Chemical Engineering(all), Renewable Energy, Sustainability and the Environment, Fuel Technology, Waste Management and Disposal, Pollution, Organic Chemistry, Inorganic Chemistry  
Keywords: Biofilm, Biofilm characterization, Co-electron acceptors, Nitrate, Selenate, Selenium removal, Sulfate  
DOIs:  
10.1002/jctb.5586  
Source: Scopus  
Source ID: 85043713774  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Design aspects of all atomic layer deposited TiO<sub>2</sub>-Fe<sub>2</sub>O<sub>3</sub> scaffold-absorber photoanodes for water splitting**

Iron and titanium oxides have attracted substantial attention in photoelectrochemical water splitting applications. However, both materials suffer from intrinsic limitations that constrain the final device performance. In order to overcome the limitations of the two materials alone, their combination has been proposed as a solution to the problems. Here we report on the fabrication of an atomic layer deposited (ALD) Fe<sub>2</sub>O<sub>3</sub> coating on porous ALD-TiO<sub>2</sub>. Our results show that successful implementation requires complete mixing of the TiO<sub>2</sub> and Fe<sub>2</sub>O<sub>3</sub> layers via annealing resulting in the formation of a photoactive iron titanium oxide on the surface. Moreover, we found that incomplete mixing leads to crystallization of Fe<sub>2</sub>O<sub>3</sub> to hematite that is detrimental to the photoelectrochemical performance. IPCE and transient photocurrent



measurements performed using UV and visible light excitation confirmed that the iron titanium oxide extends the photocurrent generation to the visible range. These measurements were complemented by transient absorption spectroscopy (TAS), which revealed a new band absent in pristine hematite or anatase TiO<sub>2</sub> that we assign to charge transfer within the structure. Taken together, these results provide design guidelines to be considered when aiming to combine TiO<sub>2</sub> and Fe<sub>2</sub>O<sub>3</sub> for photoelectrochemical applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Research group: Surface Science, Photonics, Materials Science, Research group: Plastics and Elastomer Technology

Contributors: Hiltunen, A., Ruoko, T., Iivonen, T., Lahtonen, K., Ali-Löytty, H., Sarlin, E., Valden, M., Leskelä, M., Tkachenko, N.

Pages: 2124-2130

Publication date: 31 Jul 2018

Peer-reviewed: Yes

#### Publication information

Journal: Sustainable Energy & Fuels

Volume: 2

Issue number: 9

ISSN (Print): 2398-4902

Ratings:

Scopus rating (2018): CiteScore 4.94 SNIP 0.841

Original language: English

ASJC Scopus subject areas: Electrochemistry, Renewable Energy, Sustainability and the Environment, Surfaces, Coatings and Films

Keywords: Water splitting, Atomic layer deposition (ALD), Titanium dioxide, Hematite, Cellulose, Template

DOIs:

10.1039/C8SE00252E

Research output: Contribution to journal > Article > Scientific > peer-review

#### High Bending-Mode Sensitivity of Printed Piezoelectric Poly(vinylidene fluoride- co-trifluoroethylene) Sensors

Printable piezoelectric sensors were fabricated on a flexible polyethylene terephthalate (PET) substrate. Solution-processed piezoelectric poly(vinylidene fluoride-co-trifluoroethylene) ink was used as an active layer. Evaporated silver on PET was used as the bottom electrode and the painted silver glue as the top electrode. The sensors were poled using a high dc electric field from 25 to 65 MV m<sup>-1</sup>, yielding piezoelectric normal direction sensitivities up to 25 pC N<sup>-1</sup>. Bending-mode sensitivities showed values up to 200 nC N<sup>-1</sup>, which is 4 orders of magnitude larger than the force sensitivity in the normal direction. The high bending-mode sensitivities suggest suitability for detecting small forces, such as single fiber bonds or cardiomyocyte cell-beating force.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Nokia Technologies, University of Twente

Contributors: Rajala, S., Schouten, M., Krijnen, G., Tuukkanen, S.

Number of pages: 7

Pages: 8067-8073

Publication date: 23 Jul 2018

Peer-reviewed: Yes

#### Publication information

Journal: ACS Omega

Volume: 3

Issue number: 7

ISSN (Print): 2470-1343

Ratings:

Scopus rating (2018): CiteScore 2.54 SJR 0.754 SNIP 0.673

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

Electronic versions:

full text

DOIs:

10.1021/acsomega.8b01185

URLs:

<http://urn.fi/URN:NBN:fi:tty-201808072055>

### Bibliographical note

EXT="Rajala, Satu"

Source: Scopus

Source ID: 85050457848

Research output: Contribution to journal > Article > Scientific > peer-review

### Pectin and Mucin Enhance the Bioadhesion of Drug Loaded Nanofibrillated Cellulose Films

**Purpose:** Bioadhesion is an important property of biological membranes, that can be utilized in pharmaceutical and biomedical applications. In this study, we have fabricated mucoadhesive drug releasing films with bio-based, non-toxic and biodegradable polymers that do not require chemical modifications. **Methods:** Nanofibrillar cellulose and anionic type nanofibrillar cellulose were used as film forming materials with known mucoadhesive components mucin, pectin and chitosan as functional bioadhesion enhancers. Different polymer combinations were investigated to study the adhesiveness, solid state characteristics, film morphology, swelling, mechanical properties, drug release with the model compound metronidazole and in vitro cytotoxicity using TR146 cells to model buccal epithelium. **Results:** SEM revealed lamellar structures within the films, which had a thickness ranging 40–240 µm depending on the film polymer composition. All bioadhesive components were non-toxic and showed high adhesiveness. Rapid drug release was observed, as 60–80% of the total amount of metronidazole was released in 30 min depending on the film formulation. **Conclusions:** The liquid molding used was a straightforward and simple method to produce drug releasing highly mucoadhesive films, which could be utilized in treating local oral diseases, such as periodontitis. All materials used were natural biodegradable polymers from renewable sources, which are generally regarded as safe.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Aalto University, Universita degli Studi di Padova, Italy, University of Helsinki, University of Helsinki

Contributors: Laurén, P., Paukkonen, H., Lipiäinen, T., Dong, Y., Oksanen, T., Rääkkönen, H., Ehlers, H., Laaksonen, P., Yliperttula, M., Laaksonen, T.

Publication date: 1 Jul 2018

Peer-reviewed: Yes

### Publication information

Journal: Pharmaceutical Research

Volume: 35

Issue number: 7

Article number: 145

ISSN (Print): 0724-8741

Ratings:

Scopus rating (2018): CiteScore 3.89 SJR 1.093 SNIP 1.108

Original language: English

ASJC Scopus subject areas: Biotechnology, Molecular Medicine, Pharmacology, Pharmaceutical Science, Organic Chemistry, Pharmacology (medical)

Keywords: bioadhesion, drug release, mucoadhesion, nanofibrillar cellulose, TR146

Electronic versions:

Manuscript - revised version - final. Embargo ended: 22/05/19

DOIs:

10.1007/s11095-018-2428-z

URLs:

<http://urn.fi/URN:NBN:fi:tty-201810262482>. Embargo ended: 22/05/19

Source: Scopus

Source ID: 85047448577

Research output: Contribution to journal > Article > Scientific > peer-review

### Effect of surfactant type and sonication energy on the electrical conductivity properties of nanocellulose-CNT nanocomposite films

We present a detailed study on the influence of sonication energy and surfactant type on the electrical conductivity of nanocellulose-carbon nanotube (NFC-CNT) nanocomposite films. The study was made using a minimum amount of processing steps, chemicals and materials, to optimize the conductivity properties of free-standing flexible nanocomposite films. In general, the NFC-CNT film preparation process is sensitive concerning the dispersing phase of CNTs into a solution with NFC. In our study, we used sonication to carry out the dispersing phase of processing in the presence of surfactant. In the final phase, the films were prepared from the dispersion using centrifugal cast molding. The solid films were analyzed regarding their electrical conductivity using a four-probe measuring technique. We also characterized how

conductivity properties were enhanced when surfactant was removed from nanocomposite films; to our knowledge this has not been reported previously. The results of our study indicated that the optimization of the surfactant type clearly affected the formation of freestanding films. The effect of sonication energy was significant in terms of conductivity. Using a relatively low 16 wt. % concentration of multiwall carbon nanotubes we achieved the highest conductivity value of 8.4 S/cm for nanocellulose-CNT films ever published in the current literature. This was achieved by optimizing the surfactant type and sonication energy per dry mass. Additionally, to further increase the conductivity, we defined a preparation step to remove the used surfactant from the final nanocomposite structure.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Faculty of Biomedical Sciences and Engineering, VTT Technical Research Centre of Finland

Contributors: Siljander, S., Keinänen, P., Rätty, A., Ramakrishnan, K. R., Tuukkanen, S., Kunnari, V., Harlin, A., Vuorinen, J., Kanerva, M.

Publication date: 20 Jun 2018

Peer-reviewed: Yes

#### Publication information

Journal: International Journal of Molecular Sciences

Volume: 19

Issue number: 6

Article number: 1819

ISSN (Print): 1661-6596

Ratings:

Scopus rating (2018): CiteScore 4.32 SJR 1.312 SNIP 1.224

Original language: English

ASJC Scopus subject areas: Catalysis, Molecular Biology, Spectroscopy, Computer Science Applications, Physical and Theoretical Chemistry, Organic Chemistry, Inorganic Chemistry

Keywords: Carbon nanotubes, Conductivity, Nanocellulose, Nanocomposite, Surfactant

Electronic versions:

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DOIs:

10.3390/ijms19061819

URLs:

<http://urn.fi/URN:NBN:fi:ty-201807302026>

#### Bibliographical note

INT=mol,"Rätty, Anna"

EXT="Harlin, Ali"

Source: Scopus

Source ID: 85048936349

Research output: Contribution to journal > Article > Scientific > peer-review

#### Multifunctional nitrogen sulfur co-doped reduced graphene oxide – Ag nano hybrids (sphere, cube and wire) for nonlinear optical and SERS applications

Hetero atom doped graphene - metal nanoparticle hybrids have received increasing attention owing to their unique electronic properties, large specific surface area, very high conductivity and more electronic interactions. Herein, we report for the first time a hydrothermal assisted strategy for developing novel class of nitrogen (N) and sulfur (S) co-doped graphene/Ag nano morphotypes (sphere, cube and wire) hybrids for enhanced optical limiting (OL) and surface-enhanced Raman scattering (SERS) applications. Two probe molecules, Rhodamine 6G and para-aminothiophenol, are chosen to determine the enhancement performance of the as-prepared SERS-active substrate. Our results signified that the Ag nanocube-N, S codoped graphene hybrid based SERS-active substrate presents excellent performances for sensing R6G with an enhancement factor of  $1.07 \times 10^7$ . Further, this SERS substrate reveals outstanding capability to detect P-ATP molecules with detection limit of approximately  $1.0 \times 10^{-12}$  M. Moreover, the non-linear optical absorption studies results show that the OL properties were appreciably enhanced after the insertion of Ag nanostructures on the NSG surface. Thus, OL properties of the two-dimensional N, S-codoped graphene can be effectively modified by absorbing AgNPs of different morphology on its surface. All of the results signify that these hybrid structures will show extended applications for SERS sensing and optoelectronic fields.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Mahatma Gandhi University, St Teresas's College, Ultra-Fast and Nonlinear Optical Lab, Raman Research Institute, CNRS Centre National de la Recherche Scientifique

Contributors: Nair, A. K., Bhavitha, K. B., Perumbilavil, S., Sankar, P., Rouxel, D., Kala, M. S., Thomas, S., Kalarikkal, N.  
Number of pages: 14  
Pages: 380-393  
Publication date: 1 Jun 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Carbon  
Volume: 132  
ISSN (Print): 0008-6223  
Ratings:

Scopus rating (2018): CiteScore 7.42 SJR 2.116 SNIP 1.695

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Ag nanomorphotypes, Nitrogen sulfur co-doped graphene, Optical limiting, Rhodamine 6G, Surface enhanced Raman scattering

DOIs:

10.1016/j.carbon.2018.02.068

Source: Scopus

Source ID: 85042707462

Research output: Contribution to journal > Article > Scientific > peer-review

#### Photo-antimicrobial efficacy of zinc complexes of porphyrin and phthalocyanine activated by inexpensive consumer LED lamp

The properties and antimicrobial efficacies of zinc complexes of tetrakis(N-methylpyridinium-4-yl) tetraiodide porphyrin and tetrakis(N-methylpyridinium-4-yl) tetraiodide phthalocyanine impregnated to paper were evaluated. Photo-inactivation of microbes using inexpensive consumer light-emitting diode lamp was assessed on surface of dyed papers. Antimicrobial experiments of phthalocyanine-dyed paper by live cell assessment through colony forming units counting demonstrated 3.72 and 4.01 log reduction against *Escherichia coli* (*E. coli*) and *Acinetobacter baylyi* (*A. baylyi*) respectively after 1 h of illumination with 35 mW/cm<sup>2</sup> light. The porphyrin-dyed paper exhibited 1.66 and 2.01 log reduction in colony forming units against *E. coli* and *A. baylyi* respectively after 1 h exposure with 4 mW/cm<sup>2</sup> light. Both dyed papers were photo-stable after 64 h of continuous exposure with 42 mW/cm<sup>2</sup> light, while phthalocyanine-dyed paper exhibited superior leaching stability in phosphate-buffered saline.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Research group: Bio- and Circular Economy

Contributors: George, L., Hiltunen, A., Santala, V., Efimov, A.

Number of pages: 7

Pages: 94-100

Publication date: 1 Jun 2018

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Inorganic Biochemistry

Volume: 183

ISSN (Print): 0162-0134

Ratings:

Scopus rating (2018): CiteScore 3.16 SJR 0.655 SNIP 0.895

Original language: English

ASJC Scopus subject areas: Biochemistry, Inorganic Chemistry

DOIs:

10.1016/j.jinorgbio.2018.03.015

Source: Scopus

Source ID: 85044575449

Research output: Contribution to journal > Article > Scientific > peer-review

#### Acquiring respiration rate from photoplethysmographic signal by recursive bayesian tracking of intrinsic modes in time-frequency spectra

Respiration rate (RR) provides useful information for assessing the status of a patient. We propose RR estimation based on photoplethysmography (PPG) because the blood perfusion dynamics are known to carry information on breathing, as respiration-induced modulations in the PPG signal. We studied the use of amplitude variability of transmittance mode finger PPG signal in RR estimation by comparing four time-frequency (TF) representation methods of the signal cascaded

with a particle filter. The TF methods compared were short-time Fourier transform (STFT) and three types of synchrosqueezing methods. The public VORTAL database was used in this study. The results indicate that the advanced frequency reallocation methods based on synchrosqueezing approach may present improvement over linear methods, such as STFT. The best results were achieved using wavelet synchrosqueezing transform, having a mean absolute error and median error of 2.33 and 1.15 breaths per minute, respectively. Synchrosqueezing methods were generally more accurate than STFT on most of the subjects when particle filtering was applied. While TF analysis combined with particle filtering is a promising alternative for real-time estimation of RR, artefacts and non-respiration-related frequency components remain problematic and impose requirements for further studies in the areas of signal processing algorithms and PPG instrumentation.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Sensor Technology and Biomeasurements (STB)

Contributors: Pirhonen, M., Peltokangas, M., Vehkaoja, A.

Publication date: 1 Jun 2018

Peer-reviewed: Yes

### Publication information

Journal: Sensors

Volume: 18

Issue number: 6

Article number: 1693

ISSN (Print): 1424-8220

Ratings:

Scopus rating (2018): CiteScore 3.72 SJR 0.592 SNIP 1.576

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Atomic and Molecular Physics, and Optics, Biochemistry, Instrumentation, Electrical and Electronic Engineering

Keywords: Particle filters, Photoplethysmography, Respiration, Synchrosqueezing, Time-frequency analysis

Electronic versions:

sensors-18-01693

DOIs:

10.3390/s18061693

URLs:

<http://urn.fi/URN:NBN:fi:tty-201806212010>

### Bibliographical note

int=TUT-BMT,"Pirhonen, Mikko"

Source: Scopus

Source ID: 85047608517

Research output: Contribution to journal > Article > Scientific > peer-review

### Evaluation of dry electrodes in canine heart rate monitoring

The functionality of three dry electrocardiogram electrode constructions was evaluated by measuring canine heart rate during four different behaviors: Standing, sitting, lying and walking. The testing was repeated ( $n = 9$ ) in each of the 36 scenarios with three dogs. Two of the electrodes were constructed with spring-loaded test pins while the third electrode was a molded polymer electrode with Ag/AgCl coating. During the measurement, a specifically designed harness was used to attach the electrodes to the dogs. The performance of the electrodes was evaluated and compared in terms of heartbeat detection coverage. The effect on the respective heart rate coverage was studied by computing the heart rate coverage from the measured electrocardiogram signal using a pattern-matching algorithm to extract the R-peaks and further the beat-to-beat heart rate. The results show that the overall coverage ratios regarding the electrodes varied between 45-95% in four different activity modes. The lowest coverage was for lying and walking and the highest was for standing and sitting.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Pervasive Computing, Research group: Sensor Technology and Biomeasurements (STB), University of Helsinki, Institute of Biomedical Engineering and Informatics, University of Tampere (UTA), Research Group for Emotions

Contributors: Virtanen, J., Somppi, S., Törnqvist, H., Jeyhani, V., Fiedler, P., Gizatdinova, Y., Majoranta, P., Väättäjä, H., Cardó, A. V., Lekkala, J., Tuukkanen, S., Surakka, V., Vainio, O., Vehkaoja, A.

Publication date: 1 Jun 2018

Peer-reviewed: Yes

### Publication information

Journal: Sensors

Volume: 18

Issue number: 6

Article number: 1757

ISSN (Print): 1424-8220

Ratings:

Scopus rating (2018): CiteScore 3.72 SJR 0.592 SNIP 1.576

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Atomic and Molecular Physics, and Optics, Biochemistry, Instrumentation, Electrical and Electronic Engineering

Keywords: Dry electrode, Heart rate canine

Electronic versions:

sensors-18-01757-v2

DOIs:

10.3390/s18061757

URLs:

<http://urn.fi/URN:NBN:fi:tty-201806212014>

Source: Scopus

Source ID: 85047961818

Research output: Contribution to journal › Article › Scientific › peer-review

### Effect of Co-Adsorbate and Hole Transporting Layer on the Photoinduced Charge Separation at the TiO<sub>2</sub>-Phthalocyanine Interface

Understanding the primary processes of charge separation (CS) in solid-state dye-sensitized solar cells (DSSCs) and, in particular, analysis of the efficiency losses during these primary photoreactions is essential for designing new and efficient photosensitizers. Phthalocyanines (Pcs) are potentially interesting sensitizers having absorption in the red side of the optical spectrum and known to be efficient electron donors. However, the efficiencies of Pc-sensitized DSSCs are lower than that of the best DSSCs, which is commonly attributed to the aggregation tendency of Pcs. In this study, we employ ultrafast spectroscopy to discover why and how much does the aggregation affect the efficiency. The samples were prepared on a standard fluorine-doped tin oxide (FTO) substrates covered by a porous layer of TiO<sub>2</sub> nanoparticles, functionalized by a Pc sensitizer and filled by a hole transporting material (Spiro-MeOTAD). The study demonstrates that the aggregation can be suppressed gradually by using co-adsorbates, such as chenodeoxycholic acid (CDCA) and oleic acid, but rather high concentrations of co-adsorbate is required. Gradually, a few times improvement of quantum efficiency was observed at sensitizer/co-adsorbate ratio Pc/CDCA = 1:10 and higher. The time-resolved spectroscopy studies were complemented by standard photocurrent measurements of the same sample structures, which also confirmed gradual increase in photon-to-current conversion efficiency on mixing Pc with CDCA.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Universidad Autónoma de Madrid, Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Departamento de Química Orgánica

Contributors: Virkki, K., Tervola, E., Medel, M., Torres, T., Tkachenko, N. V.

Number of pages: 12

Pages: 4947-4958

Publication date: 31 May 2018

Peer-reviewed: Yes

### Publication information

Journal: ACS Omega

Volume: 3

Issue number: 5

ISSN (Print): 2470-1343

Ratings:

Scopus rating (2018): CiteScore 2.54 SJR 0.754 SNIP 0.673

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

DOIs:

10.1021/acsomega.8b00600

Source: Scopus

Source ID: 85046661219

### **A Ceramide-Regulated Element in the Late Endosomal Protein LAPT4B Controls Amino Acid Transporter Interaction**

Membrane proteins are functionally regulated by the composition of the surrounding lipid bilayer. The late endosomal compartment is a central site for the generation of ceramide, a bioactive sphingolipid, which regulates responses to cell stress. The molecular interactions between ceramide and late endosomal transmembrane proteins are unknown. Here, we uncover in atomistic detail the ceramide interaction of Lysosome Associated Protein Transmembrane 4B (LAPT4B), implicated in ceramide-dependent cell death and autophagy, and its functional relevance in lysosomal nutrient signaling. The ceramide-mediated regulation of LAPT4B depends on a sphingolipid interaction motif and an adjacent aspartate residue in the protein's third transmembrane (TM3) helix. The interaction motif provides the preferred contact points for ceramide while the neighboring membrane-embedded acidic residue confers flexibility that is subject to ceramide-induced conformational changes, reducing TM3 bending. This facilitates the interaction between LAPT4B and the amino acid transporter heavy chain 4F2hc, thereby controlling mTORC signaling. These findings provide mechanistic insights into how transmembrane proteins sense and respond to ceramide.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, University of Helsinki Faculty of Medicine, Minerva Foundation Institute for Medical Research Helsinki, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Laboratory of Physics, Abo Akademi University, Queens College, City University of New York, University of Helsinki

Contributors: Zhou, K., Dichlberger, A., Martinez-Seara, H., Nyholm, T. K., Li, S., Kim, Y. A., Vattulainen, I., Ikonen, E., Blom, T.

Number of pages: 11

Pages: 548-558

Publication date: 23 May 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: ACS Central Science

Volume: 4

Issue number: 5

ISSN (Print): 2374-7943

Ratings:

Scopus rating (2018): CiteScore 8 SJR 4.94 SNIP 2.027

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

DOIs:

10.1021/acscentsci.7b00582

Source: Scopus

Source ID: 85047534763

Research output: Contribution to journal › Article › Scientific › peer-review

### **Wet etching of dilute nitride GaInNAs, GaInNAsSb, and GaNAsSb alloys lattice-matched to GaAs**

We have studied the etching of GaInNAs, GaInNAsSb, and GaNAsSb alloys by  $\text{NH}_4\text{OH}$ ,  $\text{H}_2\text{SO}_4$ , and  $\text{H}_3\text{PO}_4$  based solutions.  $\text{NH}_4\text{OH}$  based solutions resulted in smooth surface, while other solutions created rougher and granular surfaces. The etch rates were found to increase with the Sb content. For GaInNAs, x-ray photoelectron spectroscopy revealed the enrichment of In on the etched surfaces, indicating In or In oxides having a smaller removal rate compared to Ga or Ga oxides. The enrichment of In was associated with smoother surfaces after etching and an enhanced photoluminescence caused by lower surface recombination due to reduced surface state density.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Research group: ORC, Department of Physics and Astronomy, University of Turku, Turun Yliopisto/Turun Biomateriaalikeskus

Contributors: Raappana, M., Polojärvi, V., Aho, A., Mäkelä, J., Aho, T., Tukiainen, A., Laukkanen, P., Guina, M.

Number of pages: 7

Pages: 268-274

Publication date: 15 May 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: Corrosion Science

Volume: 136  
ISSN (Print): 0010-938X  
Ratings:

Scopus rating (2018): CiteScore 6.76 SJR 2.131 SNIP 2.595

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all), Materials Science(all)

Keywords: A. Alloy, B. AFM, B. XPS, C. Acid corrosion, C. Alkaline corrosion, C. Passivity

DOIs:

10.1016/j.corsci.2018.03.018

#### **Bibliographical note**

EXT="Mäkelä, Jaakko"

EXT="Laukkanen, Pekka"

Source: Scopus

Source ID: 85044276587

Research output: Contribution to journal > Article > Scientific > peer-review

#### **Free amino acids and 5'-nucleotides in Finnish forest mushrooms**

Edible mushrooms are valued because of their umami taste and good nutritional values. Free amino acids, 5'-nucleotides and nucleosides were analyzed from four Nordic forest mushroom species (*Lactarius camphoratus*, *Boletus edulis*, *Cantharellus cibarius*, *Craterellus tubaeformis*) using high precision liquid chromatography analysis. To our knowledge, these taste components were studied for the first time from *Craterellus tubaeformis* and *Lactarius camphoratus*. The focus was on the umami amino acids and 5'-nucleotides. The free amino acid and 5'-nucleotide/nucleoside contents of studied species differed from each other. In all studied samples, umami amino acids were among five major free amino acids. The highest concentration of umami amino acids was on *L. camphoratus* whereas *B. edulis* had the highest content of sweet amino acids and *C. cibarius* had the highest content of bitter amino acids. The content of umami enhancing 5'-nucleotides were low in all studied species.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Turun Yliopisto/Turun Biomateriaalikeskus

Contributors: Manninen, H., Rotola-Pukkila, M., Aisala, H., Hopia, A., Laaksonen, T.

Number of pages: 6

Pages: 23-28

Publication date: May 2018

Peer-reviewed: Yes

Early online date: 7 Dec 2017

#### **Publication information**

Journal: Food Chemistry

Volume: 247

ISSN (Print): 0308-8146

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Scopus rating (2018): CiteScore 5.8 SJR 1.768 SNIP 2.17

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Food Science

Keywords: 5'-Nucleotides, Amino acids, Mushrooms, Umami

Electronic versions:

Manuscript\_Free amino acids and 5'-nucleotides in Finnish forest mushrooms\_revised. Embargo ended: 13/12/18

DOIs:

10.1016/j.foodchem.2017.12.014

URLs:

<http://urn.fi/URN:NBN:fi:tty-201810262481>. Embargo ended: 13/12/18

Source: Scopus

Source ID: 85037999138

Research output: Contribution to journal > Article > Scientific > peer-review

#### **Characteristics of nFOG, an aerosol-based wet thin film coating technique**

An atmospheric pressure aerosol-based wet thin film coating technique called the nFOG is characterized and applied in polymer film coatings. In the nFOG, a fog of droplets is formed by two air-assist atomizers oriented toward each other inside a deposition chamber. The droplets settle gravitationally and deposit on a substrate, forming a wet film. In this study, the continuous deposition mode of the nFOG is explored. We determined the size distribution of water droplets



inside the chamber in a wide size range of 0.1–100  $\mu\text{m}$  and on the substrate using aerosol measurement instruments and optical microscopy, respectively. The droplet size distribution was found to be bimodal with droplets of approximately 30–50  $\mu\text{m}$  contributing the most to the mass of the formed wet film. The complementary measurement methods allow us to estimate the role of different droplet deposition mechanisms. The obtained results suggest that the deposition velocity of the droplets is lower than the calculated terminal settling velocity, likely due to the flow fields inside the chamber. Furthermore, the mass flux of the droplets onto the substrate is determined to be in the order of  $1\text{ g/m}^3\text{s}$ , corresponding to a wet film growth rate of  $1\text{ }\mu\text{m/s}$ . Finally, the nFOG technique is demonstrated by preparing polymer films with thicknesses in the range of approximately 0.1–20  $\mu\text{m}$ .

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Materials Science, RISE Bioscience and Materials, Research Institutes of Sweden, Lund University

Contributors: Harra, J., Tuominen, M., Juuti, P., Rissler, J., Koivuluoto, H., Haapanen, J., Niemelä-Anttonen, H., Stenroos, C., Teisala, H., Lahti, J., Kuusipalo, J., Vuoristo, P., Mäkelä, J. M.

Number of pages: 10

Pages: 623-632

Publication date: May 2018

Peer-reviewed: Yes

Early online date: 1 Feb 2018

### Publication information

Journal: Journal of Coatings Technology Research

Volume: 15

Issue number: 3

ISSN (Print): 1547-0091

Ratings:

Scopus rating (2018): CiteScore 1.66

Original language: English

ASJC Scopus subject areas: Chemistry(all), Surfaces and Interfaces, Surfaces, Coatings and Films, Colloid and Surface Chemistry

Keywords: Aerosol measurement, Droplet size distribution, nFOG, Polymer film, Wet coating technique

DOIs:

10.1007/s11998-017-0022-7

### Bibliographical note

EXT="Tuominen, Mikko"

Source: Scopus

Source ID: 85045145179

Research output: Contribution to journal > Article > Scientific > peer-review

### Accurate Binding of Sodium and Calcium to a POPC Bilayer by Effective Inclusion of Electronic Polarization

Binding affinities and stoichiometries of  $\text{Na}^+$  and  $\text{Ca}^{2+}$  ions to phospholipid bilayers are of paramount significance in the properties and functionality of cellular membranes. Current estimates of binding affinities and stoichiometries of cations are, however, inconsistent due to limitations in the available experimental and computational methods. In this work, we improve the description of the binding details of  $\text{Na}^+$  and  $\text{Ca}^{2+}$  ions to a 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) bilayer by implicitly including electronic polarization as a mean field correction, known as the electronic continuum correction (ECC). This is applied by scaling the partial charges of a selected state-of-the-art POPC lipid model for molecular dynamics simulations. Our improved ECC-POPC model reproduces not only the experimentally measured structural parameters for the ion-free membrane, but also the response of lipid headgroup to a strongly bound cationic amphiphile, as well as the binding affinities of  $\text{Na}^+$  and  $\text{Ca}^{2+}$  ions. With our new model, we observe on the one side negligible binding of  $\text{Na}^+$  ions to POPC bilayer, while on the other side stronger interactions of  $\text{Ca}^{2+}$  primarily with phosphate oxygens, which is in agreement with the previous interpretations of the experimental spectroscopic data. The present model results in  $\text{Ca}^{2+}$  ions forming complexes with one to three POPC molecules with almost equal probabilities, suggesting more complex binding stoichiometries than those from simple models used to interpret the NMR data previously. The results of this work pave the way to quantitative molecular simulations with realistic electrostatic interactions of complex biochemical systems at cellular membranes.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: Biological Physics and Soft Matter, Research area: Computational Physics, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Department of Physical Chemistry, University of Helsinki Institute of Biotechnology

Contributors: Melcr, J., Martinez-Seara, H., Nencini, R., Kolafa, J., Jungwirth, P., Ollila, O. H. S.  
Number of pages: 12  
Pages: 4546-4557  
Publication date: 26 Apr 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry B

Volume: 122

Issue number: 16

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2018): CiteScore 3.03 SJR 1.109 SNIP 0.965

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry  
DOIs:

10.1021/acs.jpcc.7b12510

#### Bibliographical note

EXT="Martinez-Seara, Hector"

EXT="Ollila, O. H. Samuli"

Source: Scopus

Source ID: 85046019210

Research output: Contribution to journal > Article > Scientific > peer-review

#### Composite Hydrogels Using Bioinspired Approach with in Situ Fast Gelation and Self-Healing Ability as Future Injectable Biomaterial

Biopolymers are attractive candidates to fabricate biocompatible hydrogels, but the low water solubility of most of them at physiological pH has hindered their applications. To prepare a water-soluble derivative of chitosan (WSC) biopolymer, it was grafted with a small anionic amino acid, L-glutamic acid, using a single-step 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide coupling reaction. This resulted in a zwitterion-tethered structure onto the polymer backbone. The degree of substitution range was  $13\text{--}16 \pm 1.25\%$ , which was controlled by varying the feeding reagent ratios. Differential scanning calorimetry- and X-ray diffraction-based analysis confirmed a transition from amorphous into a moderately amorphous/crystalline morphology after amino acid grafting, which made the derivative water-soluble at physiological pH. Composite hydrogels gelled within 60 s when using this WSC together with benzaldehyde-terminated 4-arm poly(ethylene glycol) as cross-linker. The compressive modulus of these hydrogels could be easily tuned between  $4.0 \pm 1.0$  and  $31 \pm 2.5$  kPa, either by changing the cross-linker concentration or total solid content in the final gel. The gels were injectable at the lowest cross-linker as well as total solid content, due to the enhanced elastic behavior. These hydrogels showed biodegradability during a 1 month incubation period in phosphate-buffered saline with weight remaining of  $60 \pm 1.5$  and  $44 \pm 1.45\%$  at pHs 7.4 and 6.5, respectively. The cytocompatibility of the gels was tested using the fibroblast cell line (i.e., WI-38), which showed good cell viability on the gel surface. Therefore, these hydrogels could be an important injectable biomaterial for delivery purpose in the future.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Chemistry and Bioengineering, Materials Science, Research group: Biomaterials and Tissue Engineering Group, BioMediTech, Institute of Chemical Sciences, 25120 Peshawar, Pakistan

Contributors: Khan, M., Koivisto, J., Hukka, T., Hokka, M., Kellomäki, M.

Pages: 11950-11960

Publication date: 11 Apr 2018

Peer-reviewed: Yes

Early online date: 15 Mar 2018

#### Publication information

Journal: ACS Applied Materials & Interfaces

Volume: 10

Issue number: 14

ISSN (Print): 1944-8244

Ratings:

Scopus rating (2018): CiteScore 8.69 SJR 2.596 SNIP 1.539

Original language: English

ASJC Scopus subject areas: Materials Science(all), Chemistry(all)

DOIs:

**Membrane bound COMT isoform is an interfacial enzyme: General mechanism and new drug design paradigm**

The enzyme catechol-O-methyltransferase (COMT) has water soluble (S-COMT) and membrane associated (MB-COMT), bitopic, isoforms. Of these MB-COMT is a drug target in relation to the treatment of Parkinson's disease. Using a combination of computational and experimental protocols, we have determined the substrate selection mechanism specific to MB-COMT. We show: (1) substrates with preferred affinity for MB-COMT over S-COMT orient in the membrane in a fashion conducive to catalysis from the membrane surface and (2) binding of COMT to its cofactor ADOMET induces conformational change that drives the catalytic surface of the protein to the membrane surface, where the substrates and  $Mg^{2+}$  ions, required for catalysis, are found. Bioinformatics analysis reveals evidence of this mechanism in other proteins, including several existing drug targets. The development of new COMT inhibitors with preferential affinity for MB-COMT over S-COMT is now possible and insight of broader relevance, into the function of bitopic enzymes, is provided.

**General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Universite de Geneve

Contributors: Magarkar, A., Parkkila, P., Viitala, T., Lajunen, T., Mobarak, E., Licari, G., Cramariuc, O., Vauthey, E., Róg, T., Bunker, A.

Number of pages: 4

Pages: 3440-3443

Publication date: 11 Apr 2018

Peer-reviewed: Yes

**Publication information**

Journal: Chemical Communications

Volume: 54

Issue number: 28

ISSN (Print): 1359-7345

Ratings:

Scopus rating (2018): CiteScore 6.12 SJR 2.177 SNIP 1.133

Original language: English

ASJC Scopus subject areas: Catalysis, Electronic, Optical and Magnetic Materials, Ceramics and Composites, Chemistry(all), Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry

DOIs:

10.1039/c8cc00221e

Source: Scopus

Source ID: 85044968200

Research output: Contribution to journal › Article › Scientific › peer-review

**Properties of HVOF-sprayed Stellite-6 coatings**

Stellite-6 coatings were deposited onto AISI 304 stainless steel substrate by gas-fueled HVOF spraying, systematically varying the process parameter settings. By operating the HVOF torch with a fuel-rich mixture, dense coatings (<1% porosity) are produced, containing up to  $\approx 3$  vol% oxide inclusions. A substantial amount of a Cr-rich f.c.c. phase is found, mainly produced by quenching of molten lamellae, and distinct from the equilibrium, Co-based f.c.c. solid solution retained in unmelted particles. These coatings exhibit pseudo-passive behavior and survive 5 cycles (100 h) of the Corrodokote test (ASTM B380-97) with no substrate corrosion. Coatings obtained from oxygen-rich mixtures, on the other hand, contain fewer oxide inclusions but also greater porosity, and do not protect the substrate against corrosion. The wear behavior of the coatings is less influenced by deposition conditions. In ball-on-disk dry sliding tests, all coatings exhibit wear rates of  $2-3 \times 10^{-5} \text{ mm}^3/(\text{N}\cdot\text{m})$ , higher than those reported for bulk or clad Stellite, because of interlamellar delamination. Strain-induced, "martensitic" phase transformation from the f.c.c. structure to a h.c.p. one is observed over a 1–2  $\mu\text{m}$  depth below the contact surface. Additional tribo-oxidation is onset when frictional heat dissipation has heated the wear debris enough to trigger its reaction with the environment. Correspondingly, a transition to a regime of higher friction occurs (from  $\approx 0.6$  to  $\approx 0.8$ ). At 400 °C, lamellar delamination is suppressed but wear rates rise to  $5-8 \times 10^{-5} \text{ mm}^3/(\text{N}\cdot\text{m})$  because of abrasive and adhesive wear. At 800 °C, a dense "glaze" tribofilm is formed by sintered debris particles, firmly bonded to a thermally grown oxide scale on the underlying metal surface. The "glaze" protects the coating, lowering the wear rate to  $\approx 1 \times 10^{-5} \text{ mm}^3/(\text{N}\cdot\text{m})$  and the friction coefficient to <0.45. Under high-stress particle abrasion conditions, wear rates of  $\approx 1 \times 10^{-3} \text{ mm}^3/(\text{N}\cdot\text{m})$  are found.

**General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Materials Characterization, Università degli Studi di Modena e Reggio Emilia, Il Sentiero International Campus S.r.l., Univ of Oulu, ECOR Research SpA  
Contributors: Sassatelli, P., Bolelli, G., Lassinantti Gualtieri, M., Heinonen, E., Honkanen, M., Lusvarghi, L., Manfredini, T., Rigon, R., Vippola, M.  
Number of pages: 18  
Pages: 45-62  
Publication date: 25 Mar 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Surface and Coatings Technology

Volume: 338

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2018): CiteScore 3.44 SJR 0.973 SNIP 1.435

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry

Keywords: Dry particles abrasion, Electrochemical corrosion test, High velocity oxygen-fuel (HVOF), High-temperature tribology, Sliding wear, Stellite coating

DOIs:

10.1016/j.surfcoat.2018.01.078

Source: Scopus

Source ID: 85041473768

Research output: Contribution to journal > Article > Scientific > peer-review

#### Thermal Isomerization of Hydroxyazobenzenes as a Platform for Vapor Sensing

Photoisomerization of azobenzene derivatives is a versatile tool for devising light-responsive materials for a broad range of applications in photonics, robotics, microfabrication, and biomaterials science. Some applications rely on fast isomerization kinetics, while for others, bistable azobenzenes are preferred. However, solid-state materials where the isomerization kinetics depends on the environmental conditions have been largely overlooked. Herein, an approach to utilize the environmental sensitivity of isomerization kinetics is developed. It is demonstrated that thin polymer films containing hydroxyazobenzenes offer a conceptually novel platform for sensing hydrogen-bonding vapors in the environment. The concept is based on accelerating the thermal cis-trans isomerization rate through hydrogen-bond-catalyzed changes in the thermal isomerization pathway, which allows for devising a relative humidity sensor with high sensitivity and quick response to relative humidity changes. The approach is also applicable for detecting other hydrogen-bonding vapors such as methanol and ethanol. Employing isomerization kinetics of azobenzenes for vapor sensing opens new intriguing possibilities for using azobenzene molecules in the future.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Aalto University

Contributors: Poutanen, M., Ahmed, Z., Rautkari, L., Ikkala, O., Priimägi, A.

Number of pages: 6

Pages: 381-386

Publication date: 20 Mar 2018

Peer-reviewed: Yes

#### Publication information

Journal: ACS Macro Letters

Volume: 7

Issue number: 3

ISSN (Print): 2161-1653

Ratings:

Scopus rating (2018): CiteScore 5.82 SJR 2.201 SNIP 1.255

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Polymers and Plastics, Inorganic Chemistry, Materials Chemistry

Electronic versions:

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DOIs:

10.1021/acsmacrolett.8b00093

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201901111060>

Source: Scopus

Source ID: 85044222959

Research output: Contribution to journal > Article > Scientific > peer-review

### Improving the high temperature abrasion resistance of thermally sprayed Cr<sub>3</sub>C<sub>2</sub>-NiCr coatings by WC addition

Two experimental agglomerated and sintered (a&s) feedstock powders were prepared, in order to reveal the role of WC addition on the microstructure, hardness, and the abrasion resistance of HVOF-sprayed Cr<sub>3</sub>C<sub>2</sub>-NiCr coatings. These powders contained 10 wt.% of sub-micron WC, 20 or 10 wt.% of nickel binder, and Cr<sub>3</sub>C<sub>2</sub> as balance. Experimental coatings were deposited by a liquid fueled high velocity oxygen-fuel (HVOF) spray process and subsequently heat treated at 800 °C for 8 h to simulate elevated temperature service conditions. The microstructures of the powders and coatings were studied by SEM and X-ray diffraction, and the hardnesses of coatings were probed by means of micro and nanoindentation. In addition, the high stress abrasion resistance was tested in a temperature range from room temperature up to 800 °C. The microstructural characterization of the coatings displayed the presence of WC and tungsten containing Cr<sub>3</sub>C<sub>2</sub> grains. The coating hardness increased after heat treatment, which stemmed from precipitation of secondary carbides and solid solution strengthening of the binder by tungsten. In addition, the study revealed that both experimental coatings have high wear resistance at room and elevated temperatures.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Surface Engineering, Viktor-Kaplan-Straße 2/C, Fraunhofer Institut für Keramische Technologien und Systeme, Fraunhofer Institut für Werkstoff- und Strahltechnik, Treibacher Industrie AG

Contributors: Janka, L., Berger, L. M., Norpoth, J., Trache, R., Thiele, S., Tomastik, C., Matikainen, V., Vuoristo, P.

Number of pages: 10

Pages: 296-305

Publication date: 15 Mar 2018

Peer-reviewed: Yes

#### Publication information

Journal: Surface and Coatings Technology

Volume: 337

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2018): CiteScore 3.44 SJR 0.973 SNIP 1.435

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry

Keywords: Abrasive wear, CrC-NiCr, Hardmetal, High temperature, Thermal spray, WC

DOIs:

10.1016/j.surfcoat.2018.01.035

Source: Scopus

Source ID: 85041378943

Research output: Contribution to journal > Article > Scientific > peer-review

### Soft hydrazone crosslinked hyaluronan- and alginate-based hydrogels as 3D supportive matrices for human pluripotent stem cell-derived neuronal cells

Regenerative medicine, especially cell therapy combined with a supportive biomaterial scaffold, is considered to be a potential treatment for various deficits in humans. Here, we have produced and investigated the detailed properties of injectable hydrazone crosslinked hyaluronan-polyvinyl alcohol (HA-PVA) and alginate-polyvinyl alcohol (AL-PVA) hydrogels to be used as a supportive biomaterial for 3D neural cell cultures. To the best of our knowledge, this is the first time the polymerization and properties of hydrazone crosslinked AL-PVA hydrogel have been reported. The effect of the degree of substitution and molecular weight of the polymer components as well as the polymer concentration of the hydrogel on the swelling, degradation and mechanical properties of the hydrogels is reported. Furthermore, we studied the effect of the above parameters on the growth of human pluripotent stem cell-derived neuronal cells. The most neural cell supportive HA-PVA hydrogel was composed of high molecular weight HA component with brain-mimicking mechanical properties and decreased polymer concentration. AL-PVA hydrogel, with stiffness quite similar to brain tissue, was also shown to be similarly supportive. Neuronal spreading and 3D network formation was enhanced inside the softest hydrogels.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Biomaterials and Tissue Engineering Group, BioMediTech Institute and Faculty of Medicine and Life Sciences

Contributors: Karvinen, J., Joki, T., Ylä-Outinen, L., Koivisto, J. T., Narkilahti, S., Kellomäki, M.  
Number of pages: 11  
Pages: 29-39  
Publication date: 1 Mar 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Reactive and Functional Polymers

Volume: 124

ISSN (Print): 1381-5148

Ratings:

Scopus rating (2018): CiteScore 3.21 SJR 0.712 SNIP 0.901

Original language: English

ASJC Scopus subject areas: Chemistry(all), Environmental Chemistry, Biochemistry, Chemical Engineering(all), Polymers and Plastics, Materials Chemistry

Keywords: 3D neuronal culture, Alginate, Hyaluronan, Hydrazone, Hydrogel

DOIs:

10.1016/j.reactfunctpolym.2017.12.019

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<http://www.scopus.com/inward/record.url?scp=85040229275&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 85040229275

Research output: Contribution to journal > Article > Scientific > peer-review

#### Improved Stability of Atomic Layer Deposited Amorphous TiO<sub>2</sub> Photoelectrode Coatings by Thermally Induced Oxygen Defects

Amorphous titanium dioxide (a-TiO<sub>2</sub>) combined with an electrocatalyst has shown to be a promising coating for stabilizing traditional semiconductor materials used in artificial photosynthesis for efficient photoelectrochemical solar-to-fuel energy conversion. In this study we report a detailed analysis of two methods of modifying an undoped thin film of atomic layer deposited (ALD) a-TiO<sub>2</sub> without an electrocatalyst to affect its performance in water splitting reaction as a protective photoelectrode coating. The methods are high-temperature annealing in ultrahigh vacuum and atomic hydrogen exposure. A key feature in both methods is that they preserve the amorphous structure of the film. Special attention is paid to the changes in the molecular and electronic structure of a-TiO<sub>2</sub> induced by these treatments. On the basis of the photoelectrochemical results, the a-TiO<sub>2</sub> is susceptible to photocorrosion but significant improvement in stability is achieved after heat treatment in vacuum at temperatures above 500 °C. On the other hand, the hydrogen treatment does not increase the stability despite the ostensibly similar reduction of a-TiO<sub>2</sub>. The surface analysis allows us to interpret the improved stability to the thermally induced formation of O<sup>-</sup> species within a-TiO<sub>2</sub> that are essentially electronic defects in the anionic framework.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Materials Science

Contributors: Hannula, M., Ali-Löyty, H., Lahtonen, K., Sarlin, E., Saari, J., Valden, M.

Number of pages: 10

Pages: 1199-1208

Publication date: 27 Feb 2018

Peer-reviewed: Yes

#### Publication information

Journal: Chemistry of Materials

Volume: 30

Issue number: 4

ISSN (Print): 0897-4756

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Scopus rating (2018): CiteScore 9.92 SJR 4.224 SNIP 1.769

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all), Materials Chemistry

Electronic versions:

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URLs:

<http://urn.fi/URN:NBN:fi:tty-201809032259>

Source: Scopus

Source ID: 85042704048

Research output: Contribution to journal › Article › Scientific › peer-review

### **An activity recognition framework deploying the random forest classifier and a single optical heart rate monitoring and triaxial accelerometer wrist-band**

Wrist-worn sensors have better compliance for activity monitoring compared to hip, waist, ankle or chest positions. However, wrist-worn activity monitoring is challenging due to the wide degree of freedom for the hand movements, as well as similarity of hand movements in different activities such as varying intensities of cycling. To strengthen the ability of wrist-worn sensors in detecting human activities more accurately, motion signals can be complemented by physiological signals such as optical heart rate (HR) based on photoplethysmography. In this paper, an activity monitoring framework using an optical HR sensor and a triaxial wrist-worn accelerometer is presented. We investigated a range of daily life activities including sitting, standing, household activities and stationary cycling with two intensities. A random forest (RF) classifier was exploited to detect these activities based on the wrist motions and optical HR. The highest overall accuracy of  $89.6 \pm 3.9\%$  was achieved with a forest of a size of 64 trees and 13-s signal segments with 90% overlap. Removing the HR-derived features decreased the classification accuracy of high-intensity cycling by almost 7%, but did not affect the classification accuracies of other activities. A feature reduction utilizing the feature importance scores of RF was also carried out and resulted in a shrunken feature set of only 21 features. The overall accuracy of the classification utilizing the shrunken feature set was  $89.4 \pm 4.2\%$ , which is almost equivalent to the above-mentioned peak overall accuracy.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: BioMediTech, Faculty of Biomedical Sciences and Engineering, Research group: Personal Health Informatics-PHI, Department of Future Technologies

Contributors: Mehrang, S., Pietilä, J., Korhonen, I.

Publication date: 22 Feb 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: Sensors

Volume: 18

Issue number: 2

Article number: 613

ISSN (Print): 1424-8220

Ratings:

Scopus rating (2018): CiteScore 3.72 SJR 0.592 SNIP 1.576

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Atomic and Molecular Physics, and Optics, Biochemistry, Instrumentation, Electrical and Electronic Engineering

Keywords: Accelerometer, Activity recognition, Context awareness, Machine learning, Photoplethysmography, Random forest, Wrist-worn sensors

Electronic versions:

sensors-18-00613-v2

DOIs:

10.3390/s18020613

URLs:

<http://urn.fi/URN:NBN:fi:itty-201803141373>

Source: Scopus

Source ID: 85042489750

Research output: Contribution to journal › Article › Scientific › peer-review

### **UV-Blocking Synthetic Biopolymer from Biomass-Based Bifuran Diester and Ethylene Glycol**

A furan-based synthetic biopolymer composed of a bifuran monomer and ethylene glycol was synthesized through melt polycondensation, and the resulting polyester was found to have promising thermal and mechanical properties. The bifuran monomer, dimethyl 2,2'-bifuran-5,5'-dicarboxylate, was prepared using a palladium-catalyzed, phosphine ligand-free direct coupling protocol. A titanium-catalyzed polycondensation procedure was found effective at polymerizing the bifuran monomer with ethylene glycol. The prepared bifuran polyester exhibited several intriguing properties including high tensile modulus. In addition, the bifuran monomer furnished the polyester with a relatively high glass transition temperature. Films prepared from the new polyester also had excellent oxygen and water barrier properties, which were found to be superior to those of poly(ethylene terephthalate). Moreover, the novel polyester also has good ultraviolet radiation blocking properties.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, University of Oulu, Research Unit of Sustainable Chemistry, P.O. Box 3000, FI-90014 Oulu, University of Oulu, Fibre and Particle Engineering Research Unit, P.O. Box 4300, FI-90014 Oulu

Contributors: Kainulainen, T. P., Sirviö, J. A., Sethi, J., Hukka, T. I., Heiskanen, J. P.

Number of pages: 8

Pages: 1822-1829

Publication date: 21 Feb 2018

Peer-reviewed: Yes

Early online date: 21 Feb 2018

#### Publication information

Journal: Macromolecules

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Scopus rating (2018): CiteScore 5.88 SJR 2.243 SNIP 1.475

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all)

Keywords: Biopolymers, Synthesis, Characterization, Thermal analysis, Spectroscopy

DOIs:

10.1021/acs.macromol.7b02457

Research output: Contribution to journal > Article > Scientific > peer-review

#### Pot-economy autooxidative condensation of 2-Aryl-2-lithio-1,3-dithianes

The autooxidative condensation of 2-aryl-2-lithio-1,3-dithianes is here reported. Treatment of 2-aryl-1,3-dithianes with n-BuLi in the absence of any electrophile leads to condensation of three molecules of 1,3-dithianes and formation of highly functionalized  $\alpha$ -thioether ketones orthothioesters in 51-89% yields upon air exposure. The method was further expanded to benzaldehyde dithioacetals, affording corresponding orthothioesters and  $\alpha$ -thioether ketones in 48-97% yields. The experimental results combined with density functional theory studies support a mechanism triggered by the autooxidation of 2-aryl-2-lithio-1,3-dithianes to yield a highly reactive thioester that undergoes condensation with two other molecules of 2-aryl-2-lithio-1,3-dithiane.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Faculdade de Farmacia da Universidade de Lisboa, Jyväskylän yliopisto

Contributors: Vale, J. R., Rimpiläinen, T., Sievänen, E., Rissanen, K., Afonso, C. A., Candeias, N. R.

Number of pages: 11

Pages: 1948-1958

Publication date: 16 Feb 2018

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Organic Chemistry

Volume: 83

Issue number: 4

ISSN (Print): 0022-3263

Ratings:

Scopus rating (2018): CiteScore 4.57 SJR 1.607 SNIP 0.952

Original language: English

ASJC Scopus subject areas: Organic Chemistry

Electronic versions:

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DOIs:

10.1021/acs.joc.7b02896

URLs:

<http://urn.fi/URN:NBN:fi:tty-201809032260>

#### Bibliographical note

INT=keb,"Vale, Joao R."



Source: Scopus

Source ID: 85042195347

Research output: Contribution to journal > Article > Scientific > peer-review

### **Entrapped Styrene Butadiene Polymer Chains by Sol-Gel-Derived Silica Nanoparticles with Hierarchical Raspberry Structures**

A sol-gel transformation of liquid silica precursor to solid silica particles was carried out in a one-pot synthesis way, where a solution of styrene butadiene elastomer was present. The composites, thus produced, offered remarkable improvements of mechanical and dynamic mechanical performances compared to precipitated silica. The morphological analysis reveals that the alkoxy-based silica particles resemble a raspberry structure when the synthesis of the silica was carried out in the presence of polymer molecules and represent a much more open silica-network structure. However, in the absence of the polymer, the morphology of the silica particles is found to be different. It is envisaged that the special morphology of the in situ synthesized silica particles contributes to the superior reinforcement effects, which are associated with a strong silica-rubber interaction by rubber chains trapped inside the raspberry-like silica aggregates. Therefore, the interfaces are characterized in detail by low-field solid-state  $^1\text{H}$  NMR spectroscopy,  $^{29}\text{Si}$  solid-state NMR spectroscopy, and energy-dispersive X-ray spectroscopy. Low-field  $^1\text{H}$  NMR-based double-quantum experiments provide a quantitative information about the cross-link density of the silica-filled rubber composites and about the influence of silane coupling agent on the chemical cross-link density of the network and correlates well with equilibrium swelling measurements. The special microstructure of the alkoxy-based silica was found to be associated with the interaction between alkoxy-based silica and rubber chains as a consequence of particle growth in the presence of rubber chains.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems, Martin-Luther-Universität Halle-Wittenberg

Contributors: Vaikuntam, S. R., Stöckelhuber, K. W., Subramani Bhagavatheswaran, E., Wießner, S., Scheler, U., Saalwächter, K., Formanek, P., Heinrich, G., Das, A.

Number of pages: 13

Pages: 2010-2022

Publication date: 15 Feb 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry B

Volume: 122

Issue number: 6

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2018): CiteScore 3.03 SJR 1.109 SNIP 0.965

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry  
DOIs:

10.1021/acs.jpcc.7b11792

Source: Scopus

Source ID: 85042152539

Research output: Contribution to journal > Article > Scientific > peer-review

### **MetrIntSimil-an accurate and robust metric for comparison of similarity in intelligence of any number of cooperative multiagent systems**

Intelligent cooperative multiagent systems are applied for solving a large range of real-life problems, including in domains like biology and healthcare. There are very few metrics able to make an effective measure of the machine intelligence quotient. The most important drawbacks of the designed metrics presented in the scientific literature consist in the limitation in universality, accuracy, and robustness. In this paper, we propose a novel universal metric called MetrIntSimil capable of making an accurate and robust symmetric comparison of the similarity in intelligence of any number of cooperative multiagent systems specialized in difficult problem solving. The universality is an important necessary property based on the large variety of designed intelligent systems. MetrIntSimil makes a comparison by taking into consideration the variability in intelligence in the problem solving of the compared cooperativemultiagent systems. It allows a classification of the cooperativemultiagent systems based on their similarity in intelligence. A cooperative multiagent system has variability in the problem solving intelligence, and it can manifest lower or higher intelligence in different problem solving tasks. More cooperative multiagent systems with similar intelligence can be included in the same class. For the evaluation of the proposed metric, we conducted a case study for more intelligent cooperative multiagent systems composed of simple computing agents applied for solving the Symmetric Travelling Salesman Problem (STSP) that is a class of NP-hard problems. STSP is the problem of finding the shortest Hamiltonian cycle/tour in a weighted undirected graph that does not have loops or multiple edges. The distance between two cities is the same in each opposite direction.

Two classes of similar intelligence denoted IntClassA and IntClassB were identified. The experimental results show that the agent belonging to IntClassA intelligence class is less intelligent than the agents that belong to the IntClassB intelligence class.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Computational Medicine and Statistical Learning Laboratory (CMSL), Faculty of Biomedical Sciences and Engineering, Petru Maior University, University of Applied Sciences Upper Austria, Nankai University, Institute for Bioinformatics and Translational Research

Contributors: Iantovics, L. B., Dehmer, M., Emmert-Streib, F.

Publication date: 1 Feb 2018

Peer-reviewed: Yes

#### Publication information

Journal: Symmetry

Volume: 10

Issue number: 2

Article number: 48

ISSN (Print): 2073-8994

Ratings:

Scopus rating (2018): CiteScore 2.28 SJR 0.287 SNIP 1.046

Original language: English

ASJC Scopus subject areas: Computer Science (miscellaneous), Chemistry (miscellaneous), Mathematics(all), Physics and Astronomy (miscellaneous)

Keywords: Computational-hard problem, Cooperative problem solving, Diversity of intelligent systems, Machine intelligence measure, Similarity in intelligence, Symmetric travelling salesman problem

Electronic versions:

symmetry-10-00048-v2

DOIs:

10.3390/sym10020048

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201803141374>

Source: Scopus

Source ID: 85042547076

Research output: Contribution to journal > Article > Scientific > peer-review

#### Controlled Growth of Supported ZnO Inverted Nanopyramids with Downward Pointing Tips

High purity porous ZnO nanopyramids with controllable properties are grown on their tips on Si(100) substrates by means of a catalyst-free vapor phase deposition route in a wet oxygen reaction environment. The system degree of preferential [001] orientation, as well as nanopyramid size, geometrical shape, and density distribution, can be finely tuned by varying the growth temperature between 300 and 400 °C, whereas higher temperatures lead to more compact systems with a three-dimensional (3D) morphology. A growth mechanism of the obtained ZnO nanostructures based on a self-catalytic vapor-solid (VS) mode is proposed, in order to explain the evolution of nanostructure morphologies as a function of the adopted process conditions. The results obtained by a thorough chemico-physical characterization enable us to get an improved control over the properties of ZnO nanopyramids grown by this technique. Taken together, they are of noticeable importance not only for fundamental research on ZnO nanomaterials with controlled nano-organization but also to tailor ZnO functionalities in view of various potential applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Supramolecular photochemistry, Chemistry and Bioengineering, Università degli Studi di Padova, Italy, Universiteit Antwerpen, VTT Technical Research Centre of Finland

Contributors: Barreca, D., Carraro, G., Maccato, C., Altantzis, T., Kaunisto, K., Gasparotto, A.

Number of pages: 9

Pages: 2579-2587

Publication date: Feb 2018

Peer-reviewed: Yes

#### Publication information

Journal: Crystal Growth and Design

Volume: 18

Issue number: 4

ISSN (Print): 1528-7483

Ratings:

Scopus rating (2018): CiteScore 4.01 SJR 1.046 SNIP 1.107

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics

DOIs:

10.1021/acs.cgd.8b00198

Source: Scopus

Source ID: 85044992194

Research output: Contribution to journal › Article › Scientific › peer-review

### **Temperature scanning stress relaxation of an autonomous self-healing elastomer containing non-covalent reversible network junctions**

In this work, we report about the mechanical relaxation characteristics of an intrinsically self-healable imidazole modified commercial rubber. This kind of self-healing rubber was prepared by melt mixing of 1-butyl imidazole with bromo-butyl rubber (bromine modified isoprene-isobutylene copolymer, BIIR). By this melt mixing process, the reactive allylic bromine of bromo-butyl rubber was converted into imidazole bromide salt. The resulting development of an ionic character to the polymer backbone leads to an ionic association of the groups which ultimately results to the formation of a network structure of the rubber chains. The modified BIIR thus behaves like a robust crosslinked rubber and shows unusual self-healing properties. The non-covalent reversible network has been studied in detail with respect to stress relaxation experiments, scanning electron microscopic and X-ray scattering.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Vodafone Department of Mobile Communications Systems, University of Applied Sciences Osnabrück, Leibniz-Institut für Polymerforschung Dresden E.V.

Contributors: Das, A., Sallat, A., Böhme, F., Sarlin, E., Vuorinen, J., Vennemann, N., Heinrich, G., Stöckelhuber, K. W.

Publication date: 19 Jan 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: Polymers

Volume: 10

Issue number: 1

Article number: 94

ISSN (Print): 2073-4360

Ratings:

Scopus rating (2018): CiteScore 3.25 SJR 0.724 SNIP 1.057

Original language: English

ASJC Scopus subject areas: Chemistry(all), Polymers and Plastics

Keywords: Bromo-butyl rubber, Ionic modification, Reversible polymer network, Self-healing, Stress-relaxation

Electronic versions:

polymers-10-00094-v2

DOIs:

10.3390/polym10010094

URLs:

<http://urn.fi/URN:NBN:fi:ty-201802071195>

Source: Scopus

Source ID: 85040774453

Research output: Contribution to journal › Article › Scientific › peer-review

### **Concentration-dependent photophysical switching in mixed self-assembled monolayers of pentacene and perylenediimide on gold nanoclusters**

Photophysical control and switching on organic-inorganic hybrid interfaces are of great interest in diverse fundamental and applicative research areas. 6,13-Bis(triisopropylsilylethynyl)pentacene (TP) is well-known to exhibit efficient singlet fission (SF) for generation of high-yield triplet excited states in aggregated forms, whereas perylenediimide (PDI) ensembles show the characteristic excimer formation. Additionally, a combination of pentacene (electron donor: D) and PDI (electron acceptor: A) is expected to undergo an efficient photoinduced electron transfer (PET), and absorption of two chromophores combined covers the entire visible region. Therefore, the concentration-dependent mixed self-assembled monolayers (SAMs) composed of two chromophores enable us to control and switch the photophysical processes on a surface. In this work, a series of mixed SAMs composed of TP and PDI units on gold nanoclusters (GNCs) were newly synthesized by changing the relative molecular concentration ratios. Structural control of mixed SAMs on a gold surface based on the concentration ratios was successfully achieved. Time-resolved femtosecond and nanosecond transient absorption measurements clearly demonstrate photophysical control and switching of the above competitive reactions

such as SF, electron transfer (ET) and excimer formation. The maximum quantum yields of triplet states ( $\Phi_T = \sim 170\%$ ) and electron transfer ( $\Phi_{ET} = \sim 95\%$ ) were quantitatively evaluated by changing the concentration ratios. The rate constants of SF and excimer processes are largely dependent on the concentration ratios, whereas the rate constants of ET processes approximately remain constant. These findings are also discussed based on the statistical framework of the assembly of chromophores on the gold surface.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Keio University, Tohoku University

Contributors: Kato, D., Sakai, H., Araki, Y., Wada, T., Tkachenko, N. V., Hasobe, T.

Number of pages: 12

Pages: 8695-8706

Publication date: 1 Jan 2018

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

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Issue number: 13

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2018): CiteScore 3.69 SJR 1.31 SNIP 0.981

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1039/c8cp00174j

Source: Scopus

Source ID: 85044838671

Research output: Contribution to journal > Article > Scientific > peer-review

#### Upconversion from fluorophosphate glasses prepared with NaYF<sub>4</sub>:Er<sup>3+</sup>,Yb<sup>3+</sup> nanocrystals

The direct doping method was applied to fabricate upconverter fluorophosphate glasses in the system (90NaPO<sub>3</sub>-(10-x)Na<sub>2</sub>O-xNaF) (mol%) by adding NaYF<sub>4</sub>:Er<sup>3+</sup>,Yb<sup>3+</sup> nanocrystals. An increase in the network connectivity, a red shift of the optical band gap and a decrease in the thermal properties occur when Na<sub>2</sub>O is progressively replaced by NaF. To ensure the survival and the dispersion of the nanocrystals in the glasses with  $x = 0$  and 10, three doping temperatures ( $T_{\text{doping}}$ ) (525, 550 and 575 °C) at which the nanocrystals were added in the glass melt after melting and 2 dwell times (3 and 5 minutes) before quenching the glasses were tested. Using 5 wt% of the NaYF<sub>4</sub>:Er<sup>3+</sup>,Yb<sup>3+</sup> nanocrystals, green emission from the NaYF<sub>4</sub>:Er<sup>3+</sup>,Yb<sup>3+</sup> nanocrystals-containing glasses was observed using a 980 nm pumping, the intensity of which depends on the glass composition and on the direct doping parameters ( $T_{\text{doping}}$  and dwell time). The strongest upconversion was obtained from the glass with  $x = 10$  prepared using a  $T_{\text{doping}}$  of 550 °C and a 3 min dwell time. Finally, we showed that the upconversion, the emission at 1.5  $\mu\text{m}$  and of the transmittance spectra of the nanocrystals-containing glasses could be measured to verify if decomposition of the nanocrystals occurred in glass melts during the preparation of the glasses.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, University of Turku

Contributors: Ojha, N., Tuomisto, M., Lastusaari, M., Petit, L.

Number of pages: 11

Pages: 19226-19236

Publication date: 1 Jan 2018

Peer-reviewed: Yes

#### Publication information

Journal: RSC Advances

Volume: 8

Issue number: 34

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2018): CiteScore 3.16 SJR 0.807 SNIP 0.785

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

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URLs:

<http://urn.fi/URN:NBN:fi:tty-201806252018>

Source: Scopus

Source ID: 85047563423

Research output: Contribution to journal > Article > Scientific > peer-review

### **Ortho-Fluorination of azophenols increases the mesophase stability of photoresponsive hydrogen-bonded liquid crystals**

Photoresponsive liquid crystals (LCs) whose alignment can be controlled with UV-Visible light are appealing for a range of photonic applications. From the perspective of exploring the interplay between the light response and the self-assembly of the molecular components, supramolecular liquid crystals are of particular interest. They allow elaborating the structure-property relationships that govern the optical performance of LC materials by subtle variation of the chemical structures of the building blocks. Herein we present a supramolecular system comprising azophenols and stilbazoles as hydrogen-bond donors and acceptors, respectively, and show that ortho-fluorination of the azophenol dramatically increases the thermal stability of the LC phases, an important characteristics in their further utilization in photonics. The systems exhibit fast photoinduced order-disorder transitions, and rapid recovery of the liquid-crystalline state once the light irradiation is ceased, due to the photochemical properties of azophenols.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, University of Duisburg-Essen

Contributors: Saccone, M., Kuntze, K., Ahmed, Z., Siiskonen, A., Giese, M., Priimagi, A.

Number of pages: 6

Pages: 9958-9963

Publication date: 1 Jan 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Materials Chemistry C

Volume: 6

Issue number: 37

ISSN (Print): 2050-7534

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Scopus rating (2018): CiteScore 6.28 SJR 1.885 SNIP 1.321

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Chemistry

Electronic versions:

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DOIs:

10.1039/c8tc02611d

URLs:

<http://urn.fi/URN:NBN:fi:tty-201901111059>. Embargo ended: 30/08/19

Source: Scopus

Source ID: 85054152271

Research output: Contribution to journal > Article > Scientific > peer-review

### **Improved electromechanical response in acrylic rubber by different carbon-based fillers**

Dielectric elastomers are materials often utilized for the fabrication of electroactive actuators. Acrylic rubber (ACM) is very widely used in dielectric elastomer actuators (DEAs). However, its overall good performance is limited by the high operating electric field required. In the present work, we compare the effect of different types of conventionally used carbon black (CB) as well as other carbon-based fillers on the dielectric and actuation properties of ACM in order to show that performance of DEAs can be improved by the development of ACM composites. Indeed, addition of CB, carbon nanotubes (CNTs), and synthetic graphite leads to an increase in the relative dielectric permittivity of elastomeric material. Moreover, incorporation of nanodiamonds results in reduction of dielectric losses. Finally, actuation stress is remarkably improved by CNTs and different grades of CB.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Plastics and Elastomer Technology, Leibniz Institute of Polymer Research Dresden  
Contributors: Shakun, A., Poikelispää, M., Das, A., Vuorinen, J.  
Pages: 395-404  
Publication date: 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Polymer Engineering and Science  
Volume: 58  
Issue number: 3  
ISSN (Print): 0032-3888  
Ratings:  
Scopus rating (2018): CiteScore 1.96 SJR 0.491 SNIP 1.016  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Polymers and Plastics, Materials Chemistry  
DOIs:  
10.1002/pen.24586  
Source: Scopus  
Source ID: 85017528518  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Modification of epoxy resin by silane-coupling agent to improve tensile properties of viscose fabric composites

The modification of epoxy resin by 3-aminopropyltriethoxysilane (APTES) to improve the tensile properties of warp knitted viscose fabric composites is reported in this study. The study evaluates the efficiency of modification methods adopted to modify the epoxy resin and the influence of the resin modification on various properties of the cured castings. The influence of matrix resin modification on the tensile properties of viscose fabric composite is compared to those prepared from chemically modified fibre. The efficiency of the modification was determined through titration method to determine the epoxide content of epoxy resin, viscosity measurement and FTIR. The effect of APTES modification on various properties of cured castings is studied through differential scanning calorimeter, contact angle measurement and tensile testing. The addition of APTES into the epoxy resin decreased the epoxide content in the resin as evident from the titration method. The tensile strength of cured castings decreased after the resin modification. The tensile strength and elongation at break of the viscose fabric composites prepared from modified resin, increased up to 14 and 41%, respectively. The improved adhesion of APTES-modified epoxy resin to the viscose fibre is confirmed from SEM analysis of tensile fracture surface.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Materials Science, Research group: Plastics and Elastomer Technology, Centria University of Applied Sciences, Royal Commission Yanbu Colleges and Institutes, Swerea IVF AB, Jozef Stefan Institute, Swedish Centre for Resource Recovery, University of Borås  
Contributors: Rajan, R., Rainosalu, E., Thomas, S. P., Ramamoorthy, S. K., Zavašnik, J., Vuorinen, J., Skrifvars, M.  
Number of pages: 29  
Pages: 167–195  
Publication date: 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Polymer Bulletin  
Volume: 75  
Issue number: 1  
ISSN (Print): 0170-0839  
Ratings:  
Scopus rating (2018): CiteScore 1.71 SJR 0.414 SNIP 0.718  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Polymers and Plastics, Materials Chemistry  
Keywords: APTES, Composites, Epoxy, Modification, Regenerated cellulose, Silane coupling agent, Tensile, Viscose  
Electronic versions:  
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DOIs:  
10.1007/s00289-017-2022-2  
URLs:  
<http://urn.fi/URN:NBN:fi:itty-201706051574>. Embargo ended: 20/04/18

### Bibliographical note

EXT="Skrifvars, Mikael"

Source: Scopus

Source ID: 85018515485

Research output: Contribution to journal › Article › Scientific › peer-review

### Adsorption of furfural from torrefaction condensate using torrefied biomass

Torrefaction is a biomass energy densification process that generates a major byproduct in the form of torrefaction condensate. Microbial conversion of torrefaction condensate could be an attractive option for energy integration within torrefaction process. However, torrefaction condensate contains several compounds, such as furfural, 5-hydroxymethylfurfural and guaiacol that are inhibitory to microbes. In this study, for the first time, we reported detoxification of torrefaction condensate, by removing the major inhibitory compound furfural, using torrefied biomass and later used the detoxified torrefaction condensate for anaerobic digestion. The effect of varying torrefaction temperature (225–300 °C), torrefied biomass dosage (25–250 g/L), initial pH (2.0–9.0), and contact time (1–12 h) on furfural adsorption was studied with batch adsorption experiments. The furfural adsorption on torrefied biomass was best represented by pseudo second order kinetic model. The adsorption of furfural and other inhibitory compounds on torrefied biomass was likely a hydrophobic interaction. A maximum of 60% of furfural was adsorbed from torrefaction condensate containing 9000 mg furfural/L using 250 g/L of torrefied biomass in batch adsorption. For, column (20 mm internal diameter and 200 mm bed height), the saturation time for furfural adsorption was around 50 min. Anaerobic digestion of the detoxified torrefaction condensate shows that the lag phase in methane production was reduced from 25 d to 15 d for 0.2 volatile solid (VS)<sub>substrate</sub>:VS<sub>inoculum</sub> loading. The study shows that torrefaction condensate can be effectively detoxified using torrefied biomass for microbial conversion and can be integrated within the torrefied biomass pellet production process.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Helmholtz-Zentrum Dresden-Rossendorf, Univ of Oulu

Contributors: Doddapaneni, T. R. K. C., Jain, R., Praveenkumar, R., Rintala, J., Romar, H., Konttinen, J.

Number of pages: 11

Pages: 558-568

Publication date: 2018

Peer-reviewed: Yes

Early online date: 2017

### Publication information

Journal: Chemical Engineering Journal

Volume: 334

ISSN (Print): 1385-8947

Ratings:

Scopus rating (2018): CiteScore 8.47 SJR 2.066 SNIP 1.941

Original language: English

ASJC Scopus subject areas: Chemistry(all), Environmental Chemistry, Chemical Engineering(all), Industrial and Manufacturing Engineering

Keywords: Anaerobic digestion, Detoxification, Energy densification, Pellets, Torrefaction volatiles

DOIs:

10.1016/j.cej.2017.10.053

Source: Scopus

Source ID: 85033666908

Research output: Contribution to journal › Article › Scientific › peer-review

### Regeneration of sulfur-poisoned Pd-based catalyst for natural gas oxidation

Sulfur deactivation and regeneration behavior of the Pd/Al<sub>2</sub>O<sub>3</sub> catalyst has been investigated via experimental characterization and density functional theory (DFT) simulations. During the sulfur exposure, PdO crystallites grow slightly while bulk Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> forms on the support. DFT calculations indicate that SO<sub>x</sub> species interact strongly with the catalyst surface making it chemically inactive in agreement with the experimental results. During the regeneration treatment (CH<sub>4</sub> conditions), PdO particles reduce, Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> is partially removed, and the activity for CH<sub>4</sub> conversion is increased. No full recovery can be observed due to remaining Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>, the formation of encapsulating sulfur species, and the partial reduction of PdO particles. To reoxidize Pd, the catalyst is further regenerated (O<sub>2</sub> conditions). The resulting CH<sub>4</sub> conversion is at the same level than with the regenerated catalyst. Thus, a small amount of Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> appears to have a stronger effect on the performance than the state of Pd.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Materials Characterization, Physics, Research area: Computational Physics, Research group: Materials and Molecular Modeling, Univ of Oulu, Aalto University, Dinex Ecocat Oy, Norwegian University of Science and Technology

Contributors: Honkanen, M., Wang, J., Kärkkäinen, M., Huuhtanen, M., Jiang, H., Kallinen, K., Keiski, R. L., Akola, J., Vippola, M.

Number of pages: 13

Pages: 253-265

Publication date: 2018

Peer-reviewed: Yes

Early online date: 4 Jan 2018

### Publication information

Journal: Journal of Catalysis

Volume: 358

ISSN (Print): 0021-9517

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Original language: English

ASJC Scopus subject areas: Catalysis, Physical and Theoretical Chemistry

Keywords: Catalytic testing, Density functional theory simulations, Fourier transform infrared spectrometry, Pd-based catalyst, Regeneration, Sulfur poisoning, Transmission electron microscopy

DOIs:

10.1016/j.jcat.2017.12.021

Source: Scopus

Source ID: 85039986144

Research output: Contribution to journal > Article > Scientific > peer-review

### Composition and role of the attached and planktonic microbial communities in mesophilic and thermophilic xylose-fed microbial fuel cells

A mesophilic (37 °C) and a thermophilic (55 °C) two-chamber microbial fuel cell (MFC) were studied and compared for their power production from xylose and the microbial communities involved. The anode-Attached, membrane-Attached, and planktonic microbial communities, and their respective active subpopulations, were determined by next generation sequencing (Illumina MiSeq), based on the presence and expression of the 16S rRNA gene. Geobacteraceae accounted for 65% of the anode-Attached active microbial community in the mesophilic MFC, and were associated to electricity generation likely through direct electron transfer, resulting in the highest power production of 1.1 W m<sup>-3</sup>. A lower maximum power was generated in the thermophilic MFC (0.2 W m<sup>-3</sup>), likely due to limited acetate oxidation and the competition for electrons by hydrogen oxidizing bacteria and hydrogenotrophic methanogenic archaea. Aerobic microorganisms, detected among the membrane-Attached active community in both the mesophilic and thermophilic MFC, likely acted as a barrier for oxygen flowing from the cathodic chamber through the membrane, favoring the strictly anaerobic exoelectrogenic microorganisms, but competing with them for xylose and its degradation products. This study provides novel information on the active microbial communities populating the anodic chamber of mesophilic and thermophilic xylose-fed MFCs, which may help in developing strategies to favor exoelectrogenic microorganisms at the expenses of competing microorganisms.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Natl. University of Ireland, Galway, Institute for Water Education, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education

Contributors: Dessì, P., Porca, E., Haavisto, J., Lakaniemi, A., Collins, G., Lens, P. N.

Number of pages: 12

Pages: 3069-3080

Publication date: 2018

Peer-reviewed: Yes

### Publication information

Journal: RSC Advances

Volume: 8

Issue number: 6

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2018): CiteScore 3.16 SJR 0.807 SNIP 0.785

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)



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<http://urn.fi/URN:NBN:fi:ty-201802081202>

Source: Scopus

Source ID: 85040867034

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Decomposition of persistent luminescent microparticles in corrosive phosphate glass melt**

Findings on the decomposition of persistent luminescent (PeL)  $\text{SrAl}_2\text{O}_4:\text{Eu}^{2+},\text{Dy}^{3+}$  microparticles (MPs) in phosphate glass melt under static condition are reported. PeL phosphate glasses with the composition (50 $\text{P}_2\text{O}_5$ -10 $\text{Na}_2\text{O}$ -40 $\text{SrO}$ ) (in mol%) were prepared by adding the MPs in the glass melt. The decomposition of the MPs occurs during the preparation of the glass and leads to changes in the  $\text{Eu}^{2+}$  sites and to the formation of  $\text{Eu}^{3+}$  which decreases the PeL properties of the glasses. The decomposition of the MPs depends on the temperature at which the MPs are added in the melt and also on the time before casting the melts.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Research group: Nanophotonics, Turun Yliopisto/Turun Biomateriaalikeskus

Contributors: Ojha, N., Nguyen, H., Laihininen, T., Salminen, T., Lastusaari, M., Petit, L.

Pages: 207-214

Publication date: 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: Corrosion Science

Volume: 135

ISSN (Print): 0010-938X

Ratings:

Scopus rating (2018): CiteScore 6.76 SJR 2.131 SNIP 2.595

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all), Materials Science(all)

Keywords: Corrosion, Decomposition, Persistent luminescence, Phosphate glasses,  $\text{SrAlO}:\text{Eu},\text{Dy}$  microparticles

DOIs:

10.1016/j.corsci.2018.02.050

#### **Bibliographical note**

INT=fot,"Nguyen, H."

Source: Scopus

Source ID: 85042665831

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Convenient extraction method for quantification of thin zinc patina layers**

Synthetic zinc patina was grown on galvanized steel sheets in supercritical carbon dioxide atmosphere. Different patina compounds were dissolved and quantified using a stepwise immersion and dissolution procedure. The distinct patina components, namely anhydrous zinc carbonate (a dense layer adjacent to metallic zinc) and zinc hydroxy carbonate (nanowires on the surface), were dissolved in glycine solutions, followed by quantification of  $\text{Zn}^{2+}$  in the solutes by X-ray fluorescence. The zinc hydroxy carbonate nanowires were readily glycine soluble, and the anhydrous zinc carbonate showed scarce glycine solubility, which enabled their selective quantification. The amount of the remaining (anhydrous) zinc carbonate after glycine extraction was determined from the glycine-soluble zinc oxide after calcination (heat treatment for 10 minutes at 350°C). The results were verified by scanning electron microscopy imaging and Fourier transform infrared spectroscopy measurements.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science

Contributors: Saarimaa, V., Kaleva, A., Paunikallio, T., Nikkanen, J., Heinonen, S., Levänen, E., Väisänen, P., Markkula, A.

Pages: 564-570

Publication date: 2018

Peer-reviewed: Yes  
Early online date: 1 Jan 2018

### Publication information

Journal: Surface and Interface Analysis

Volume: 50

Issue number: 5

ISSN (Print): 0142-2421

Ratings:

Scopus rating (2018): CiteScore 1.44 SJR 0.451 SNIP 0.64

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry

Keywords: Galvanized steel, Glycine, Supercritical carbon dioxide, Zinc carbonate, Zinc nanowires, Zinc oxide

DOIs:

10.1002/sia.6429

Source: Scopus

Source ID: 85044219012

Research output: Contribution to journal › Article › Scientific › peer-review

### Gloriosa superba Mediated Synthesis of Platinum and Palladium Nanoparticles for Induction of Apoptosis in Breast Cancer

Green chemistry approaches for designing therapeutically significant nanomedicine have gained considerable attention in the past decade. Herein, we report for the first time on anticancer potential of phytogetic platinum nanoparticles (PtNPs) and palladium nanoparticles (PdNPs) using a medicinal plant *Gloriosa superba* tuber extract (GSTE). The synthesis of the nanoparticles was completed within 5 hours at 100°C which was confirmed by development of dark brown and black colour for PtNPs and PdNPs, respectively, along with enhancement of the peak intensity in the UV-visible spectra. High-resolution transmission electron microscopy (HRTEM) showed that the monodispersed spherical nanoparticles were within a size range below 10 nm. Energy dispersive spectra (EDS) confirmed the elemental composition, while dynamic light scattering (DLS) helped to evaluate the hydrodynamic size of the particles. Anticancer activity against MCF-7 (human breast adenocarcinoma) cell lines was evaluated using MTT assay, flow cytometry, and confocal microscopy. PtNPs and PdNPs showed  $49.65 \pm 1.99\%$  and  $36.26 \pm 0.91\%$  of anticancer activity. Induction of apoptosis was most predominant in the underlying mechanism which was rationalized by externalization of phosphatidyl serine and membrane blebbing. These findings support the efficiency of phytogetic fabrication of nanoscale platinum and palladium drugs for management and therapy against breast cancer.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Modern College of Arts, Savitribai Phule Pune University, Indian Institute of Science, Bangalore, Department of Biomedical Sciences and Engineering, Defense Institute of Advanced Technology, Indian Institute of Technology Bombay, RK University

Contributors: Rokade, S. S., Joshi, K. A., Mahajan, K., Patil, S., Tomar, G., Dubal, D. S., Parihar, V. S., Kitture, R., Bellare, J. R., Ghosh, S.

Publication date: 2018

Peer-reviewed: Yes

### Publication information

Journal: Bioinorganic Chemistry and Applications

Volume: 2018

Article number: 4924186

ISSN (Print): 1565-3633

Ratings:

Scopus rating (2018): CiteScore 2.05 SJR 0.383 SNIP 0.886

Original language: English

ASJC Scopus subject areas: Biochemistry, Organic Chemistry, Inorganic Chemistry

Electronic versions:

4924186

DOIs:

10.1155/2018/4924186

URLs:

<http://urn.fi/URN:NBN:fi:itty-201808102060>

Source: Scopus

Source ID: 85050376240

### **A Bioscreening Technique for Ultraviolet Irradiation Protective Natural Substances**

Ultraviolet radiation (UV-R) causes genotoxic and aging effects on skin, and sunscreens are used to alleviate the damage. However, sunscreens contain synthetic shielding agents that can cause harmful effects in the environment. Nature-derived substances may have potential as replacement materials for the harmful sunscreen chemicals. However, screening of a broad range of samples is tedious, and often requires a separate genotoxicity assessment. We describe a simple microplate technique for the screening of UV protective substances using a recombinant *Escherichia coli* biosensor. Both absorbance-based and bioactivity-based shields can be detected with simultaneous information about the sample genotoxicity. With this technique, a controversial sunscreen compound, oxybenzone offers physical or absorbance-based shield but appears genotoxic at higher concentrations (3.3 mg/mL). We also demonstrate that pine needle extract (Pi<sub>Ne</sub>) shields the biosensor from UV-R in a dose-dependent manner without showing genotoxicity. The physical shield of 5 mg/mL Pi<sub>Ne</sub> was similar to that of one of the most common UV-shielding compound TiO<sub>2</sub> concentration 0.80 mg/mL. The bioactivity-based shield of Pi<sub>Ne</sub> also reaches the extent of the physical shield with the highest concentration (3.3 mg/mL). We conclude that our technique is suitable in detecting the UV-shielding potential of natural substances, and gives simultaneous information on genotoxicity.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Natural Resources Institute Finland (Luke)

Contributors: Tienaho, J., Poikulainen, E., Sarjala, T., Muilu-Mäkelä, R., Santala, V., Karp, M.

Pages: 1273-1280

Publication date: 2018

Peer-reviewed: Yes

Early online date: 2018

#### **Publication information**

Journal: Photochemistry and Photobiology

Volume: 94

Issue number: 6

ISSN (Print): 0031-8655

Ratings:

Scopus rating (2018): CiteScore 2.35 SJR 0.806 SNIP 0.883

Original language: English

ASJC Scopus subject areas: Biochemistry, Physical and Theoretical Chemistry

DOIs:

10.1111/php.12954

#### **Bibliographical note**

INT=keb,"Poikulainen, Emmi"

Source: Scopus

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Research output: Contribution to journal › Article › Scientific › peer-review

### **Detection and characterization at nM concentration of oligomers formed by hIAPP, A $\beta$ (1-40) and their equimolar mixture using SERS and MD simulations**

We report a structural investigation on IAPP, A $\beta$ (1-40) and their equi-molar mixture aggregation pathway at nano-molar concentration using the Surface Enhanced Raman Spectroscopy (SERS) effect induced by silver metal colloids prepared by laser processes in solution and molecular dynamics simulations. Our data show the ability of silver NPs coupled with SERS to detect secondary structures of IAPP, A $\beta$ (1-40) and their 1:1 molar ratio mixture in the oligomeric state. The preparation of silver colloids shows superior performance with respect to chemically prepared nano-particles. SERS spectroscopy shows both selectivity and sensitivity in detecting the secondary structures of hIAPP and A $\beta$ (1-40) and to recognize both proteins in their mixture. On the other hand, molecular dynamics simulations confirm SERS structural data and the given atomistic details about the structural organization of IAPP and A $\beta$ (1-40) oligomers. Our study shows an inhomogeneity in the chemical composition of IAPP/A $\beta$ (1-40) oligomer aggregates.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Department of Chemical Sciences

Contributors: D'Urso, L., Condorelli, M., Puglisi, O., Tempra, C., Lolicato, F., Compagnini, G., La Rosa, C.

Number of pages: 9

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Peer-reviewed: Yes

#### Publication information

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Volume: 20

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Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

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Source ID: 85051509553

Research output: Contribution to journal > Article > Scientific > peer-review

#### Stable carbon isotopic composition of peat columns, subsoil and vegetation on natural and forestry-drained boreal peatlands

We studied natural and forestry-drained peatlands to examine the effect of over 34 years lowered water table on the  $\delta^{13}\text{C}$  values of vegetation, bulk peat and subsoil. In the seven studied sites,  $\delta^{13}\text{C}$  in the basal peat layer was 1.1 and 1.2 ‰ lower than that of the middle-layer and surface layer, respectively. Furthermore, there was a positive correlation between the  $\delta^{13}\text{C}$  values of the basal and surface peat layers, possibly due to carbon (C) recycling within the peat column. In the same mire complex, natural fen peat  $\delta^{13}\text{C}$  values were lower than those of the nearby bog, possibly due to the dominance of vascular plants on fen and the generally larger share of recycled C in the fens than in the bogs. Furthermore, natural and 51 years previously drained fen and bog, on the opposite sides of a ditch on the same mire complex, showed no significant differences in  $\delta^{13}\text{C}$  values. Plant  $\delta^{13}\text{C}$  values were lower, while  $\delta^{13}\text{C}$  values of subsoil were higher in the drained than in the natural site of the fen.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, University of Eastern Finland, University of Jyväskylä

Contributors: Nykänen, H., Mpamah, P. A., Rissanen, A. J.

Publication date: 2018

Peer-reviewed: Yes

Early online date: 2018

#### Publication information

Journal: Isotopes in Environmental and Health Studies

Volume: 54

Issue number: 6

ISSN (Print): 1025-6016

Ratings:

Scopus rating (2018): CiteScore 1.6 SJR 0.666 SNIP 0.804

Original language: English

ASJC Scopus subject areas: Environmental Chemistry, Environmental Science(all), Inorganic Chemistry

Keywords: Biogeochemistry, bog, carbon cycle, carbon dioxide, carbon-13, diagenesis, drainage, fen, isotope ecology, Sphagnum, Suess effect

DOIs:

10.1080/10256016.2018.1523158

Source: Scopus

Source ID: 85053893057

Research output: Contribution to journal > Article > Scientific > peer-review

#### Optical frequency comb photoacoustic spectroscopy

We report the first photoacoustic detection scheme using an optical frequency comb - optical frequency comb photoacoustic spectroscopy (OFC-PAS). OFC-PAS combines the broad spectral coverage and the high resolution of OFCs with the small sample volume of cantilever-enhanced PA detection. In OFC-PAS, a Fourier transform spectrometer (FTS) is used to modulate the intensity of the exciting comb source at a frequency determined by its scanning speed. One of the FTS outputs is directed to the PA cell and the other is measured simultaneously with a photodiode and used to normalize the PA signal. The cantilever-enhanced PA detector operates in a non-resonant mode, enabling detection of a

broadband frequency response. The broadband and the high-resolution capabilities of OFC-PAS are demonstrated by measuring the rovibrational spectra of the fundamental C-H stretch band of CH<sub>4</sub>, with no instrumental line shape distortions, at total pressures of 1000 mbar, 650 mbar, and 400 mbar. In this first demonstration, a spectral resolution two orders of magnitude better than previously reported with broadband PAS is obtained, limited by the pressure broadening. A limit of detection of 0.8 ppm of methane in N<sub>2</sub> is accomplished in a single interferogram measurement (200 s measurement time, 1000 MHz spectral resolution, 1000 mbar total pressure) for an exciting power spectral density of 42 μW/cm<sup>-1</sup>. A normalized noise equivalent absorption of 8 × 10<sup>-10</sup> W cm<sup>-1</sup> Hz<sup>-1/2</sup> is obtained, which is only a factor of three higher than the best reported with PAS based on continuous wave lasers. A wide dynamic range of up to four orders of magnitude and a very good linearity (limited by the Beer-Lambert law) over two orders of magnitude are realized. OFC-PAS extends the capability of optical sensors for multispecies trace gas analysis in small sample volumes with high resolution and selectivity.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Energy Technology and Thermal Process Chemistry, Laboratory of Photonics, University of Helsinki

Contributors: Sadiq, I., Mikkonen, T., Vainio, M., Toivonen, J., Foltynowicz, A.

Number of pages: 7

Pages: 27849-27855

Publication date: 2018

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 20

Issue number: 44

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2018): CiteScore 3.69 SJR 1.31 SNIP 0.981

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

Electronic versions:

c8cp05666h

DOIs:

10.1039/c8cp05666h

URLs:

<http://urn.fi/URN:NBN:fi:ty-201812212894>

Source: Scopus

Source ID: 85056520950

Research output: Contribution to journal › Article › Scientific › peer-review

#### Efficient photon upconversion at remarkably low annihilator concentrations in a liquid polymer matrix: when less is more

A green-to-blue triplet-triplet annihilation upconversion of 24.5% quantum yield was achieved at a remarkably low 600 μM annihilator concentration in a viscous polymer matrix. This was made possible by utilizing a ZnTPP-based photosensitizer with exceptionally long 11 ms phosphorescence lifetime. Higher 3 mM annihilator concentration resulted in lower 24% upconversion quantum yield.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering

Contributors: Durandin, N. A., Isokuortti, J., Efimov, A., Vuorimaa-Laukkanen, E., Tkachenko, N. V., Laaksonen, T.

Number of pages: 4

Pages: 14029-14032

Publication date: 2018

Peer-reviewed: Yes

#### Publication information

Journal: Chemical Communications

Volume: 54

Issue number: 99

ISSN (Print): 1359-7345

Ratings:

Scopus rating (2018): CiteScore 6.12 SJR 2.177 SNIP 1.133

Original language: English

ASJC Scopus subject areas: Catalysis, Electronic, Optical and Magnetic Materials, Ceramics and Composites, Chemistry(all), Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry

Keywords: triplet-triplet annihilation, triplet-triplet energy transfer, triplet state lifetime, upconversion, triplet fusion

DOIs:

10.1039/c8cc07592a

URLs:

<http://urn.fi/URN:NBN:fi:ttty-201901141089>. Embargo ends: 22/11/19

Source: Scopus

Source ID: 85058301188

Research output: Contribution to journal > Article > Scientific > peer-review

### On the molecular optical nonlinearity of halogen-bond-forming azobenzenes

We study hyper-Rayleigh scattering and computed molecular hyperpolarizability in a series of azobenzene chromophores in chloroform and dimethylformamide as solvents. The chromophores form halogen or hydrogen bonds of varying strength with dimethylformamide molecules, differently from what is expected for chloroform. We show that hyperpolarizability is unaffected or slightly lower with the azobenzene forming the strongest halogen bond. Solid supramolecular polymers with the same chromophores have previously demonstrated clearly higher second-order nonlinear responses when a halogen-bond-accepting polymer is used, the larger increase being associated with the stronger halogen bond. The present study proves that the higher optical nonlinearity in polymers lies in the better ordering of the chromophores instead of changes in molecular hyperpolarizability, highlighting the unique properties of halogen bonding in supramolecular chemistry.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Photonics, Research group: Nonlinear Optics, Research group: Chemistry & Advanced Materials, Claude Bernard-University, Università degli Studi di Milano, Politecnico di Milano

Contributors: Virkki, M., Maurice, A., Forni, A., Sironi, M., Dichiarante, V., Brevet, P. F., Metrangolo, P., Kauranen, M., Priimagi, A.

Number of pages: 8

Pages: 28810-28817

Publication date: 2018

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 20

Issue number: 45

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2018): CiteScore 3.69 SJR 1.31 SNIP 0.981

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1039/c8cp05392h

Source: Scopus

Source ID: 85056802102

Research output: Contribution to journal > Article > Scientific > peer-review

### Supercritical carbon dioxide treatment of hot dip galvanized steel as a surface treatment before coating

Supercritical carbon dioxide (scCO<sub>2</sub>) treatment was employed for rapid formation of a zinc patina layer on hot dip galvanized (HDG) steel. In the presence of H<sub>2</sub>O and a Cu precursor, an artificial patina consisting of two distinctive phases was formed: a dense ~ 1 μm layer of anhydrous ZnCO<sub>3</sub> adjacent to native zinc coating, and a needle-like porous structure showing resemblance to hydrozincite (Zn<sub>5</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>6</sub>). The artificial patina layer significantly decreased the surface free energy of HDG, which was evidenced also by good wettability by a polyester melamine coating. Furthermore, the needle-like patina surface structure stayed intact through the coating process, indicating improved coating adhesion. ScCO<sub>2</sub> treatment facilitates rapid and impurity-free surface treatment of hot dip galvanized steel, and could be used to tailor novel adhesion and corrosion promoting surface morphologies.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Ceramic materials, Top Analytica Oy, SSAB

Contributors: Saarimaa, V., Kaleva, A., Nikkanen, J., Heinonen, S., Levänen, E., Väisänen, P., Markkula, A., Juhanoja, J.

Number of pages: 6  
Pages: 137-142  
Publication date: 15 Dec 2017  
Peer-reviewed: Yes

#### Publication information

Journal: Surface and Coatings Technology  
Volume: 331  
ISSN (Print): 0257-8972  
Ratings:

Scopus rating (2017): CiteScore 3.08 SJR 0.928 SNIP 1.565

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry

Keywords: Basic zinc carbonate, Coatings, Corrosion resistance, Hot dip galvanized steel, Patina, Supercritical carbon dioxide, Zinc

DOIs:

10.1016/j.surfcoat.2017.10.047

Source: Scopus

Source ID: 85032293898

Research output: Contribution to journal > Article > Scientific > peer-review

#### Time-Resolved Fluorescence Spectroscopy Reveals Fine Structure and Dynamics of Poly(L-lysine) and Polyethylenimine Based DNA Polyplexes

Structural dynamics of the polyethylenimine-DNA and poly(L-lysine)-DNA complexes (polyplexes) was studied by steady-state and time-resolved fluorescence spectroscopy using the fluorescence resonance energy transfer (FRET) technique. During the formation of the DNA polyplexes, the negative phosphate groups (P) of DNA are bound by the positive amine groups (N) of the polymer. At N/P ratio 2, nearly all of the DNA's P groups are bound by the polymer N groups: These complexes form the core of the polyplexes. The excess polymer, added to this system to increase the N/P ratio to the values giving efficient gene delivery, forms a positively charged shell around the core polyplex. We investigated whether the exchange between the core and shell regions of PEI and PLL polyplexes takes place. Our results demonstrated a clear difference between the two studied polymers. Shell PEI can replace PEIs previously attached to DNA in the polyplex core, while PLL cannot. Such a dynamic structure of PEI polyplexes compared to a more static one found for PLL polyplexes partially explains the observed difference in the DNA transfection efficiency of these polyplexes. Moreover, the time-resolved fluorescence spectroscopy revealed additional details on the structure of PLL polyplexes: In between the core and shell, there is an intermediate layer where both core and shell PLLs or their parts overlap.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Centre for Drug Research, University of Helsinki, Ita-Suomen yliopisto, Universita degli Studi di Padova, Italy

Contributors: Lisitsyna, E. S., Ketola, T., Morin-Picardat, E., Liang, H., Hanzlíková, M., Urtti, A., Yliperttula, M., Vuorimaa-Laukkanen, E.

Number of pages: 11

Pages: 10782-10792

Publication date: 7 Dec 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry B

Volume: 121

Issue number: 48

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2017): CiteScore 3.13 SJR 1.331 SNIP 0.996

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry

DOIs:

10.1021/acs.jpccb.7b08394

Source: Scopus

Source ID: 85037731381

Research output: Contribution to journal > Article > Scientific > peer-review

### Mapping microscale wetting variations on biological and synthetic water-repellent surfaces

Droplets slip and bounce on superhydrophobic surfaces, enabling remarkable functions in biology and technology. These surfaces often contain microscopic irregularities in surface texture and chemical composition, which may affect or even govern macroscopic wetting phenomena. However, effective ways to quantify and map microscopic variations of wettability are still missing, because existing contact angle and force-based methods lack sensitivity and spatial resolution. Here, we introduce wetting maps that visualize local variations in wetting through droplet adhesion forces, which correlate with wettability. We develop scanning droplet adhesion microscopy, a technique to obtain wetting maps with spatial resolution down to 10  $\mu\text{m}$  and three orders of magnitude better force sensitivity than current tensiometers. The microscope allows characterization of challenging non-flat surfaces, like the butterfly wing, previously difficult to characterize by contact angle method due to obscured view. Furthermore, the technique reveals wetting heterogeneity of micropillared model surfaces previously assumed to be uniform.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Micro and Nanosystems Research Group, Research group: Bioinspired Materials and Robotics (BMR), Aalto University, Helsinki University of Technology

Contributors: Liimatainen, V., Vuckovac, M., Jokinen, V., Sariola, V., Hokkanen, M. J., Zhou, Q., Ras, R. H.

Publication date: 1 Dec 2017

Peer-reviewed: Yes

#### Publication information

Journal: Nature Communications

Volume: 8

Issue number: 1

Article number: 1798

ISSN (Print): 2041-1723

Ratings:

Scopus rating (2017): CiteScore 12.41 SJR 6.582 SNIP 2.934

Original language: English

ASJC Scopus subject areas: Chemistry(all), Biochemistry, Genetics and Molecular Biology(all), Physics and Astronomy(all)

Electronic versions:

article

DOIs:

10.1038/s41467-017-01510-7

URLs:

<http://urn.fi/URN:NBN:fi:tty-201712112320>

#### Bibliographical note

EXT="Zhou, Quan"

Source: Scopus

Source ID: 85035320075

Research output: Contribution to journal > Article > Scientific > peer-review

### Carbazole-based small molecule electron donors: Syntheses, characterization, and material properties

Efficient synthetic methods for carbazole-based small molecule electron donors with donor-acceptor (D-A) and A-D-A type structures were developed. In order to study the relation between chemical structures and material properties, the prepared compounds were characterized in detail using absorption spectroscopy, differential pulse voltammetry, and computational methods. In addition, symmetrical A-D-A type compounds were tested as an active layer component in bulk heterojunction based organic solar cell (OSC) devices with conventional structure. The results show that the two compound types have many similar properties. However, the extended molecular structure of A-D-A type compounds offer better film forming properties and higher molar absorption coefficients compared with the D-A type materials. Furthermore, the attachment of fluoro substituents in the A units has a positive effect on all solar cell device parameters. Moreover, the computational studies revealed that the molecular structures are twisted between the central carbazole D unit and  $\pi$ -bridge which may result in inefficient intramolecular charge transfer and, also, relatively limited short-circuit currents in OSC devices.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials, Research Unit of Sustainable Chemistry, IMEC PV Department



Contributors: Sippola, R. J., Hadipour, A., Kastinen, T., Vivo, P., Hukka, T. I., Aernouts, T., Heiskanen, J. P.  
Number of pages: 10  
Pages: 79-88  
Publication date: 8 Nov 2017  
Peer-reviewed: Yes  
Early online date: 8 Nov 2017

#### Publication information

Journal: Dyes and Pigments  
Volume: 150  
Article number: j.dyepig.2017.11.014  
ISSN (Print): 0143-7208  
Ratings:

Scopus rating (2017): CiteScore 3.59 SJR 0.819 SNIP 1.005

Original language: English

ASJC Scopus subject areas: Chemistry(all), Energy(all)

Keywords: Absorption, DFT, Electron donor, Organic solar cell, Suzuki-Miyaura, Synthesis

DOIs:

10.1016/j.dyepig.2017.11.014

Research output: Contribution to journal > Article > Scientific > peer-review

#### DoGlycans-Tools for Preparing Carbohydrate Structures for Atomistic Simulations of Glycoproteins, Glycolipids, and Carbohydrate Polymers for GROMACS

Carbohydrates constitute a structurally and functionally diverse group of biological molecules and macromolecules. In cells they are involved in, e.g., energy storage, signaling, and cell-cell recognition. All of these phenomena take place in atomistic scales, thus atomistic simulation would be the method of choice to explore how carbohydrates function.

However, the progress in the field is limited by the lack of appropriate tools for preparing carbohydrate structures and related topology files for the simulation models. Here we present tools that fill this gap. Applications where the tools discussed in this paper are particularly useful include, among others, the preparation of structures for glycolipids, nanocellulose, and glycans linked to glycoproteins. The molecular structures and simulation files generated by the tools are compatible with GROMACS.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: Biological Physics and Soft Matter, University of Helsinki, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, MEMPHYS - Centre for Biomembrane Physics, University of Southern Denmark, Laboratory of Physics

Contributors: Danne, R., Poojari, C., Martinez-Seara, H., Rissanen, S., Lolicato, F., Róg, T., Vattulainen, I.

Number of pages: 6

Pages: 2401-2406

Publication date: 23 Oct 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chemical Information and Modeling

Volume: 57

Issue number: 10

ISSN (Print): 1549-9596

Ratings:

Scopus rating (2017): CiteScore 3.9 SJR 1.349 SNIP 1.216

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all), Computer Science Applications, Library and Information Sciences

DOIs:

10.1021/acs.jcim.7b00237

Source: Scopus

Source ID: 85031999962

Research output: Contribution to journal > Article > Scientific > peer-review

#### Systematic analysis of coating-substrate interactions in the presence of flow localization

Localized deformation and cracking in a system of thermally sprayed hard metal coating overlaid on a low alloy steel is studied by means of bend testing. In-situ digital image correlation measurements are used to characterize material strain field near the coating/substrate interface. The studied substrate undergoes softening upon yielding which manifests itself as narrow bands of localized shear deformation. The measurements show that the coating cracks and the substrate shear

bands interact. When the coating starts cracking during the elastic loading of the substrate, the formed cracks function as nucleation points for the shear bands. In contrast, if the coating resists cracking until the yielding of the substrate, the coating cracks and substrate shear bands form simultaneously. Based on the experiments, continuum-scale finite element model of the system is developed, validated and then used for a systematic numerical analysis of the effects of substrate shear banding on the measurement of coating properties. Based on the results of this work, three main effects can be identified. Firstly, the flow localization in the substrate can increase the measured apparent (macroscopic) surface strain of the coating, if not accounted for by using microscopic techniques. Secondly, substrate shear bands increase the interfacial loading, which may cause unexpected delamination of the coating and thus affect the evaluation of the interfacial strength. Finally, substrate shear bands affect the stress state within the coating and may thus affect the cracking morphology in the coating. Therefore, based on the results of this study, if the coating and interfacial strengths are of similar magnitude with the substrate yield strength, the possible tendency of the substrate towards flow localization should be taken into account in the analysis of the coating behavior.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Surface Engineering, Ernst-Mach-Institut

Contributors: Isakov, M., Matikainen, V., Koivuluoto, H., May, M.

Number of pages: 17

Pages: 264-280

Publication date: 15 Sep 2017

Peer-reviewed: Yes

#### Publication information

Journal: Surface and Coatings Technology

Volume: 324

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2017): CiteScore 3.08 SJR 0.928 SNIP 1.565

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry

Keywords: Bending, Digital image correlation, Finite element method, Hard metal coating, Interfacial strength, Shear band

Electronic versions:

Isakov\_et\_al\_2017\_SurfCoatTech\_POST-PRINT\_Author. Embargo ended: 3/06/19

DOIs:

10.1016/j.surfcoat.2017.05.040

URLs:

<http://urn.fi/URN:NBN:fi:tty-201712202430>. Embargo ended: 3/06/19

Source: Scopus

Source ID: 85019992522

Research output: Contribution to journal › Article › Scientific › peer-review

#### Membrane Binding of Recoverin: From Mechanistic Understanding to Biological Functionality

Recoverin is a neuronal calcium sensor involved in vision adaptation that reversibly associates with cellular membranes via its calcium-activated myristoyl switch. While experimental evidence shows that the myristoyl group significantly enhances membrane affinity of this protein, molecular details of the binding process are still under debate. Here, we present results of extensive molecular dynamics simulations of recoverin in the proximity of a phospholipid bilayer. We capture multiple events of spontaneous membrane insertion of the myristoyl moiety and confirm its critical role in the membrane binding. Moreover, we observe that the binding strongly depends on the conformation of the N-terminal domain. We propose that a suitable conformation of the N-terminal domain can be stabilized by the disordered C-terminal segment or by binding of the target enzyme, i.e., rhodopsin kinase. Finally, we find that the presence of negatively charged lipids in the bilayer stabilizes a physiologically functional orientation of the membrane-bound recoverin.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Institute of Experimental Botany of the Academy of Sciences of the Czech Republic, University of Stuttgart, University of Helsinki

Contributors: Timr, Š., Pleskot, R., Kadlec, J., Kohagen, M., Magarkar, A., Jungwirth, P.

Number of pages: 7

Pages: 868-874

Publication date: 23 Aug 2017

Peer-reviewed: Yes

## Publication information

Journal: ACS Central Science

Volume: 3

Issue number: 8

ISSN (Print): 2374-7943

Ratings:

Scopus rating (2017): CiteScore 6.55 SJR 5.022 SNIP 2.01

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all)

DOIs:

10.1021/acscentsci.7b00210

Source: Scopus

Source ID: 85028063042

Research output: Contribution to journal › Article › Scientific › peer-review

## Exhaust emissions of non-road mobile machine: Real-world and laboratory studies with diesel and HVO fuels

Exhaust emissions emitted by a non-road mobile machine were studied chasing a tractor in real-world conditions and repeating the same transient tests with a similar engine on an engine dynamometer where additionally, non-road steady state tests were carried out. The engines were equipped with an oxidation catalyst (DOC) and a selective catalytic reduction (SCR) system, and they were fuelled by fossil diesel fuel with ultra-low sulphur content and hydrotreated vegetable oil (HVO). By substituting diesel fuel with HVO the on-road emissions of nitrogen oxides ( $\text{NO}_x$ ) reduced 20% and particle number 44%, the emission factors being  $\text{EF}_{\text{NO}_x} = 1.62 \pm 0.04 \text{ g/kWh}$  and  $\text{EF}_N = (28.2 \pm 7.8) \times 10^{13} \text{ \#kWh}$ . Similar trend was observed for  $\text{NO}_x$  at laboratory although the emissions were somewhat smaller than on-road. In contrast to real-world, in the laboratory experiment the  $\text{EF}_N$  was only 2% smaller with HVO than with diesel, and these emission factors were almost one order of magnitude smaller than observed on-road. The number size distribution and volatility measurements showed that in real-world experiments small nucleation mode particles were formed during uphill and during downhill in engine braking conditions. These were not observed at laboratory. However, nucleation mode particles were observed in the laboratory experiments at high load steady driving conditions. At steady state tests the emissions strongly depended on engine load and engine speed with both fuels.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research area: Aerosol Physics, University of Helsinki, Turku University of Applied Sciences

Contributors: Pirjola, L., Rönkkö, T., Saukko, E., Parviainen, H., Malinen, A., Alanen, J., Saveljeff, H.

Number of pages: 11

Pages: 154-164

Publication date: 15 Aug 2017

Peer-reviewed: Yes

## Publication information

Journal: Fuel

Volume: 202

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2017): CiteScore 5.4 SJR 1.891 SNIP 2.127

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Fuel Technology, Energy Engineering and Power Technology, Organic Chemistry

Keywords: Diesel engine, Exhaust emissions, HVO, NO, Particle size distribution, Real-world emissions, Tractor

Electronic versions:

Fuel\_Pirjola\_rev2\_TUTCRIS. Embargo ended: 13/04/19

DOIs:

10.1016/j.fuel.2017.04.029

URLs:

<http://urn.fi/URN:NBN:fi:tty-201712192400>. Embargo ended: 13/04/19

Additional files:

Appendix A\_Pirjola\_rev\_TUTCRIS

Source: Scopus

Source ID: 85017566506

Research output: Contribution to journal › Article › Scientific › peer-review

### **Feed-hopper level estimation and control in cone crushers**

This paper describes a novel feed-hopper level estimation and control scheme for addressing the known problem of unreliable and occasionally corrupted feed-hopper level measurement in a cone crusher. The approach involves estimating the feed-hopper level with an adaptive time-variant state estimator. The proposed scheme delivers asymptotically unbiased feed-hopper level estimates, despite using an inherently biased state estimator with biased measurement(s) and/or model, and therefore addresses the common pitfall of state estimators. The paper details the entire control system design procedure, from the fundamental theory, through dynamic modeling and estimator/controller tuning, to the design validation and control performance evaluation. The performance of the proposed scheme is evaluated through extensive full-scale tests in various production scenarios, including process start-up, level setpoint changes, and mass flow disturbance rejection. The full-scale tests revealed a number of benefits compared to the straightforward level control implementation. These benefits include the possibility of recovering from a temporary loss of measurement signal, smaller control effort, and increased system robustness due to an increased ability to withstand measurement errors. Therefore, the proposed scheme will enable more consistent size reduction and provide protection against performance degradation and process down-time.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Automation and Hydraulic Engineering, Chalmers University of Technology

Contributors: Itävuori, P., Hulthén, E., Vilkkio, M.

Number of pages: 14

Pages: 82-95

Publication date: 15 Aug 2017

Peer-reviewed: Yes

#### **Publication information**

Journal: Minerals Engineering

Volume: 110

ISSN (Print): 0892-6875

Ratings:

Scopus rating (2017): CiteScore 2.99 SJR 1.248 SNIP 2.073

Original language: English

ASJC Scopus subject areas: Control and Systems Engineering, Chemistry(all), Geotechnical Engineering and Engineering Geology, Mechanical Engineering

Keywords: Adaptive state estimation, Cone crusher, Dynamic modeling, Level control, System identification

DOIs:

10.1016/j.mineng.2017.04.010

Source: Scopus

Source ID: 85018328452

Research output: Contribution to journal > Article > Scientific > peer-review

### **Configurational Disorder of Water Hydrogen-Bond Network at the Protein Dynamical Transition**

We introduce a novel strategy to quantify the disorder of extended water-water hydrogen-bond (HB) networks sampled in particle-based computer simulations. The method relies on the conformational clustering of the HB connectivity states. We successfully applied it to unveil the fine relationship among the protein dynamical transition in hydrated powder, which marks the activation of protein flexibility at  $T_g \approx 240$  K, and the sudden increase in the configurational disorder of the water HB network enveloping the proteins. Our finding links, in the spirit of the Adam-Gibbs relationship, the diffusivity of protein atoms, as quantified by the hydrogen mean-square displacements, and the thermodynamic solvent configurational entropy.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Bauhaus-Universität Weimar, Université Paris Diderot, Università di Perugia

Contributors: Rahaman, O., Kalimeri, M., Katava, M., Paciaroni, A., Sterpone, F.

Number of pages: 7

Pages: 6792-6798

Publication date: 20 Jul 2017

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry Part B

Volume: 121

Issue number: 28

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2017): CiteScore 3.13 SJR 1.331 SNIP 0.996

Original language: English

ASJC Scopus subject areas: Surfaces, Coatings and Films, Physical and Theoretical Chemistry, Materials Chemistry

DOIs:

10.1021/acs.jpcc.7b03888

Source: Scopus

Source ID: 85025646989

Research output: Contribution to journal > Article > Scientific > peer-review

### **Vegetable fillers for electric stimuli responsive elastomers**

Dielectric elastomer actuators (DEAs) have been studied widely in recent years for artificial muscle applications, but their implementation into production is limited due to high operating voltages required. The actuation behavior of dielectric elastomer under an applied electric field is predicted by Maxwell's pressure and thickness strain equations. According to these equations, the best electromechanical response is achieved when the relative permittivity is high and elastic modulus is low. The potential source for additives increasing the relative permittivity of rubbers can be vegetable powders that have much higher dielectric constant than common elastomers. In the present research, the dielectric and actuation properties of polyacrylate rubber (ACM) were studied after the addition of different vegetable-based fillers such as potato starch, corn starch, garlic, and paprika. The results were compared to ACM filled with barium titanate. The compounds containing vegetable fillers showed higher relative dielectric permittivity at 1 Hz frequency than the compounds containing barium titanate due to higher interfacial polarization. The actuation studies showed that lower electric fields are required to generate certain actuation forces when the starches and garlic are used in the rubber instead of barium titanate. Therefore, the vegetable-based fillers can be used to improve actuation performance of DEAs.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Plastics and Elastomer Technology, Department of Elastomers, Leibniz-Institut für Polymerforschung Dresden E.V.

Contributors: Poikelispää, M., Shakun, A., Sarlin, E., Das, A., Vuorinen, J.

Publication date: 20 Jul 2017

Peer-reviewed: Yes

Early online date: 2017

### **Publication information**

Journal: Journal of Applied Polymer Science

Volume: 134

Issue number: 28

Article number: 45081

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2017): CiteScore 1.87 SJR 0.543 SNIP 0.773

Original language: English

ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry

Keywords: biomaterials, dielectric properties, elastomers, mechanical properties, sensors and actuators

DOIs:

10.1002/app.45081

### **Bibliographical note**

INT=mol,"Poikelispää, Minna"

Source: Scopus

Source ID: 85016434216

Research output: Contribution to journal > Article > Scientific > peer-review

### **Electropolymerized polyazulene as active material in flexible supercapacitors**

We report the capacitive behavior of electrochemically polymerized polyazulene films in different ionic liquids. The ionic liquids in this study represent conventional imidazolium based ionic liquids with tetrafluoroborate and bis(trifluoromethylsulfonyl)imide anions as well as an unconventional choline based ionic liquid. The effect of different ionic liquids on the polymerization and capacitive performance of polyazulene films is demonstrated by cyclic voltammetry and electrochemical impedance spectroscopy in a 3-electrode cell configuration. The films exhibit the highest capacitances in the lowest viscosity ionic liquid ( $92 \text{ mF cm}^{-2}$ ), while synthesis in high viscosity ionic liquid shortens the conjugation length and results in lower electroactivity ( $25 \text{ mF cm}^{-2}$ ). The obtained films also show good cycling stabilities retaining over 90% of their initial capacitance over 1200 p-doping cycles. We also demonstrate, for the first time, flexible polyazulene supercapacitors of symmetric and asymmetric configurations using the choline based ionic liquid as electrolyte. In asymmetric configuration, capacitance of  $55 \text{ mF}$  ( $27 \text{ mF cm}^{-2}$ ) with an equivalent series resistance of  $19 \Omega$  is obtained at

operating voltage of 1.5 V. Upon increasing the operating voltage up to 2.4 V, the capacitance increases to 72 mF (36 mF cm<sup>-2</sup>).

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Electronics and Communications Engineering, Faculty of Biomedical Sciences and Engineering, Research area: Microsystems, Research area: Measurement Technology and Process Control, Research group: Sensor Technology and Biomeasurements (STB), BioMediTech, Turun Yliopisto/Turun Biomateriaalikeskus

Contributors: Suominen, M., Lehtimäki, S., Yewale, R., Damlin, P., Tuukkanen, S., Kvarnström, C.

Number of pages: 10

Pages: 181-190

Publication date: 15 Jul 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Power Sources

Volume: 356

ISSN (Print): 0378-7753

Ratings:

Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.557

Original language: English

ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Energy Engineering and Power Technology, Physical and Theoretical Chemistry, Electrical and Electronic Engineering

Keywords: Choline, Electropolymerization, Flexible supercapacitor, Ionic liquid, Polyazulene

Electronic versions:

Suominen\_2017\_Revised\_Manuscript. Embargo ended: 15/07/19

Suominen\_2017\_Supplementary\_information. Embargo ended: 15/07/19

DOIs:

10.1016/j.jpowsour.2017.04.082

URLs:

<http://urn.fi/URN:NBN:fi:tty-201706021571>. Embargo ended: 15/07/19

URLs:

<http://www.scopus.com/inward/record.url?scp=85019024216&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 85019024216

Research output: Contribution to journal › Article › Scientific › peer-review

#### Dynamics of a True Moving Bed separation process: Linear model identification and advanced process control

The control of Simulated Moving Bed (SMB) units is challenging due to their complex dynamic behaviour and the difficulty of measuring their main properties. Furthermore, for the SMB units, the transfer function identification when the unit is operating at its optimal point is not easy to be done through the usual way. This work presents the development of a novel strategy to identify transfer functions of TMB/SMB and its application on classical linear model predictive controllers (MPC). However, for the process in study, due its unique dynamics, only the identification of the linear model is not enough to solve its control problem. Therefore, it is proposed a modification in the MPC prediction, that consists in a strategy based on a switching system where the most adequate transfer function is employed in the controller to overcome the problems related with the process dynamic behaviour. The results show that the used methodology enables the easy identification of transfer functions at the process optimal operating point and that the MPC can control the process in both the servo and regulator problem cases. It is also showed that the transfer function identified can be applied in the control of a SMB unit with four columns, under its optimal conditions.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Automation and Hydraulic Engineering, Research area: Information Systems in Automation

Contributors: Nogueira, I. B., Ribeiro, A. M., Martins, M. A., Rodrigues, A. E., Koivisto, H., Loureiro, J. M.

Publication date: 30 Jun 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chromatography A

Volume: 1504

ISSN (Print): 0021-9673

Ratings:

Scopus rating (2017): CiteScore 3.81 SJR 1.378 SNIP 1.23

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Biochemistry, Organic Chemistry

Keywords: Enantiomers separation, Model predictive control, Process transfer function, Simulated moving bed

DOIs:

10.1016/j.chroma.2017.04.060

Source: Scopus

Source ID: 85019248239

Research output: Contribution to journal > Article > Scientific > peer-review

### Long-Range Observation of Exciplex Formation and Decay Mediated by One-Dimensional Bridges

We report herein unprecedented long-range observation of both formation and decay of the exciplex state in donor (D)-bridge (B)-acceptor (A) linked systems. Zinc porphyrins (ZnP) as a donor were tethered to single-walled carbon nanotube (SWNT) as an acceptor through oligo(*p*-phenylene)s (ZnP-ph<sub>*n*</sub>-SWNT) or oligo(*p*-xylene)s (ZnP-xy<sub>*n-1*</sub>-ph<sub>*1*</sub>-SWNT) with systematically varied lengths (*n* = 1-5) to address the issue. Exponential dependencies of rate constants for the exciplex formation (*k*<sub>FEX</sub>) and decay (*k*<sub>DEX</sub>) on the edge-to-edge separation distance between ZnP and SWNT through the bridges were unambiguously derived from time-resolved spectroscopies. Distance dependencies (i.e., attenuation factor,  $\beta$ ) of *k*<sub>FEX</sub> and *k*<sub>DEX</sub> in ZnP-ph<sub>*n*</sub>-SWNT were found to be considerably small ( $\beta = 0.10$  for *k*<sub>FEX</sub> and  $0.12 \text{ \AA}^{-1}$  for *k*<sub>DEX</sub>) compared to those for charge separation and recombination ( $0.2\text{-}0.8 \text{ \AA}^{-1}$ ) in D-B-A systems with the same oligo(*p*-phenylene) bridges. The small  $\beta$  values may be associated with the exciplex state with mixed characters of charge-transfer and excited states. In parallel, the substantially nonconjugated bridge of oligo(*p*-xylene)s exhibited larger attenuation values ( $\beta = 0.12$  for *k*<sub>FEX</sub> and  $0.14 \text{ \AA}^{-1}$  for *k*<sub>DEX</sub>). These results provide deep insight into the unique photodynamics of electronically strongly coupled D-B-A systems involving exciplex.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Kyoto Women's University

Contributors: Baek, J., Umeyama, T., Stranius, K., Yamada, H., Tkachenko, N. V., Imahori, H.

Number of pages: 10

Pages: 13952-13961

Publication date: 29 Jun 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 121

Issue number: 25

ISSN (Print): 1932-7447

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Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.135

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Surfaces, Coatings and Films, Physical and Theoretical Chemistry

DOIs:

10.1021/acs.jpcc.7b04483

Source: Scopus

Source ID: 85022231305

Research output: Contribution to journal > Article > Scientific > peer-review

### Comparison of starch and gelatin hydrogels for non-toxic supercapacitor electrolytes

Starch and gelatin are two of the most abundantly available natural polymers. Their non-toxicity, low cost, and compatibility with aqueous solvents make them ideal for use in ubiquitous, environmentally friendly electronics systems. This work presents the results of conductivity measurements through impedance spectroscopy for gelatin- and starch-based aqueous gel electrolytes. The NaCl-based gels were physically cross-linked. The conductivity values were 84.6 mS/cm at  $1.5 \text{ mol L}^{-1}$  and 71.5 mS/cm at  $2 \text{ mol L}^{-1}$  for gelatin and starch, respectively. The mechanical properties of gelatin were found preferable to those of starch, although they deteriorated significantly when the salt concentration exceeded  $2 \text{ mol L}^{-1}$ . The ability of the gels to successfully act as a supercapacitor electrolyte was demonstrated with printed electrodes on plastic substrate. The devices were characterized through cyclic voltammetry measurements. The results imply that these polymer gel electrolytes are very promising for replacing the traditional aqueous liquid electrolytes in supercapacitors in applications where, for example, user and environmental safety is essential.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Electronics and Communications Engineering, Research group: Laboratory for Future Electronics

Contributors: Railanmaa, A., Lehtimäki, S., Lupo, D.

Publication date: 1 Jun 2017

Peer-reviewed: Yes

### Publication information

Journal: Applied Physics A-Materials Science and Processing

Volume: 123

Issue number: 6

Article number: 459

ISSN (Print): 0947-8396

Ratings:

Scopus rating (2017): CiteScore 1.62

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all)

DOIs:

10.1007/s00339-017-1068-1

Source: Scopus

Source ID: 85020029646

Research output: Contribution to journal › Article › Scientific › peer-review

### Catalytic Activity of AuCu Clusters on MgO(100): Effect of Alloy Composition for CO Oxidation

Density functional simulations have been performed for Au<sub>7</sub>Cu<sub>23</sub> and Au<sub>23</sub>Cu<sub>7</sub> clusters on MgO(100) supports to probe their catalytic activity for CO oxidation. The adsorption of reactants, O<sub>2</sub> and CO, and potential O<sub>2</sub> dissociation have been investigated in detail by tuning the location of vacancies (F-center, V-center) in MgO(100). The total charge on Au<sub>7</sub>Cu<sub>23</sub> and Au<sub>23</sub>Cu<sub>7</sub> is negative on all supports, regardless of the presence of vacancies, but the effect is significantly amplified on the F-center. Au<sub>7</sub>Cu<sub>23</sub>/MgO(100) and Au<sub>23</sub>Cu<sub>7</sub>/MgO(100) with an F-center are the only systems to bind O<sub>2</sub> more strongly than CO. In each case, O<sub>2</sub> can be effectively activated upon adsorption and dissociated to 2 × O atoms. The different reaction paths based on the Langmuir-Hinshelwood (LH) and Eley-Rideal (ER) mechanisms for CO oxidation have been explored on the Au<sub>7</sub>Cu<sub>23</sub> and Au<sub>23</sub>Cu<sub>7</sub> clusters on F-centers, and the results are compared with the previous findings for Au<sub>15</sub>Cu<sub>15</sub>. Overall, the reaction barriers are small, but the changes in the Au:Cu ratio tune the reactant adsorption energies and sites considerably, showing also varying selectivity for CO and O<sub>2</sub>. The microkinetic model built on the basis of the above results shows a pronounced CO<sub>2</sub> production rate at low temperature for the clusters on F-centers.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: Materials and Molecular Modeling, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Aalto University, Norwegian Univ. of Sci. and Technol.

Contributors: Ma, L., Laasonen, K., Akola, J.

Number of pages: 11

Pages: 10876-10886

Publication date: 25 May 2017

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physical Chemistry C

Volume: 121

Issue number: 20

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.135

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Surfaces, Coatings and Films,

Physical and Theoretical Chemistry

Electronic versions:

Catalytic Activity of AuCu Clusters on MgO(100) Effect of Alloy Composition for CO Oxidation. Embargo ended: 17/02/18

DOIs:

10.1021/acs.jpcc.6b12054

URLs:

<http://urn.fi/URN:NBN:fi:tty-201905021452>. Embargo ended: 17/02/18



Source: Scopus

Source ID: 85020757142

Research output: Contribution to journal › Article › Scientific › peer-review

### **Geometric Structure and Chemical Ordering of Large AuCu Clusters: A Computational Study**

Understanding the structure and composition of nanosized gold-copper (AuCu) clusters is crucial for designing an effective AuCu catalyst. Global optimization of AuCu clusters using atomistic force fields is a viable solution for clusters with at least a few nm sizes, because of its fast computation. Here we develop an atomistic many-body potential for AuCu on the basis of the second-moment approximation to the tight-binding model. We show that our potential is in good agreement with density-functional theory calculations, and use it to study the structure and chemical ordering of clusters of sizes up to ~4 nm by means of global optimization searches. We show that the clusters present a surface enrichment in Au, while subsurface and central sites are enriched in Cu. Surface enrichment in Au and center enrichment in Cu are stronger in icosahedra. Surface Cu atoms prefer terrace sites on (111) facets. Both atomistic and DFT calculations show that  $L1_0$  and  $L1_2$  ordered phases are not favorable, even at their ideal compositions for these sizes, because of the tendency of Au to surface segregation. The stability range of icosahedral structures is wider in AuCu nanoalloys than in Au and Cu pure clusters.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Aalto University, Università di Genova

Contributors: Goh, J., Akola, J., Ferrando, R.

Number of pages: 8

Pages: 10809-10816

Publication date: 25 May 2017

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry C

Volume: 121

Issue number: 20

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.135

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Physical and Theoretical Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/acs.jpcc.6b11958

Source: Scopus

Source ID: 85016919329

Research output: Contribution to journal › Article › Scientific › peer-review

### **Nematicon-enhanced spontaneous symmetry breaking**

We investigate topological and optical spontaneous symmetry breaking in nematic liquid crystals subject to the Fréedericksz transition. Specular nematicon states couple to mirrored distributions of the director due to symmetry breaking, with transverse velocities controlled by beam power in the strong nonlinear regime. Hysteresis in transverse velocity versus incidence angle is observed in the soliton regime.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, University "Roma Tre", University of Southampton, United Kingdom, Centro S3, Nonlinear Optics and OptoElectronics Lab, Optics Laboratory, Department of Physics, Tampere University of Technology

Contributors: Piccardi, A., Alberucci, A., Kravets, N., Buchnev, O., Assanto, G.

Number of pages: 7

Pages: 59-65

Publication date: 24 May 2017

Peer-reviewed: Yes

#### **Publication information**

Journal: Molecular Crystals and Liquid Crystals

Volume: 649

Issue number: 1  
ISSN (Print): 1542-1406  
Ratings:

Scopus rating (2017): CiteScore 0.59 SJR 0.216 SNIP 0.348

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics

Keywords: liquid crystals, nonlinear optics, solitons, Spontaneous symmetry breaking

DOIs:

10.1080/15421406.2017.1303916

Source: Scopus

Source ID: 85028756273

Research output: Contribution to journal > Article > Scientific > peer-review

### Density functional study of structure and dynamics in liquid antimony and $Sb_n$ clusters

Density functional/molecular dynamics simulations have been performed on liquid antimony (588 atoms and six temperatures between 600 K and 1300 K) and on neutral Sb clusters with up to 14 atoms. We study structural patterns (coordination numbers, bond angles, and ring patterns, structure factors, pair distribution functions) and dynamical properties (vibration frequencies, diffusion constants, power spectra, dynamical structure factors, viscosity) and compare with available experimental results and with the results of our previous simulations on Bi. Three short covalent bonds characteristic of pnictogens are common in the clusters, and higher temperatures lead in the liquid to broader bond angle distributions, larger total cavity volumes, and weaker correlations between neighboring bond lengths. There are clear similarities between the properties of Sb and Bi aggregates.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Forschungszentrum Jülich (FZJ), Norwegian Univ. of Sci. and Technol., COMP Centre of Excellence, Department of Applied Physics, Aalto University, Aalto University

Contributors: Jones, R. O., Ahlstedt, O., Akola, J., Ropo, M.

Publication date: 21 May 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chemical Physics

Volume: 146

Issue number: 19

Article number: 194502

ISSN (Print): 0021-9606

Ratings:

Scopus rating (2017): CiteScore 2.5 SJR 1.252 SNIP 0.971

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1063/1.4983219

Source: Scopus

Source ID: 85029897404

Research output: Contribution to journal > Article > Scientific > peer-review

### The effects of calcium and potassium on $CO_2$ gasification of birch wood in a fluidized bed

Birch wood was leached of its naturally occurring ash forming elements and doped with three concentrations of calcium or potassium before being gasified in a laboratory bubbling fluidized bed reactor. The wood samples were pelletized and inserted into a fluidized bed reactor where they were first pyrolyzed with  $N_2$  and then gasified with  $CO_2$ . In addition to tracking the gas concentration of the exit gas, char samples were taken from the fluidized bed and analyzed to study the char properties. The presence of potassium in the biomass was found to have a significant influence on the structure of the resulting char, however potassium did not have an observable catalytic effect on the overall gasification reaction rate with  $CO_2$  due to the formation of a unreactive coke layer on the char surface. In contrast, calcium did increase the char conversion rate and is likely the primary active catalyst in gasification of birch wood with  $CO_2$ .

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Industrial Bioengineering and Applied Organic Chemistry, Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology, Universidad de Sevilla, Johan Gadolin Process Chemistry Centre, Abo Akademi University, Univ of Oulu

Contributors: Kramb, J., Gómez-Barea, A., DeMartini, N., Romar, H., Doddapaneni, T. R. K. C., Kontinen, J.  
Number of pages: 10  
Pages: 398-407  
Publication date: 15 May 2017  
Peer-reviewed: Yes

#### Publication information

Journal: Fuel  
Volume: 196  
ISSN (Print): 0016-2361  
Ratings:

Scopus rating (2017): CiteScore 5.4 SJR 1.891 SNIP 2.127

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Fuel Technology, Energy Engineering and Power Technology, Organic Chemistry

Keywords: Biomass, Catalysts, Char, Fluidized bed, Gasification

DOIs:

10.1016/j.fuel.2017.01.101

Source: Scopus

Source ID: 85012050856

Research output: Contribution to journal > Article > Scientific > peer-review

#### Photoinduced Electron Injection from Zinc Phthalocyanines into Zinc Oxide Nanorods: Aggregation Effects

Phthalocyanines (Pc) are well-known light-harvesting compounds. However, despite the tremendous efforts on phthalocyanine synthesis, the achieved energy conversion efficiencies for Pc-based dye-sensitized solar cells are moderate. To cast light on the factors reducing the conversion efficiency, we have undertaken a time-resolved spectroscopy study of the primary photoinduced reactions at a semiconductor-Pc interface. ZnO nanorods were chosen as a model semiconductor substrate with enhanced specific surface area. The use of a nanostructured oxide surface allows to extend the semiconductor-dye interface with a hole transporting layer (spiro-MeOTAD) in a controlled way, making the studied system closer to a solid-state dye-sensitized solar cell. Four zinc phthalocyanines are compared in this study. The compounds are equipped with bulky peripheral groups designed to reduce the self-aggregation of the Pcs. Almost no signs of aggregation can be observed from the absorption spectra of the Pcs assembled on a ZnO surface. Nevertheless, the time-resolved spectroscopy indicates that there are inter-Pc charge separation-recombination processes in the time frame of 1-100 ps. This may reduce the electron injection efficiency into the ZnO by more than 50%, pointing out to a remaining aggregation effect. Surprisingly, the electron injection time does not correlate with the length of the linker connecting the Pc to ZnO. A correlation between the electron injection time and the "bulkiness" of the peripheral groups was observed. This correlation is further discussed with the use of computational modeling of the Pc arrangements on the ZnO surface. (Figure Presented).

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Universidad Autónoma de Madrid, Mersin University, South-Ukrainian National Pedagogical University

Contributors: Virkki, K., Hakola, H., Urbani, M., Tejerina, L., Ince, M., Martínez-Díaz, M. V., Torres, T., Golovanova, V., Golovanov, V., Tkachenko, N. V.

Number of pages: 12

Pages: 9594-9605

Publication date: 4 May 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 121

Issue number: 17

ISSN (Print): 1932-7447

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Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.135

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Surfaces, Coatings and Films, Physical and Theoretical Chemistry

DOIs:

10.1021/acs.jpcc.7b01562

Source: Scopus

Source ID: 85020915273

Research output: Contribution to journal › Article › Scientific › peer-review

### **Electron microscopic studies of natural gas oxidation catalyst – Effects of thermally accelerated aging on catalyst microstructure**

Structural changes of PtPd nanoparticles in a natural gas oxidation catalyst were studied at elevated temperatures in air and low-oxygen conditions and in situ using environmental transmission electron microscopy (ETEM). The fresh catalyst shows x particles on the  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> support. At 700 °C, the noble metal oxide decomposes and Pt gets trapped by PdO particles followed by formation of metallic Pd and Pt containing particles. At 1000 °C, the particles had a metallic Pd and Pt containing core surrounded by PdO particles. In addition, the presence of

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Materials Characterization, Danmarks Tekniske Universitet, DTU Informatik, Aalto University, Univ of Oulu, Dinex Ecocat Oy

Contributors: Honkanen, M., Hansen, T. W., Jiang, H., Kärkkäinen, M., Huuhtanen, M., Heikkinen, O., Kallinen, K., Lahtinen, J., Keiski, R. L., Wagner, J. B., Vippola, M.

Number of pages: 11

Pages: 19-29

Publication date: 1 May 2017

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Catalysis

Volume: 349

ISSN (Print): 0021-9517

Ratings:

Scopus rating (2017): CiteScore 6.99 SJR 2.397 SNIP 1.839

Original language: English

ASJC Scopus subject areas: Catalysis, Physical and Theoretical Chemistry

Keywords: Environmental transmission electron microscope, Low-oxygen conditions, Natural gas oxidation, Palladium, Platinum, Sintering, Thermal aging

DOIs:

10.1016/j.jcat.2017.03.003

Source: Scopus

Source ID: 85016079754

Research output: Contribution to journal › Article › Scientific › peer-review

### **Elucidation of Compression-Induced Surface Crystallization in Amorphous Tablets Using Sum Frequency Generation (SFG) Microscopy**

Purpose: To investigate the effect of compression on the crystallization behavior in amorphous tablets using sum frequency generation (SFG) microscopy imaging and more established analytical methods. Method: Tablets containing neat amorphous griseofulvin with/without excipients (silica, hydroxypropyl methylcellulose acetate succinate (HPMCAS), microcrystalline cellulose (MCC) and polyethylene glycol (PEG)) were prepared. They were analyzed upon preparation and storage using attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy, scanning electron microscopy (SEM) and SFG microscopy. Results: Compression-induced crystallization occurred predominantly on the surface of the neat amorphous griseofulvin tablets, with minimal crystallinity being detected in the core of the tablets. The presence of various types of excipients was not able to mitigate the compression-induced surface crystallization of the amorphous griseofulvin tablets. However, the excipients affected the crystallization rate of amorphous griseofulvin in the core of the tablet upon compression and storage. Conclusions: SFG microscopy can be used in combination with ATR-FTIR spectroscopy and SEM to understand the crystallization behaviour of amorphous tablets upon compression and storage. When selecting excipients for amorphous formulations, it is important to consider the effect of the excipients on the physical stability of the amorphous formulations.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, University of Helsinki, Division of Biopharmaceutical Sciences, Biomedical Imaging Unit, FIN-00014 University of Helsinki

Contributors: Mah, P. T., Novakovic, D., Saarinen, J., van Landeghem, S., Peltonen, L., Laaksonen, T., Isomäki, A., Strachan, C. J.

Number of pages: 14

Pages: 957-970  
Publication date: May 2017  
Peer-reviewed: Yes  
Early online date: 13 Oct 2016

#### Publication information

Journal: Pharmaceutical Research  
Volume: 34

Issue number: 5  
ISSN (Print): 0724-8741

Ratings:

Scopus rating (2017): CiteScore 3.3 SJR 1.077 SNIP 1.054

Original language: English

ASJC Scopus subject areas: Biotechnology, Molecular Medicine, Pharmacology, Pharmaceutical Science, Organic Chemistry, Pharmacology (medical)

DOIs:

10.1007/s11095-016-2046-6

Source: Scopus

Source ID: 84991051806

Research output: Contribution to journal > Article > Scientific > peer-review

#### Hexaphyrin as a Potential Theranostic Dye for Photothermal Therapy and $^{19}\text{F}$ Magnetic Resonance Imaging

Two features of meso-Aryl-substituted expanded porphyrins suggest suitability as theranostic agents. They have excellent absorption in near infrared (NIR) region, and they offer the possibility of introduction of multiple fluorine atoms at structurally equivalent positions. Here, hexaphyrin (hexa) was synthesized from 2,6-bis(trifluoromethyl)-4-formyl benzoate and pyrrole and evaluated as a novel expanded porphyrin with the above features. Under NIR illumination hexa showed intense photothermal and weak photodynamic effects, which were most likely due to its low excited states, close to singlet oxygen. The sustained photothermal effect caused ablation of cancer cells more effectively than the photodynamic effect of indocyanine green (a clinical dye). In addition, hexa showed potential for use in the visualization of tumors by  $^{19}\text{F}$  magnetic resonance imaging (MRI), because of the multiple fluorine atoms. Our results strongly support the utility of expanded porphyrins as theranostic agents in both photothermal therapy and  $^{19}\text{F}$  MRI.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Kyoto Women's University, Toyama Prefectural University

Contributors: Higashino, T., Nakatsuji, H., Fukuda, R., Okamoto, H., Imai, H., Matsuda, T., Tochio, H., Shirakawa, M., Tkachenko, N. V., Hashida, M., Murakami, T., Imahori, H.

Number of pages: 9

Pages: 951-959

Publication date: 24 Mar 2017

Peer-reviewed: Yes

#### Publication information

Journal: ChemBioChem

Volume: 18

Issue number: 10

ISSN (Print): 1439-4227

Ratings:

Scopus rating (2017): CiteScore 2.64 SJR 1.407 SNIP 0.726

Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Medicine, Molecular Biology, Organic Chemistry

Keywords: expanded porphyrin, fluorine, MRI, NMR spectroscopy, photochemistry, theranostics

DOIs:

10.1002/cbic.201700071

Source: Scopus

Source ID: 85016610793

Research output: Contribution to journal > Article > Scientific > peer-review

#### Calcium Directly Regulates Phosphatidylinositol 4,5-Bisphosphate Headgroup Conformation and Recognition

The orchestrated recognition of phosphoinositides and concomitant intracellular release of  $\text{Ca}^{2+}$  is pivotal to almost every aspect of cellular processes, including membrane homeostasis, cell division and growth, vesicle trafficking, as well as secretion. Although  $\text{Ca}^{2+}$  is known to directly impact phosphoinositide clustering, little is known about the molecular basis for this or its significance in cellular signaling. Here, we study the direct interaction of  $\text{Ca}^{2+}$  with phosphatidylinositol 4,5-

bisphosphate (PI(4,5)P<sub>2</sub>), the main lipid marker of the plasma membrane. Electrokinetic potential measurements of PI(4,5)P<sub>2</sub> containing liposomes reveal that Ca<sup>2+</sup> as well as Mg<sup>2+</sup> reduce the zeta potential of liposomes to nearly background levels of pure phosphatidylcholine membranes. Strikingly, lipid recognition by the default PI(4,5)P<sub>2</sub> lipid sensor, phospholipase C delta 1 pleckstrin homology domain (PLC δ1-PH), is completely inhibited in the presence of Ca<sup>2+</sup>, while Mg<sup>2+</sup> has no effect with 100 nm liposomes and modest effect with giant unilamellar vesicles. Consistent with biochemical data, vibrational sum frequency spectroscopy and atomistic molecular dynamics simulations reveal how Ca<sup>2+</sup> binding to the PI(4,5)P<sub>2</sub> headgroup and carbonyl regions leads to confined lipid headgroup tilting and conformational rearrangements. We rationalize these findings by the ability of calcium to block a highly specific interaction between PLC δ1-PH and PI(4,5)P<sub>2</sub>, encoded within the conformational properties of the lipid itself. Our studies demonstrate the possibility that switchable phosphoinositide conformational states can serve as lipid recognition and controlled cell signaling mechanisms.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, German Center for Diabetes Research (DZD e.V.), Institute of Experimental Botany of the Academy of Sciences of the Czech Republic, Pennsylvania State University, University of Wrocław, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, J. Heyrovský Institute of Physical Chemistry, University of Helsinki, MEMPHYS, University of Southern Denmark

Contributors: Bilkova, E., Pleskot, R., Rissanen, S., Sun, S., Czogalla, A., Cwiklik, L., Róg, T., Vattulainen, I., Cremer, P. S., Jungwirth, P., Coskun, Ü.

Number of pages: 6

Pages: 4019-4024

Publication date: 22 Mar 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of the American Chemical Society

Volume: 139

Issue number: 11

ISSN (Print): 0002-7863

Ratings:

Scopus rating (2017): CiteScore 14.05 SJR 8.127 SNIP 2.633

Original language: English

ASJC Scopus subject areas: Catalysis, Chemistry(all), Biochemistry, Colloid and Surface Chemistry

DOIs:

10.1021/jacs.6b11760

#### Bibliographical note

EXT="Cwiklik, Lukasz"

Source: Scopus

Source ID: 85016148911

Research output: Contribution to journal > Article > Scientific > peer-review

#### Hierarchical Self-Assembly of Halogen-Bonded Block Copolymer Complexes into Upright Cylindrical Domains

Self-assembly of block copolymers into well-defined, ordered arrangements of chemically distinct domains is a reliable strategy for preparing tailored nanostructures. Microphase separation results from the system, minimizing repulsive interactions between dissimilar blocks and maximizing attractive interactions between similar blocks. Supramolecular methods have also achieved this separation by introducing small-molecule additives binding specifically to one block by noncovalent interactions. Here, we use halogen bonding as a supramolecular tool that directs the hierarchical self-assembly of low-molecular-weight perfluorinated molecules and diblock copolymers. Microphase separation results in a lamellar-within-cylindrical arrangement and promotes upright cylindrical alignment in films upon rapid casting and without further annealing. Such cylindrical domains with internal lamellar self-assemblies can be cleaved by solvent treatment of bulk films, resulting in separated and segmented cylindrical micelles stabilized by halogen-bond-based supramolecular crosslinks. These features, alongside the reversible nature of halogen bonding, provide a robust modular approach for nanofabrication.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, VTT Technical Research Centre of Finland, Aalto University, Politecnico di Milano, Italian Institute of Technology, Università del Salento

Contributors: Milani, R., Houbenov, N., Fernandez-Palacio, F., Cavallo, G., Luzio, A., Haataja, J., Giancane, G., Saccone, M., Priimägi, A., Metrangolo, P., Ikkala, O.

Number of pages: 10

Pages: 417-426  
Publication date: 9 Mar 2017  
Peer-reviewed: Yes

#### Publication information

Journal: CheM  
Volume: 2  
Issue number: 3  
ISSN (Print): 2451-9294  
Ratings:

Scopus rating (2017): CiteScore 7.23 SJR 5.295 SNIP 2.263

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all), Biochemistry, Environmental Chemistry, Materials Chemistry, Biochemistry, medical

Keywords: block copolymers, halogen bond, hierarchical self-assembly, nanofabrication, supramolecular complexes  
Electronic versions:

Hierarchical Self-Assembly of Halogen-Bonded Block Copolymer Complexes into Upright Cylindrical Domains

DOIs:

10.1016/j.chempr.2017.02.003

URLs:

<http://urn.fi/URN:NBN:fi:tty-201703281227>

Source: Scopus

Source ID: 85014778403

Research output: Contribution to journal > Article > Scientific > peer-review

#### Membrane cholesterol access into a G-protein-coupled receptor

Cholesterol is a key component of cell membranes with a proven modulatory role on the function and ligand-binding properties of G-protein-coupled receptors (GPCRs). Crystal structures of prototypical GPCRs such as the adenosine  $A_{2A}$  receptor ( $A_{2A}$  R) have confirmed that cholesterol finds stable binding sites at the receptor surface suggesting an allosteric role of this lipid. Here we combine experimental and computational approaches to show that cholesterol can spontaneously enter the  $A_{2A}$  R-binding pocket from the membrane milieu using the same portal gate previously suggested for opsin ligands. We confirm the presence of cholesterol inside the receptor by chemical modification of the  $A_{2A}$  R interior in a biotinylation assay. Overall, we show that cholesterol's impact on  $A_{2A}$  R-binding affinity goes beyond pure allosteric modulation and unveils a new interaction mode between cholesterol and the  $A_{2A}$  R that could potentially apply to other GPCRs.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research area: Computational Physics, Charité-Universitätsmedizin Berlin, Universidad de Castilla-La Mancha, Universitat Pompeu Fabra

Contributors: Guixà-González, R., Albasanz, J. L., Rodríguez-Espigares, I., Pastor, M., Sanz, F., Martí-Solano, M., Manna, M., Martínez-Seara, H., Hildebrand, P. W., Martín, M., Selent, J.

Publication date: 21 Feb 2017

Peer-reviewed: Yes

#### Publication information

Journal: Nature Communications

Volume: 8

Article number: 14505

ISSN (Print): 2041-1723

Ratings:

Scopus rating (2017): CiteScore 12.41 SJR 6.582 SNIP 2.934

Original language: English

ASJC Scopus subject areas: Chemistry(all), Biochemistry, Genetics and Molecular Biology(all), Physics and Astronomy(all)

Electronic versions:

Membrane cholesterol access into a G-protein-coupled receptor

DOIs:

10.1038/ncomms14505

URLs:

<http://urn.fi/URN:NBN:fi:tty-201703081123>

Source: Scopus

Source ID: 85013391445

### **Magnetic routing of light-induced waveguides**

Among photofunctional materials that can be employed to control the propagation of light by modifying their properties, soft dielectrics such as nematic liquid crystals (NLCs) stand out for their large all-optical response. Through reorientation, the molecular distribution of NLCs can be modified by the electric field of light, permitting functional operations and supporting self-localized light beams or spatial optical solitons. To date, the generation and routing of such solitons have been limited by the boundary conditions employed to tailor the properties of NLCs in planar cells or capillaries. Here we report on spatial solitons in bulk NLCs with no lateral anchoring, where the application of an external magnetic field effectively controls the direction of propagation and the angular steering of the self-trapped wavepackets. Our results entail a completely new approach to the routing of self-localized beams and light-induced waveguides in three dimensions, without the usual limitations imposed by transverse boundary conditions.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Australian National University, Nonlinear Optics and OptoElectronics Lab, University "Roma Tre", Texas A and M University at Qatar

Contributors: Izdebskaya, Y., Shvedov, V., Assanto, G., Krolikowski, W.

Publication date: 15 Feb 2017

Peer-reviewed: Yes

#### **Publication information**

Journal: Nature Communications

Volume: 8

Article number: 14452

ISSN (Print): 2041-1723

Ratings:

Scopus rating (2017): CiteScore 12.41 SJR 6.582 SNIP 2.934

Original language: English

ASJC Scopus subject areas: Chemistry(all), Biochemistry, Genetics and Molecular Biology(all), Physics and Astronomy(all)

Electronic versions:

Magnetic routing of light-induced waveguides

DOIs:

10.1038/ncomms14452

URLs:

<http://urn.fi/URN:NBN:fi:tty-201703081124>

Source: Scopus

Source ID: 85012921190

Research output: Contribution to journal › Article › Scientific › peer-review

### **Benchmarking DFT methods with small basis sets for the calculation of halogen-bond strengths**

In recent years, halogen bonding has become an important design tool in crystal engineering, supramolecular chemistry and biosciences. The fundamentals of halogen bonding have been studied extensively with high-accuracy computational methods. Due to its non-covalency, the use of triple-zeta (or larger) basis sets is often recommended when studying halogen bonding. However, in the large systems often encountered in supramolecular chemistry and biosciences, large basis sets can make the calculations far too slow. Therefore, small basis sets, which would combine high computational speed and high accuracy, are in great demand. This study focuses on comparing how well density functional theory (DFT) methods employing small, double-zeta basis sets can estimate halogen-bond strengths. Several methods with triple-zeta basis sets are included for comparison. Altogether, 46 DFT methods were tested using two data sets of 18 and 33 halogen-bonded complexes for which the complexation energies have been previously calculated with the high-accuracy CCSD(T)/CBS method. The DGDZVP basis set performed far better than other double-zeta basis sets, and it even outperformed the triple-zeta basis sets. Due to its small size, it is well-suited to studying halogen bonding in large systems.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Siiskonen, A., Priimägi, A.

Publication date: 1 Feb 2017

Peer-reviewed: Yes

#### **Publication information**



Journal: Journal of Molecular Modeling

Volume: 23

Issue number: 2

Article number: 50

ISSN (Print): 1610-2940

Ratings:

Scopus rating (2017): CiteScore 1.17 SJR 0.36 SNIP 0.515

Original language: English

ASJC Scopus subject areas: Catalysis, Computer Science Applications, Physical and Theoretical Chemistry, Organic Chemistry, Computational Theory and Mathematics, Inorganic Chemistry

Keywords: Basis set, Benchmarking, Density functional theory, Halogen bonding

DOIs:

10.1007/s00894-017-3212-4

Source: Scopus

Source ID: 85011684872

Research output: Contribution to journal > Article > Scientific > peer-review

### **Polarization resolved photoluminescence in GaAs<sub>1-x</sub>Bi<sub>x</sub>/GaAs quantum wells**

We have investigated polarization resolved photoluminescence (PL) of GaAs<sub>1-x</sub>Bi<sub>x</sub>/GaAs quantum wells (QWs) with different Bi concentrations in the dilute range ( $x < 10^{-2}$ ). The PL intensity of GaAs<sub>1-x</sub>Bi<sub>x</sub> QWs increase with the increase of Bi concentration. Excitonic  $g_{ex}$ -factors of 4 and 10 were obtained at 15 T for as-grown GaAs<sub>1-x</sub>Bi<sub>x</sub>/GaAs QWs with 1.2% and 1.9% Bi concentration, respectively. These values evidence an important increase of electron and hole g-factors with the introduction of Bi in GaAs.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications, Universidade Federal de São Carlos, University of Nottingham, Universidade Federal de São Carlos

Contributors: Balanta, M. A. G., Orsi Gordo, V., Carvalho, A. R. H., Puustinen, J., Alghamdi, H. M., Henini, M., Galeti, H. V. A., Guina, M., Galvão Gobato, Y.

Number of pages: 4

Pages: 49-52

Publication date: Feb 2017

Peer-reviewed: Yes

Early online date: 13 Oct 2016

#### **Publication information**

Journal: Journal of Luminescence

Volume: 182

ISSN (Print): 0022-2313

Ratings:

Scopus rating (2017): CiteScore 2.72 SJR 0.694 SNIP 1.075

Original language: English

ASJC Scopus subject areas: Biophysics, Chemistry(all), Atomic and Molecular Physics, and Optics, Biochemistry, Condensed Matter Physics

DOIs:

10.1016/j.jlumin.2016.10.008

Source: Scopus

Source ID: 84992707527

Research output: Contribution to journal > Article > Scientific > peer-review

### **Architectures and codecs for real-time light field streaming**

Light field 3D displays represent a major step forward in visual realism, providing glasses-free spatial vision of real or virtual scenes. Applications that capture and process live imagery have to process data captured by potentially tens to hundreds of cameras and control tens to hundreds of projection engines making up the human perceivable 3D light field using a distributed processing system. The associated massive data processing is difficult to scale beyond a specific number and resolution of images, limited by the capabilities of the individual computing nodes. The authors therefore analyze the bottlenecks and data flow of the light field conversion process and identify possibilities to introduce better scalability. Based on this analysis they propose two different architectures for distributed light field processing. To avoid using uncompressed video data all along the processing chain, the authors also analyze how the operation of the proposed architectures can be supported by existing image/video codecs.

#### **General information**

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Signal Processing, Research group: 3D MEDIA, Holografika, Nokia  
Contributors: Kovács, P. T., Zare, A., Balogh, T., Bregovic, R., Gotchev, A.  
Publication date: 1 Jan 2017  
Peer-reviewed: Yes

### Publication information

Journal: Journal of Imaging Science and Technology

Volume: 61

Issue number: 1

Article number: 010403

ISSN (Print): 1062-3701

Ratings:

Scopus rating (2017): CiteScore 0.59 SJR 0.237 SNIP 0.712

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Chemistry(all), Atomic and Molecular Physics, and Optics, Computer Science Applications

Electronic versions:

LF\_codecs\_1.1

DOIs:

10.2352/J.ImagingSci.Technol.2017.61.1.010403

Source: Scopus

Source ID: 85016298177

Research output: Contribution to journal > Article > Scientific > peer-review

### Improved corrosion properties of Hot Dip Galvanized Steel by nanomolecular silane layers as hybrid interface between zinc and top coatings

Thin organic coatings (TOC) or paints on hot dip galvanized steel (HDGS) improve the corrosion properties and create visually pleasing surfaces. Delamination of these coatings lead to corrosion and peeling of the paints. Hence, a novel method for improved adhesion and corrosion properties for HDGS surfaces is introduced. It is shown how the fabrication of a nanomolecular silane film as an interfacial layer between the HDGS and TOC or paint improves the corrosion properties of HDGS in different pH regimes. Understanding the corrosion behavior of ultra-thin silane layers under differing pH is crucial as subsequent coatings have different pHs. By varying the silanization parameters two different nanomolecular surface structures of aminopropyl trimethoxysilane (APS) on HDGS were fabricated: well-ordered monolayers with approximately 1 nm thickness and highly clustered APS films with a thickness in the range of 5-8 nm. To verify the nanomolecular APS structures, photoelectron spectroscopy (PES) and contact angle (CA) measurements were employed. The corrosion properties of HDGS and silanized HDGS were studied with linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS). It is shown that at pH 5 and 7 passivation behavior is observed on silanized samples but the most significant improvement in corrosion resistance is found at pH 10 where the corrosion currents of silanized samples are up to two orders of magnitude lower than on uncoated metallic samples. Also, it is demonstrated that the corrosion inhibition of APS is not only dependent on the thickness of the silane film, but also the molecular ordering at the surface. The thin, well-ordered APS monolayer is more resistant towards corrosion in NaCl solution (pH 7) than thicker clustered APS layer. This indicates that the highly ordered nanomolecular surface structure protects the HDGS-silane interface from the Cl<sup>-</sup> adsorption better than the thicker, but more randomly ordered APS layers. Nanomolecular interfacial silane films for enhanced corrosion and adhesion properties on HDGS are transferrable to industrial production lines providing a low cost and environmentally friendly method for improved HDGS products.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Surface Science, MAX IV Laboratory, Lund University

Contributors: Vuori, L., Ali-Löytty, H., Lahtonen, K., Hannula, M., Lehtonen, E., Niu, Y., Valden, M.

Publication date: 2017

Peer-reviewed: Yes

### Publication information

Journal: Corrosion

Volume: 73

Issue number: 2

ISSN (Print): 0010-9312

Ratings:

Scopus rating (2017): CiteScore 1.95 SJR 0.955 SNIP 1.376

Original language: English

ASJC Scopus subject areas: Surfaces and Interfaces, Surfaces, Coatings and Films, Electrochemistry

DOIs:

10.5006/2206

Research output: Contribution to journal > Article > Scientific > peer-review

### **Synthesis, Structural Characterization, Hirshfeld Surface and Antioxidant Activity Analysis of a Novel Organic Cation Antimonate Complex**

A new organic–inorganic hybrid material of formula  $(C_{10}H_{15}N_2)_7 Sb_2Cl_{10} Sb_2Cl_9 (SbCl_5)_2 SbCl_4 \cdot 2Cl \cdot 7H_2O$  was synthesized and characterized by an X-ray diffraction analysis. It crystallizes in the triclinic system with the P (Formula presented.) space group and the following unit cell parameters  $a = 11.8127(3) \text{ \AA}$ ,  $b = 15.7557(4) \text{ \AA}$ ,  $c = 35.4511(8) \text{ \AA}$ ,  $\alpha = 89.409(1)^\circ$ ,  $\beta = 84.04(1)^\circ$ ,  $\gamma = 71.116(1)^\circ$ ,  $Z = 2$  and  $V = 6207.3(3) \text{ \AA}^3$ . The examination of the structure shows that the two dimensional frameworks are produced by O–H...Cl, N–H...Cl and N–H...O hydrogen bonding. In addition, the most important features of crystal packing and intermolecular interactions in the title complex were quantified via Hirshfeld surface analysis. Differential scanning calorimetry has revealed a dehydration phenomenon at around 348 K. The investigation of the antioxidant activity of the title compound was carried out using the 2,2-diphenyl-1-picrylhydrazyl and ferrous iron chelating methods.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Carthage University

Contributors: Lahbib, I., Valkonen, A., Rzaigui, M., Smirani, W.

Number of pages: 14

Pages: 2239–2252

Publication date: 2017

Peer-reviewed: Yes

Early online date: 29 Apr 2017

#### **Publication information**

Journal: Journal of Cluster Science

Volume: 28

Issue number: 4

ISSN (Print): 1040-7278

Ratings:

Scopus rating (2017): CiteScore 1.4 SJR 0.332 SNIP 0.455

Original language: English

ASJC Scopus subject areas: Chemistry(all), Biochemistry, Materials Science(all), Condensed Matter Physics

Keywords: Antimonates, Antioxidant activity, Crystal structure, Hirshfeld surface, Photoluminescence

DOIs:

10.1007/s10876-017-1217-x

Source: Scopus

Source ID: 85018336645

Research output: Contribution to journal > Article > Scientific > peer-review

### **Effects of orientation at the phthalocyanine–CdSe interface on the electron transfer characteristics**

A phthalocyanine molecule adsorbed on the (1010) surface of wurtzite CdSe is theoretically modeled by the DFT method. We have found that a linker does not affect substantially the redox properties of phthalocyanine, while saturation of the macrocycle with peripheral substituent groups causes a downward shift in the energy position of its frontier orbitals that can hinder electron injection to the CdSe surface. Tilting of the phthalocyanine molecule relative to the surface also leads to the lowering of its molecular electronic levels relative to the bands of CdSe. At a tilting angle of  $30^\circ$ , the LUMO level of the dye appears to be lower than the conduction band minimum of cadmium selenide, which makes the electron transfer to its hybridized surface unfavorable. By contrast, the HOMO level of the phenylbutyric acid linker provides a suitable intermediate channel for the hole transfer from the valence band of CdSe to the phthalocyanine that points to the possible acceptor behavior of the phthalocyanine molecule in its hybrids with CdSe nanostructures.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Research

group: Electronic Structure Theory, Research area: Computational Physics, Center of Innovation Technologies

Contributors: Golovanov, V. V., Nazarchuk, B. V., Golovanova, V. V., Tkachenko, N. V., Rantala, T. T.

Number of pages: 7

Pages: 10511-10517

Publication date: 2017

Peer-reviewed: Yes

### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 19

Issue number: 16

ISSN (Print): 1463-9076

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ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1039/c7cp00833c

Source: Scopus

Source ID: 85019969347

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

### High-resolution coded-aperture design for compressive X-ray tomography using low resolution detectors

One of the main challenges in Computed Tomography (CT) is obtaining accurate reconstructions of the imaged object while keeping a low radiation dose in the acquisition process. In order to solve this problem, several researchers have proposed the use of compressed sensing for reducing the amount of measurements required to perform CT. This paper tackles the problem of designing high-resolution coded apertures for compressed sensing computed tomography. In contrast to previous approaches, we aim at designing apertures to be used with low-resolution detectors in order to achieve super-resolution. The proposed method iteratively improves random coded apertures using a gradient descent algorithm subject to constraints in the coherence and homogeneity of the compressive sensing matrix induced by the coded aperture. Experiments with different test sets show consistent results for different transmittances, number of shots and super-resolution factors.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Signal Processing

Contributors: Mojica, E., Pertuz, S., Arguello, H.

Pages: 103-109

Publication date: 2017

Peer-reviewed: Yes

### Publication information

Journal: Optics Communications

Volume: 404

ISSN (Print): 0030-4018

Ratings:

Scopus rating (2017): CiteScore 1.86 SJR 0.614 SNIP 0.933

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics, Physical and Theoretical Chemistry, Electrical and Electronic Engineering

Keywords: Coded apertures, Compressive sensing, Computed tomography, Super-resolution

DOIs:

10.1016/j.optcom.2017.06.053

Source: Scopus

Source ID: 85021667000

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

### Crystallization and sintering of borosilicate bioactive glasses for application in tissue engineering

Typical silicate bioactive glasses are known to crystallize readily during the processing of porous scaffolds. While such crystallization does not fully suppress the bioactivity, the presence of significantly large amounts of crystals leads to a decrease in the rate of reaction of the glass and an uncontrolled release of ions. Furthermore, due to the non-congruent dissolution of silicate glasses, these materials have been shown to remain within the surgical site even 14 years post-operation. Therefore, bioactive materials that can dissolve more effectively and have higher conversion rates are required. Within this work, boron was introduced, in the FDA approved S53P4 glass, at the expense of  $\text{SiO}_2$ . The crystallization and sintering-ability of the newly developed glasses were investigated by differential thermal analysis. All the glasses were found to crystallize primarily from the surface, and the crystal phase precipitation was dependent on the quantity of  $\text{B}_2\text{O}_3$  incorporated. The rate of crystallization was found to be lower for the glasses when 25, 50 and 75% of  $\text{SiO}_2$  was replaced with  $\text{B}_2\text{O}_3$ . These glasses were further sintered into porous scaffolds using simple heat sintering. The impact of glass

particle size and heat treatment temperature on the scaffold porosity and average pore size was investigated. Scaffolds with porosity ranging from 10 to 60% and compressive strength ranging from 1 to 35 MPa were produced. The scaffolds remained amorphous during processing and their ability to rapidly precipitate hydroxycarbonate apatite was maintained. This is of particular interest in the field of tissue engineering as scaffold degradation and reaction is generally faster and offers higher controllability as opposed to the current partially/fully crystallized scaffolds obtained from the FDA approved bioactive glasses.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Photonics Glasses, Faculty of Biomedical Sciences and Engineering, Research group: Computational Biophysics and Imaging Group, Materials Science, Research group: Biomaterials and Tissue Engineering Group, BioMediTech, Department of Mining and Metallurgical Engineering, UMR CNRS 6226 Sciences Chimiques de Rennes, University of Witwatersrand, University of Namibia, Department of Chemistry and Bioengineering

Contributors: Fabert, M., Ojha, N., Erasmus, E., Hannula, M., Hokka, M., Hyttinen, J., Rocherullé, J., Sigalas, I., Massera, J.

Number of pages: 12

Pages: 4514-4525

Publication date: 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Materials Chemistry B

Volume: 5

Issue number: 23

ISSN (Print): 2050-7518

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Scopus rating (2017): CiteScore 4.95 SJR 1.561 SNIP 1.024

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ASJC Scopus subject areas: Chemistry(all), Medicine(all), Biomedical Engineering, Materials Science(all)

DOIs:

10.1039/c7tb00106a

#### Bibliographical note

INT=keb,"Fabert, M."

Source: Scopus

Source ID: 85021668458

Research output: Contribution to journal > Article > Scientific > peer-review

#### Two cations, two mechanisms: Interactions of sodium and calcium with zwitterionic lipid membranes

Adsorption of metal cations onto a cellular membrane changes its properties, such as interactions with charged moieties or the propensity for membrane fusion. It is, however, unclear whether cells can regulate ion adsorption and the related functions via locally adjusting their membrane composition. We employed fluorescence techniques and computer simulations to determine how the presence of cholesterol - a key molecule inducing membrane heterogeneity - affects the adsorption of sodium and calcium onto zwitterionic phosphatidylcholine bilayers. We found that the transient adsorption of sodium is dependent on the number of phosphatidylcholine head groups, while the strong surface binding of calcium is determined by the available surface area of the membrane. Cholesterol thus does not affect sodium adsorption and only plays an indirect role in modulating the adsorption of calcium by increasing the total surface area of the membrane. These observations also indicate how lateral lipid heterogeneity can regulate various ion-induced processes including adsorption of peripheral proteins, nanoparticles, and other molecules onto membranes.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, University of Helsinki, J. Heyrovský Institute of Physical Chemistry, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Javanainen, M., Melcrová, A., Magarkar, A., Jurkiewicz, P., Hof, M., Jungwirth, P., Martinez-Seara, H.

Number of pages: 4

Pages: 5380-5383

Publication date: 2017

Peer-reviewed: Yes

#### Publication information

Journal: Chemical Communications

Volume: 53

Issue number: 39  
ISSN (Print): 1359-7345  
Ratings:

Scopus rating (2017): CiteScore 6.03 SJR 2.555 SNIP 1.127

Original language: English

ASJC Scopus subject areas: Catalysis, Electronic, Optical and Magnetic Materials, Ceramics and Composites, Chemistry(all), Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry

Electronic versions:

c7cc02208e

DOIs:

10.1039/c7cc02208e

URLs:

<http://urn.fi/URN:NBN:fi:tty-201712202418>

Source: Scopus

Source ID: 85021689400

Research output: Contribution to journal > Article > Scientific > peer-review

### **Supramolecular control of liquid crystals by doping with halogen-bonding dyes**

Introducing photochromic or polymeric dopants into nematic liquid crystals is a well-established method to create stimuli-responsive photonic materials with the ability to "control light with light". Herein, we demonstrate a new material design concept by showing that specific supramolecular interactions between the host liquid crystal and the guest dopants enhance the optical performance of the doped liquid crystals. By varying the type and strength of the dopant-host interaction, the phase-transition temperature, the order parameter of the guest molecules, and the diffraction signal in response to interference irradiation, can be accurately engineered. Our concept points out the potential of supramolecular interactions in liquid-crystal photonics, being valuable for optimizing the design of dye-doped functional liquid-crystalline systems.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials, Département de Chimie, Succ. Centre-Ville, Politecnico di Milano, Università degli Studi di Milano, Tokyo Institute of Technology, VTT Technical Research Centre of Finland

Contributors: Vapaavuori, J., Siiskonen, A., Dichiarante, V., Forni, A., Saccone, M., Pilati, T., Pellerin, C., Shishido, A., Metrangolo, P., Priimagi, A.

Number of pages: 6

Pages: 40237-40242

Publication date: 2017

Peer-reviewed: Yes

#### **Publication information**

Journal: RSC Advances

Volume: 7

Issue number: 64

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2017): CiteScore 3.01 SJR 0.863 SNIP 0.736

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

Electronic versions:

c7ra06397k

DOIs:

10.1039/c7ra06397k

URLs:

<http://urn.fi/URN:NBN:fi:tty-201712122322>

Source: Scopus

Source ID: 85028088976

Research output: Contribution to journal > Article > Scientific > peer-review

### **Photoresponsive ionic liquid crystals assembled: Via halogen bond: En route towards light-controllable ion transporters**

We demonstrate that halogen bonding (XB) can offer a novel approach for the construction of photoresponsive ionic liquid crystals. In particular, we assembled two new supramolecular complexes based on 1-ethyl-3-methylimidazolium iodides and azobenzene derivatives containing an iodotetrafluoro-benzene ring as XB donor, where the iodide anion acted as an XB acceptor. DSC and X-ray diffraction analyses revealed that the preferred stoichiometry between the XB donors and

acceptors is 2:1, and that the iodide anions act as bidentate XB-acceptors, binding two azobenzene derivatives. Due to the high directionality of the XB, calamitic superanions are obtained, while the segregation occurring between the charged and uncharged parts of the molecules gives rise to a layered structure in the crystal lattice. Despite the fact that the starting materials are non-mesomorphic, the halogen-bonded supramolecular complexes exhibited monotropic lamellar liquid-crystalline phases over broad temperature ranges, as confirmed with polarized optical microscopy. Due to the presence of the azobenzene moieties, the LCs were photoresponsive, and a LC-to-isotropic phase transition could be obtained by irradiation with UV light. We envisage that the light-induced phase transition, in combination with the ionic nature of the LC, provides a route towards light-induced control over ion transport and conductance in these supramolecular complexes.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Politecnico di Milano, Aalto University

Contributors: Saccone, M., Palacio, F. F., Cavallo, G., Dichiarante, V., Virkki, M., Terraneo, G., Priimagi, A., Metrangolo, P.

Number of pages: 16

Pages: 407-422

Publication date: 2017

Peer-reviewed: Yes

#### Publication information

Journal: Faraday Discussions

Volume: 203

ISSN (Print): 1359-6640

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1039/c7fd00120g

Source: Scopus

Source ID: 85031726639

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

#### Photophysical properties of porphyrin dimer-single-walled carbon nanotube linked systems

Porphyrin dimers were covalently grafted onto electron-accepting single-walled carbon nanotube (SWNT) sidewalls by direct aryl radical addition reaction with an m-or p-phenylene linker with the help of p-p interaction between the porphyrins. A splitting of the porphyrin Soret band and DFT calculations supported the selective formation of the porphyrin dimers on the sidewall of SWNTs. Photoexcitation of the porphyrin dimers on the SWNT resulted in the formation of the exciplex state, which directly decayed to the ground state without yielding the complete charge-separated state. Lifetimes of the porphyrin dimer-SWNT exciplex were longer than that of a porphyrin monomer-SWNT exciplex due to the stabilization by p-electron interaction over two porphyrin rings. In addition, the weaker electronic coupling through the meta-linkage than the para-one may be responsible for the exciplex lifetime of the porphyrin dimer-SWNT with the m-phenylene linker (49 ps) longer than that with the p-phenylene one (24 ps). The results obtained here provide the basic information on the effect of the donor dimerization on the photodynamic behavior of the exciplex state in donor-acceptor linked systems. [Figure presented]

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Kyoto Women's University

Contributors: Baek, J., Umeyama, T., Mizuno, S., Tkachenko, N. V., Imahori, H.

Publication date: 2017

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 121

Issue number: 39

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.135

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Physical and Theoretical Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/acs.jpcc.7b08594

Source: Scopus

Source ID: 85032629899

Research output: Contribution to journal › Article › Scientific › peer-review

### **Design of a 25 MWe Solar Thermal Power Plant in Iran with Using Parabolic Trough Collectors and a Two-Tank Molten Salt Storage System**

Nowadays, parabolic trough solar thermal plants are prevalent around the world. In different areas concerning the amount of solar radiation, their standard size is approximately between 20 and 100 MWe. Certainly, the right size of the solar field is the first selection with regard to nominal electrical power. A vast area will be economically unreasonable whereas a small area will mainly cause the power plant to operate at the part-load condition. This paper presents an economic modeling of a solar parabolic trough plant, operating at 25 MWe in Yazd, Iran. The varying types of collector dimensions have been investigated; then, by selecting autumnal equinox (22 September) at 12:00 PM as the design point, thermal performance of the solar power plant has been featured annually, in all conditions. The total operating time of the power plant is about 1726 hours (1248 hours in full-load condition). In the end, the effect of thermal storage tanks has been analyzed to save extra solar heat and use it at nights in hot months. By implementing a storage system, the total operating time will be increased to 3169 hours (2785 in full-load condition). Moreover, 7974 GJ useful thermal energy can be obtained from the solar field and storage system.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Automation and Hydraulic Engineering, University of Guilan

Contributors: Kordmahaleh, A. A., Naghashzadegan, M., Javaherdeh, K., Khoshgoftar, M.

Publication date: 2017

Peer-reviewed: Yes

#### **Publication information**

Journal: International Journal of Photoenergy

Volume: 2017

Article number: 4210184

ISSN (Print): 1110-662X

Ratings:

Scopus rating (2017): CiteScore 1.18 SJR 0.341 SNIP 0.605

Original language: English

ASJC Scopus subject areas: Chemistry(all), Atomic and Molecular Physics, and Optics, Renewable Energy, Sustainability and the Environment, Materials Science(all)

Electronic versions:

4210184

DOIs:

10.1155/2017/4210184

URLs:

<http://urn.fi/URN:NBN:fi:tty-201801081036>

#### **Bibliographical note**

INT=aut,"Kordmahaleh, Aidin Alinezhad"

Source: Scopus

Source ID: 85038904387

Research output: Contribution to journal › Article › Scientific › peer-review

### **Particle emissions characterization from a medium-speed marine diesel engine with two fuels at different sampling conditions**

Particle emission characteristics for a medium-speed four-stroke marine diesel engine were studied using a variety of sampling systems. Measurements were conducted at 25% and 75% load employing a heavy fuel oil (HFO) and a lighter marine distillate oil. The measurements, especially with HFO, revealed that marine exhaust particles mostly consist of nanometer sized ash particles on which heavy volatile species condense during exhaust dilution and cooling. The soot mode number concentration was low with both fuels tested, in particular when HFO was used. Total particle number emissions ranged in the order of  $5.2\text{--}6.9 \times 10^{15}$  per kg of fuel and formed a monomodal size distribution when a porous tube diluter combined with an ageing chamber and operating at low dilution ratio was used for sampling. The levels and size distributions obtained in the lab using a porous tube diluter were similar to the ones reported in the literature studying ship plumes following atmospheric dilution. Lab measurements with ejector-type diluters mostly led to bi-modal distributions that did not well resemble atmospheric size distributions. Moreover, the nucleation mode formed with the ejector diluters was variable in size and concentration. When used with dilution air at ambient temperature, ejector diluters were inappropriate for primary dilution due to clogging.



### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Aerosol Physics Laboratory, VTT Technical Research Centre of Finland, Finnish Meteorological Institute

Contributors: Ntziachristos, L., Saukko, E., Lehtoranta, K., Rönkkö, T., Timonen, H., Simonen, P., Karjalainen, P., Keskinen, J.

Number of pages: 10

Pages: 456-465

Publication date: 15 Dec 2016

Peer-reviewed: Yes

### Publication information

Journal: Fuel

Volume: 186

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2016): CiteScore 4.9 SJR 1.736 SNIP 2.185

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Fuel Technology, Energy Engineering and Power Technology, Organic Chemistry

Keywords: Heavy fuel oil, Light fuel oil, Marine emissions, Particle emissions, Soot particles

DOIs:

10.1016/j.fuel.2016.08.091

Source: Scopus

Source ID: 84984817885

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

### Optimization of HVOF Cr<sub>3</sub>C<sub>2</sub>-NiCr coating for increased fatigue performance

Thermally sprayed coatings are strong candidates to be used for replacement of hard chromium – process which is regarded as an environmental risk – in many sliding surfaces for engineering applications such as hydraulic cylinders and aircraft landing gears. Recent advance in thermal spraying technology, based on the increase of the spray particle velocity, has led to improved coating quality. This study focuses on the fatigue performance of structural steel coated with Cr<sub>3</sub>C<sub>2</sub>[Formula presented] coating. Coating has been produced by using high kinetic HVOF thermal spray process. First, the coating was optimized for fatigue purposes by studying the residual stress generation. The optimized coating was selected for deposition of axial fatigue tests specimens, whose fatigue performance was compared to the uncoated steel specimens having different surface treatments (turning, polishing, and shot blasting) relevant for the target applications. The results showed that by using a high kinetic energy coating, the fatigue performance of Cr<sub>3</sub>C<sub>2</sub>[Formula presented] coated structural steel was clearly improved compared to uncoated steel of similar surface quality. Increased fatigue resistance of the coated material was attributed to the substantial compressive residual stresses that hindered crack initiation and that was caused by the high velocity spray particles during the coating process.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Surface Engineering, VTT Technical Research Centre of Finland, Aalto University, Technical University of Liberec

Contributors: Varis, T., Suhonen, T., Calonijs, O., Čuban, J., Pietola, M.

Number of pages: 9

Pages: 123-131

Publication date: 15 Nov 2016

Peer-reviewed: Yes

### Publication information

Journal: Surface and Coatings Technology

Volume: 305

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2016): CiteScore 2.56 SJR 0.882 SNIP 1.379

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry

Keywords: CrC[Formula presented] coating, Fatigue performance, HVOF thermal spray, Residual stress, S-N curve, Wear resistance

DOIs:

10.1016/j.surfcoat.2016.08.012

Source: Scopus

Source ID: 84981273135

Research output: Contribution to journal > Article > Scientific > peer-review

### **Collective excitations and viscosity in liquid Bi**

The analysis of extensive density functional/molecular dynamics simulations (over 500 atoms, up to 100 ps) of liquid bismuth at four temperatures between 573 K and 1023 K has provided details of the dynamical structure factors, the dispersion of longitudinal and transverse collective modes, and related properties (power spectrum, viscosity, and sound velocity). Agreement with available inelastic x-ray and neutron scattering data and with previous simulations is generally very good. The results show that density functional/molecular dynamics simulations can give dynamical information of good quality without the use of fitting functions, even at long wavelengths.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Research group: Materials and Molecular Modeling, Forschungszentrum Jülich (FZJ)

Contributors: Ropo, M., Akola, J., Jones, R. O.

Publication date: 14 Nov 2016

Peer-reviewed: Yes

### **Publication information**

Journal: Journal of Chemical Physics

Volume: 145

Issue number: 18

Article number: 184502

ISSN (Print): 0021-9606

Ratings:

Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 1.003

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1063/1.4965429

URLs:

<http://www.scopus.com/inward/record.url?scp=84994735177&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84994735177

Research output: Contribution to journal > Article > Scientific > peer-review

### **Improvement of actuation performance of dielectric elastomers by barium titanate and carbon black fillers**

Dielectric elastomers are promising materials for actuators resembling human muscle. Among elastomers, acrylic rubbers (ACM) have shown good actuation performance but its use is limited by the high operating voltages required. The present work demonstrates that simultaneous incorporation of nanostructured carbon black and dielectric fillers offers an increase in a dielectric permittivity and a suitable modulus of the elastomers matrix, enabling an improved electro-mechanical actuation performance at low voltages. By the use of reinforcing carbon black and barium titanate in an acrylic elastomer matrix a sixfold increase in the dielectric permittivity was realized. A fine tuning of the actuation stress and, consequently, actuation strain can be done by a judicious selection of the different filler concentrations in the soft rubber matrix. Finally, a synergistic effect of the fillers was observed in the improved actuation performance of the developed materials. This work may pave the way to design dielectric elastomers for actuator fabrication.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Leibniz-Institut für Polymerforschung Dresden E.V.

Contributors: Poikelispää, M., Shakun, A., Das, A., Vuorinen, J.

Publication date: 10 Nov 2016

Peer-reviewed: Yes

### **Publication information**

Journal: Journal of Applied Polymer Science

Volume: 133

Issue number: 42

Article number: 44116  
ISSN (Print): 0021-8995  
Ratings:

Scopus rating (2016): CiteScore 1.73 SJR 0.588 SNIP 0.815

Original language: English

ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry

Keywords: actuators, dielectric properties, elastomers

Electronic versions:

poikelispaa\_Improvement of actuation performance of dielectric elastomers by barium titanate and carbon black fillers.

Embargo ended: 11/07/17

DOIs:

10.1002/app.44116

URLs:

<http://urn.fi/URN:NBN:fi:tty-201701051021>

Source: Scopus

Source ID: 84982792344

Research output: Contribution to journal > Article > Scientific > peer-review

### **Grain orientation dependent Nb-Ti microalloying mediated surface segregation on ferritic stainless steel**

Surface segregation and oxide formation anisotropy on Ti-Nb stabilized ferritic stainless steel (EN 1.4521) were studied by XPS and Electron Backscatter Diffraction. Competitive surface segregation of Si, Nb and Ti was initiated at ~550. °C, and segregation was favored to the open surface sites of  $\langle 111 \rangle$  oriented grains. Furthermore, the surface segregation of Cr was strongly limited at the locations of stable Ti(CN)- and (NbTi)C-type precipitates. Consequently, the oxidation resistance of stainless steels can be enhanced cost-efficiently, without alloy additions, by optimizing the microstructure to facilitate the fast and uniform growth of protective oxide scale.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Surface Science, Department of Materials Science,

Research group: Materials Characterization

Contributors: Ali-Löyty, H., Hannula, M., Honkanen, M., Östman, K., Lahtonen, K., Valden, M.

Pages: 204-213

Publication date: Nov 2016

Peer-reviewed: Yes

#### **Publication information**

Journal: Corrosion Science

Volume: 112

ISSN (Print): 0010-938X

Ratings:

Scopus rating (2016): CiteScore 5.19 SJR 1.891 SNIP 2.459

Original language: English

ASJC Scopus subject areas: Materials Science(all), Chemical Engineering(all), Chemistry(all)

Keywords: A. Stainless steel, B. SEM, B. XPS, C. Interfaces, C. Oxidation, C. Segregation

DOIs:

10.1016/j.corsci.2016.07.024

Source: Scopus

Source ID: 84979753478

Research output: Contribution to journal > Article > Scientific > peer-review

### **UPS and DFT investigation of the electronic structure of gas-phase trimesic acid**

Benzene-1,3,5-tricarboxylic acid (trimesic acid, TMA) molecules in gas-phase have been investigated by using valence band photoemission. The photoelectron spectrum in the binding energy region from 9 to 22 eV is interpreted based on the density functional theory calculations. The electronic configuration that makes contribution to each transition is demonstrated. Furthermore, electronic structure of TMA is compared with benzene and benzoic acid (BA) in order to demonstrate changes in molecular orbital energies induced by addition of carboxyl groups to benzene ring.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Surface Science, University of Tartu, MAX IV Laboratory, Lund University

Contributors: Reisberg, L., Pärna, R., Kikas, A., Kuusik, I., Kisand, V., Hirsimäki, M., Valden, M., Nõmmiste, E.  
Number of pages: 6  
Pages: 11-16  
Publication date: Nov 2016  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Electron Spectroscopy and Related Phenomena

Volume: 213

ISSN (Print): 0368-2048

Ratings:

Scopus rating (2016): CiteScore 1.72 SJR 0.852 SNIP 0.731

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Atomic and Molecular Physics, and Optics

Keywords: trimesic acid, molecules, electronic structure, synchrotron radiation, MAX IV Laboratory, UPS, DFT, organic acids, gas-phase, spectroscopy, photoemission

Electronic versions:

Author's post-print accepted manuscript. Embargo ended: 18/10/18

DOIs:

10.1016/j.elspec.2016.10.004

URLs:

<http://urn.fi/URN:NBN:fi:tty-201612094854>. Embargo ended: 18/10/18

Research output: Contribution to journal > Article > Scientific > peer-review

#### Increased survival rate by local release of diclofenac in a murine model of recurrent oral carcinoma

Despite aggressive treatment with radiation and combination chemotherapy following tumor resection, the 5-year survival rate for patients with head and neck cancer is at best only 50%. In this study, we examined the therapeutic potential of localized release of diclofenac from electrospun nanofibers generated from poly(d,l-lactide-co-glycolide) polymer. Diclofenac was chosen since anti-inflammatory agents that inhibit cyclooxygenase have shown great potential in their ability to directly inhibit tumor growth as well as suppress inflammation-mediated tumor growth. A mouse resection model of oral carcinoma was developed by establishing tumor growth in the oral cavity by ultrasound-guided injection of 1 million SCC-9 cells in the floor of the mouth. Following resection, mice were allocated into four groups with the following treatment: 1) no treatment, 2) implanted scaffolds without diclofenac, 3) implanted scaffolds loaded with diclofenac, and 4) diclofenac given orally. Small animal ultrasound and magnetic resonance imaging were utilized for longitudinal determination of tumor recurrence. At the end of 7 weeks following tumor resection, 33% of mice with diclofenac-loaded scaffolds had a recurrent tumor, in comparison to 90%-100% of the mice in the other three groups. At this time point, mice with diclofenac-releasing scaffolds showed 89% survival rate, while the other groups showed survival rates of 10%-25%. Immunohistochemical staining of recurrent tumors revealed a near 10-fold decrease in the proliferation marker Ki-67 in the tumors derived from mice with diclofenac-releasing scaffolds. In summary, the local application of diclofenac in an orthotopic mouse tumor resection model of oral cancer reduced tumor recurrence with significant improvement in survival over a 7-week study period following tumor resection. Local drug release of anti-inflammatory agents should be investigated as a therapeutic option in the prevention of tumor recurrence in oral squamous carcinoma.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Electronics and Communications Engineering, Clinic for Radiology and Neuroradiology, University Hospital Schleswig-Holstein, Institute of Biochemistry, University Hospital Cologne

Contributors: Will, O. M., Purcz, N., Chalaris, A., Heneweer, C., Boretius, S., Purcz, L., Nikkola, L., Ashammakhi, N., Kalthoff, H., Glüer, C. C., Wiltfang, J., Açil, Y., Tiwari, S.

Number of pages: 11

Pages: 5311-5321

Publication date: 12 Oct 2016

Peer-reviewed: Yes

#### Publication information

Journal: International Journal of Nanomedicine

Volume: 11

ISSN (Print): 1176-9114

Ratings:

Scopus rating (2016): CiteScore 4.55 SJR 1.174 SNIP 1.211

Original language: English

ASJC Scopus subject areas: Bioengineering, Biophysics, Biomaterials, Drug Discovery, Organic Chemistry

Keywords: Drug releasing polymers, Head and neck cancer, Mouse model, NSAIDs, Oral squamous cell carcinoma, Tumor recurrence

Electronic versions:

IJN-109199-increased-survival-rate-by-local-release-of-diclofenac-in-a-\_101216

DOIs:

10.2147/IJN.S109199

URLs:

<http://urn.fi/URN:NBN:fi:ty-201611304830>

Source: Scopus

Source ID: 84991726470

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Elimination of arsenic-containing emissions from gasification of chromated copper arsenate wood**

The behavior of arsenic in chromated copper arsenate containing wood during gasification was modeled using thermodynamic equilibrium calculations. The results of the model were validated using bench-scale gasification tests. It is shown that over 99.6% of arsenic can be removed from the product gas by a hot filter when the gas is cooled below the predicted condensation temperature.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Energy Technology and Thermal Process Chemistry, Gasification Technologies Inc., Gas Technology Institute

Contributors: Kramb, J., Kontinen, J., Backman, R., Salo, K., Roberts, M.

Number of pages: 6

Pages: 319-324

Publication date: 1 Oct 2016

Peer-reviewed: Yes

#### **Publication information**

Journal: Fuel

Volume: 181

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2016): CiteScore 4.9 SJR 1.736 SNIP 2.185

Original language: English

ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

Keywords: Arsenic, CCA wood, Equilibrium modeling, Gasification

DOIs:

10.1016/j.fuel.2016.04.109

Source: Scopus

Source ID: 84965081806

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Controlling the motion of multiple objects on a Chladni plate**

The origin of the idea of moving objects by acoustic vibration can be traced back to 1787, when Ernst Chladni reported the first detailed studies on the aggregation of sand onto nodal lines of a vibrating plate. Since then and to this date, the prevailing view has been that the particle motion out of nodal lines is random, implying uncontrollability. But how random really is the out-of-nodal-lines motion on a Chladni plate? Here we show that the motion is sufficiently regular to be statistically modelled, predicted and controlled. By playing carefully selected musical notes, we can control the position of multiple objects simultaneously and independently using a single acoustic actuator. Our method allows independent trajectory following, pattern transformation and sorting of multiple miniature objects in a wide range of materials, including electronic components, water droplets loaded on solid carriers, plant seeds, candy balls and metal parts.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Automation Science and Engineering, Research area: Microsystems, Helsinki University of Technology, Aalto University

Contributors: Zhou, Q., Sariola, V., Latifi, K., Liimatainen, V.

Publication date: 9 Sep 2016

Peer-reviewed: Yes

#### **Publication information**

Journal: Nature Communications

Volume: 7

Article number: 12764

ISSN (Print): 2041-1723

Ratings:

Scopus rating (2016): CiteScore 11.8 SJR 6.414 SNIP 2.882

Original language: English

ASJC Scopus subject areas: Biochemistry, Genetics and Molecular Biology(all), Chemistry(all), Physics and Astronomy(all)

Electronic versions:

Controlling the motion of multiple objects on a Chladni plate

DOIs:

10.1038/ncomms12764

URLs:

<http://urn.fi/URN:NBN:fi:ty-201609264550>

#### Bibliographical note

EXT="Zhou, Quan"

EXT="Latifi, Kouros"

Source: Scopus

Source ID: 84986907353

Research output: Contribution to journal > Article > Scientific > peer-review

#### Polyarginine Interacts More Strongly and Cooperatively than Polylysine with Phospholipid Bilayers

The interactions of two highly positively charged short peptide sequences with negatively charged lipid bilayers were explored by fluorescence binding assays and all-atom molecular dynamics simulations. The bilayers consisted of mixtures of phosphatidylglycerol (PG) and phosphatidylcholine (PC) lipids as well as a fluorescence probe that was sensitive to the interfacial potential. The first peptide contained nine arginine repeats (Arg<sub>9</sub>), and the second one had nine lysine repeats (Lys<sub>9</sub>). The experimentally determined apparent dissociation constants and Hill cooperativity coefficients demonstrated that the Arg<sub>9</sub> peptides exhibited weakly anticooperative binding behavior at the bilayer interface at lower PG concentrations, but this anticooperative effect vanished once the bilayers contained at least 20 mol % PG. By contrast, Lys<sub>9</sub> peptides showed strongly anticooperative binding behavior at all PG concentrations, and the dissociation constants with Lys<sub>9</sub> were approximately 2 orders of magnitude higher than with Arg<sub>9</sub>. Moreover, only arginine-rich peptides could bind to the phospholipid bilayers containing just PC lipids. These results along with the corresponding molecular dynamics simulations suggested two important distinctions between the behavior of Arg<sub>9</sub> and Lys<sub>9</sub> that led to these striking differences in binding and cooperativity. First, the interactions of the guanidinium moieties on the Arg side chains with the phospholipid head groups were stronger than for the amino group. This helped facilitate stronger Arg<sub>9</sub> binding at all PG concentrations that were tested. However, at PG concentrations of 20 mol % or greater, the Arg<sub>9</sub> peptides came into sufficiently close proximity with each other so that favorable like-charge pairing between the guanidinium moieties could just offset the long-range electrostatic repulsions. This led to Arg<sub>9</sub> aggregation at the bilayer surface. By contrast, Lys<sub>9</sub> molecules experienced electrostatic repulsion from each other at all PG concentrations. These insights may help explain the propensity for cell penetrating peptides containing arginine to more effectively cross cell membranes in comparison with lysine-rich peptides.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Texas A and M University, Pennsylvania State University, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Division of Organic Chemistry and Biochemistry, Bijičská Cesta 54

Contributors: Robison, A. D., Sun, S., Poyton, M. F., Johnson, G. A., Pellois, J. P., Jungwirth, P., Vazdar, M., Cremer, P. S.

Number of pages: 10

Pages: 9287-9296

Publication date: 8 Sep 2016

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 120

Issue number: 35

ISSN (Print): 1520-6106

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Scopus rating (2016): CiteScore 3.03 SJR 1.345 SNIP 1.023

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry

DOIs:

10.1021/acs.jpcc.6b05604

Source: Scopus

Source ID: 84986593892

Research output: Contribution to journal > Article > Scientific > peer-review

### **3D micro-nano structured hybrid scaffolds: An investigation into the role of nanofiber coating on viability, proliferation and differentiation of seeded mesenchymal stem cells**

The introduction of a three dimensional scaffold providing the closest analogies to extracellular matrix (ECM) is currently a key strategy for tackling many challenges in tissue repair. Here, we present a new hybrid scaffold constructed by coating electrospun chitosan/polyethylene oxide (PEO) nanofibers on commercial BioTek polystyrene (PS) scaffold obtained from Sigma Aldrich. The viability and proliferation rate of mesenchymal stem cells (MSCs) seeded on micro-nano structured hybrid scaffold (MNHS) and commercial PS scaffolds were analyzed by MTT assay. The results of the MTT assay revealed a higher degree of viability and proliferation rate in MSCs seeded on MNHS compared with the commercial PS scaffold. DAPI images also confirmed the higher degree of attachment and viability of MSCs seeded on MNHS. Moreover, MSCs on both scaffolds differentiated to osteoblasts and adipocytes cells, as reflected by the images obtained from Alizarin Red and Oil Red-O staining. Alkaline phosphatase activity (ALP) and calcium content assays revealed that the MNHS has a higher potential for osteogenic differentiation than the commercial scaffold. To quantify the osteoblast and adipocyte gene expression, quantitative RT-PCR was carried out for MNHS, commercial scaffold and Tissue culture polystyrene (TCPS). It was found that MNHS can express a higher level of Runx-related transcription factor 2 (Runx2), osteonectin and osteocalcin in osteogenic differentiation as well as increased expression of PPAR $\gamma$  and UCP-1 in adipogenic differentiation. The enhancement of the attachment, viability and proliferation as well as bi-lineage differentiation may result from the biochemical and structural analogies of MNHS to native ECM. Furthermore, it was observed that biocompatible MNHS scaffold can potentially be utilized as a suitable scaffold for bone and connective tissue engineering.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Fibre Materials, Tarbiat Modares University, Isfahan University of Medical Sciences, VTT Technical Research Centre of Finland

Contributors: Pilehrood, M. K., Atashi, A., Sadeghi-Aliabadi, H., Nousiainen, P., Harlin, A.

Number of pages: 8

Pages: 9000-9007

Publication date: 1 Sep 2016

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal Nanoscience and Nanotechnology

Volume: 16

Issue number: 9

ISSN (Print): 1533-4880

Ratings:

Scopus rating (2016): CiteScore 1.34 SJR 0.324 SNIP 0.486

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Biomedical Engineering, Materials Science(all), Condensed Matter Physics

Keywords: Adipogenic Differentiation, Hybrid Scaffold, Mesenchymal Stem Cell, Micro Porosity, Nanofiber, Osteogenic Differentiation

DOIs:

10.1166/jnn.2016.12740

#### **Bibliographical note**

EXT="Harlin, Ali"

Source: Scopus

Source ID: 84983416664

Research output: Contribution to journal > Article > Scientific > peer-review

### **Detergent impurity effect on recycled HDPE: Properties after repetitive processing**

High density polyethylene (rHDPE) is extruded 1 to 8 times, with and without detergent, to simulate the effects of impurities on the material and on the artificial ageing process. The mechanical properties, thermal stability, rheology, Fourier transform infrared spectroscopy (FTIR), and volatile organic compound (VOC) emissions are measured. According to the results, ageing of rHDPE increases tensile strength, reduces elongation, and enhances side chain branching of the

material and thus causes rheological changes. The addition of detergent reduces changes in mechanical properties and rheological behavior but accelerates thermal degradation. VOC and FTIR measurements of the samples with detergent addition show generation of harmful 1,4-dioxane. The amount of total emission, as well as emissions of important perfumes limonene and 1R- $\alpha$ -pinene, decreases during multiple extrusion cycles. Heating of the plastics is found to be a major factor in the VOC emission reduction. Impurities have a notable effect on the artificial ageing results.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, University of Helsinki, Ekokem

Contributors: Mylläri, V., Hartikainen, S., Poliakova, V., Anderson, R., Jönkkäri, I., Pasanen, P., Andersson, M., Vuorinen, J.

Publication date: 15 Aug 2016

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Applied Polymer Science

Volume: 133

Issue number: 31

Article number: 43766

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2016): CiteScore 1.73 SJR 0.588 SNIP 0.815

Original language: English

ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry

Keywords: Ageing, Degradation, Polyolefins, Recycling

DOIs:

10.1002/app.43766

Source: Scopus

Source ID: 84992303578

Research output: Contribution to journal > Article > Scientific > peer-review

#### Buckling Behavior of Cold-Formed Studs with Thermal Perforations

Studies have shown that the optimal structural scheme for low-rise buildings that meets all regulatory requirements is a frame system. In this connection, thin-walled cold-formed steel (CFS) profiles seem to be the best material for constructing light steel framed (LSF) walls. The framework of LSF walls is usually constructed from CFS C-shaped profiles. To increase the thermal effectiveness of a wall, CFS profiles usually have thermal perforations and thus are called thermoprofiles. However, these openings have a negative impact on bearing capacity of profiles and require accurate evaluation. In this article a relatively new reticular-stretched thermoprofile with diamond-shaped openings is considered. The article deals with the buckling analysis of perforated CFS C-sections subjected to compression.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Peter the Great Saint-Petersburg Polytechnic University, University of Maribor

Contributors: Garifullin, M., Sinelnikov, A., Bronzova, M., Kovacic, B., Kamnik, R.

Publication date: 11 Aug 2016

Peer-reviewed: Yes

#### Publication information

Journal: MATEC Web of Conferences

Volume: 73

Article number: 04011

ISSN (Print): 2274-7214

Ratings:

Scopus rating (2016): CiteScore 0.2 SJR 0.132 SNIP 0.346

Original language: English

ASJC Scopus subject areas: Chemistry(all), Engineering(all), Materials Science(all)

DOIs:

10.1051/mateconf/20167304011

URLs:

<http://www.scopus.com/inward/record.url?scp=84983508952&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84983508952



### Reinforced chloroprene rubber by in situ generated silica particles: Evidence of bound rubber on the silica surface

Nano silica is generated in situ inside the uncrosslinked chloroprene rubber (CR) by the sol-gel reaction of tetraethoxysilane (TEOS). This results in appreciable improvement in mechanical properties of the CR composites at relatively low filler content. Furthermore, exploitation of reactive organosilanes,  $\gamma$ -aminopropyltrimethoxysilane ( $\gamma$ -APS) in particular, in the silica synthesis process facilitates growing of spherical silica particles with a size distribution in the range of 20-50 nm. The silica particles are found to be uniformly dispersed and they do not suffer from filler-filler interaction. Additionally, it is observed that the silica particles are coated by silane and rubber chains together which are popularly known as bound rubber. The existence of the bound rubber on silica surface has been supported by the detailed investigations with transmission electron microscopy (TEM), energy filtered transmission electron microscopy (EFTEM) and energy dispersive X-ray spectroscopy (EDAX). The interaction between rubber and silica, via bi-functionality of the  $\gamma$ -APS, has been explored by detailed FTIR studies.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Visvesvaraya National Institute of Technology, Leibniz-Institut für Polymerforschung Dresden E.V., Institut für Werkstoffwissenschaft

Contributors: Kapgate, B. P., Das, C., Das, A., Basu, D., Wiessner, S., Reuter, U., Heinrich, G.

Publication date: 10 Aug 2016

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Applied Polymer Science

Volume: 133

Issue number: 30

Article number: 43717

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2016): CiteScore 1.73 SJR 0.588 SNIP 0.815

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)

Keywords: bound rubber, in situ silica and silane treatment, transmission electron microscopy

DOIs:

10.1002/app.43717

Source: Scopus

Source ID: 84964925986

Research output: Contribution to journal › Article › Scientific › peer-review

### Spontaneous formation of three-dimensionally ordered Bi-rich nanostructures within GaAs<sub>1-x</sub>Bi<sub>x</sub>/GaAs quantum wells

In this work, we report on the spontaneous formation of ordered arrays of nanometer-sized Bi-rich structures due to lateral composition modulations in Ga(As,Bi)/GaAs quantum wells grown by molecular beam epitaxy. The overall microstructure and chemical distribution is investigated using transmission electron microscopy. The information is complemented by synchrotron x-ray grazing incidence diffraction, which provides insight into the in-plane arrangement. Due to the vertical inheritance of the lateral modulation, the Bi-rich nanostructures eventually shape into a three-dimensional assembly. Whereas the Bi-rich nanostructures are created via two-dimensional phase separation at the growing surface, our results suggest that the process is assisted by Bi segregation which is demonstrated to be strong and more complex than expected, implying both lateral and vertical (surface segregation) mass transport. As demonstrated here, the inherent thermodynamic miscibility gap of Ga(As,Bi) alloys can be exploited to create highly uniform Bi-rich units embedded in a quantum confinement structure.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications, Hausvogteiplatz 5-7

Contributors: Luna, E., Wu, M., Hanke, M., Puustinen, J., Guina, M., Trampert, A.

Publication date: 1 Jul 2016

Peer-reviewed: Yes

#### Publication information

Journal: Nanotechnology

Volume: 27

Issue number: 32  
Article number: 325603  
ISSN (Print): 0957-4484  
Ratings:

Scopus rating (2016): CiteScore 2.87 SJR 1.339 SNIP 0.982

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Electrical and Electronic Engineering, Mechanical Engineering, Mechanics of Materials, Materials Science(all)

Keywords: GaAsBi, phase separation and segregation, self organization, TEM

DOIs:

10.1088/0957-4484/27/32/325603

#### Bibliographical note

EXT="Wu, M."

Source: Scopus

Source ID: 84978884196

Research output: Contribution to journal > Article > Scientific > peer-review

#### The Influence of Phosphorus Exposure on a Natural-Gas-Oxidation Catalyst

Phosphorus is found to have a deactivating effect on the catalytic activity of the studied natural-gas-oxidation catalyst. Accelerated laboratory-scale phosphorus treatment was done to the PtPd/Al<sub>2</sub>O<sub>3</sub> natural gas oxidation catalyst. The effect of phosphorus after low (0.065 M) and high (0.13 M) phosphorus concentration treatments was studied by using an inductively coupled plasma optical emission spectroscopy, N<sub>2</sub> physisorption, X-ray diffraction, field emission scanning electron microscopy, transmission electron microscopy, and X-ray photoelectron spectroscopy. In addition, the behavior of the catalyst was studied by a Gasmet FT-IR gas analyzer. Based on the received results it can be concluded that phosphorus was adsorbed on the surface by chemical bonds forming phosphates (PO<sub>4</sub>). In addition, the partial transformation of PdO to Pd was observed. Due to the phosphorus adsorption both the CO and CH<sub>4</sub> oxidation activities were lower after the phosphorus treatments compared with the fresh catalyst.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Materials Characterization, University of Oulu, Aalto University, Dinex Ecocat Oy, COMP Centre of Excellence, Department of Applied Physics, Aalto University

Contributors: Kärkkäinen, M., Kolli, T., Honkanen, M., Heikkinen, O., Väliheikki, A., Huuhtanen, M., Kallinen, K., Lahtinen, J., Vippola, M., Keiski, R. L.

Number of pages: 5

Pages: 1044-1048

Publication date: 1 Jul 2016

Peer-reviewed: Yes

#### Publication information

Journal: Topics in Catalysis

Volume: 59

Issue number: 10-12

ISSN (Print): 1022-5528

Ratings:

Scopus rating (2016): CiteScore 2.55 SJR 0.975 SNIP 0.811

Original language: English

ASJC Scopus subject areas: Catalysis, Chemistry(all)

Keywords: Methane degradation, Palladium, Platinum, Poisoning

DOIs:

10.1007/s11244-016-0587-x

Source: Scopus

Source ID: 84977071141

Research output: Contribution to journal > Article > Scientific > peer-review

#### Structurally Controlled Dynamics in Azobenzene-Based Supramolecular Self-Assemblies in Solid State

Light-responsive supramolecular self-assemblies exhibit interplay between order and dynamics of the self-assembling motifs, through which the thermal isomerization rate of azobenzene chromophores can be tuned by orders of magnitude. By using supramolecular complexes of 4-(4-alkylphenylazo)phenols hydrogen-bonded to poly(4-vinylpyridine) as model systems, we demonstrate that the thermal isomerization rate of the hydroxyazobenzene derivatives increases 5700-fold when the material undergoes a transformation from a disordered, low-azobenzene-concentration state to a high-concentration state exhibiting lamellar, smectic-like self-assembly. Drastically smaller thermal isomerization rates are observed in disordered structures. This allows us to attribute the change to a combination of increased number density of

the hydroxyazobenzenes inducing plasticization, and cooperativity created by the chromophore-chromophore interactions through self-assembled molecular order and alignment. Our results pinpoint the importance of molecular self-assembly and intermolecular interactions in modifying the dynamics in supramolecular complexes in a controlled manner. We foresee this to be important in light-controlled dynamic materials.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Aalto University

Contributors: Poutanen, M., Ikkala, O., Priimägi, A.

Number of pages: 7

Pages: 4095-4101

Publication date: 14 Jun 2016

Peer-reviewed: Yes

#### Publication information

Journal: Macromolecules

Volume: 49

Issue number: 11

ISSN (Print): 0024-9297

Ratings:

Scopus rating (2016): CiteScore 5.76 SJR 2.564 SNIP 1.483

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry

DOIs:

10.1021/acs.macromol.6b00562

Source: Scopus

Source ID: 84975044511

Research output: Contribution to journal > Article > Scientific > peer-review

#### Development of Magnetic Losses During Accelerated Corrosion Tests for Nd-Fe-B Magnets Used in Permanent Magnet Generators

Sintered Nd-Fe-B magnets are critical components in permanent magnet wind generators. They are the strongest permanent magnets available and thus enable the construction of light and effective devices, but their stability in corrosive environments is limited. In this work, the formation of corrosion losses in two types of Nd-Fe-B alloys was studied. Magnets were in a magnetized state during the corrosion test, enabling monitoring of the development of losses in magnetic flux along with those in weight. Parallel flux and weight loss measurements conducted during corrosion tests showed that percentage weight losses were lower than the total flux losses. Scanning electron microscope studies of corroded specimens disclosed that the magnets first underwent dissolution of the grain-boundary phase, followed by the detachment and movement of the loosened grains in the magnetic field. The degradation was accelerated by oxidation of the matrix phase, which introduced further damage by volume expansion.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Materials Characterization, VTT Technical Research Centre of Finland

Contributors: Isotahdon, E., Huttunen-Saarivirta, E., Kuokkala, V.

Number of pages: 10

Pages: 732-741

Publication date: 1 Jun 2016

Peer-reviewed: Yes

#### Publication information

Journal: Corrosion

Volume: 72

Issue number: 6

ISSN (Print): 0010-9312

Ratings:

Scopus rating (2016): CiteScore 2.02 SJR 1.075 SNIP 1.496

Original language: English

ASJC Scopus subject areas: Materials Science(all), Chemical Engineering(all), Chemistry(all)

Keywords: Corrosion, Corrosion losses, Highly accelerated stress test (HAST test), Improved corrosion resistance sintered Nd-Fe-B magnets, Improved stability sintered Nd-Fe-B magnets, Nd-Fe-B, Permanent magnet, Scanning electron microscopy, Thermal losses, Wind power

DOIs:

10.5006/2037

URLs:

<http://corrosionjournal.org/doi/abs/10.5006/2037>

URLs:

<http://www.scopus.com/inward/record.url?scp=84973626857&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84973626857

Research output: Contribution to journal › Article › Scientific › peer-review

### **Robust statistical approaches for RSS-based floor detection in indoor localization**

Floor detection for indoor 3D localization of mobile devices is currently an important challenge in the wireless world. Many approaches currently exist, but usually the robustness of such approaches is not addressed or investigated. The goal of this paper is to show how to robustify the floor estimation when probabilistic approaches with a low number of parameters are employed. Indeed, such an approach would allow a building-independent estimation and a lower computing power at the mobile side. Four robustified algorithms are to be presented: a robust weighted centroid localization method, a robust linear trilateration method, a robust nonlinear trilateration method, and a robust deconvolution method. The proposed approaches use the received signal strengths (RSS) measured by the Mobile Station (MS) from various heardWiFi access points (APs) and provide an estimate of the vertical position of the MS, which can be used for floor detection. We will show that robustification can indeed increase the performance of the RSS-based floor detection algorithms.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Electronics and Communications Engineering, Research group: Wireless Communications and Positioning

Contributors: Razavi, A., Valkama, M., Lohan, E. S.

Publication date: 1 Jun 2016

Peer-reviewed: Yes

### **Publication information**

Journal: Sensors

Volume: 16

Issue number: 6

Article number: 793

ISSN (Print): 1424-8220

Ratings:

Scopus rating (2016): CiteScore 2.78 SJR 0.623 SNIP 1.614

Original language: English

ASJC Scopus subject areas: Electrical and Electronic Engineering, Atomic and Molecular Physics, and Optics, Analytical Chemistry, Biochemistry

Keywords: Floor detection, Indoor localization, Robust regression, RSS-based localization, Trilateration, Weighted centroid localization

Electronic versions:

sensors-16-00793

DOIs:

10.3390/s16060793

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201606204285>

Source: Scopus

Source ID: 84971596811

Research output: Contribution to journal › Article › Scientific › peer-review

### **Effect of incorporation of CdS NPs on performance of PTB7: PCBM organic solar cells**

It has been well known that incorporation of nano-heterostructures of various metals, semiconductors and dielectric materials in the active layer of organic solar cells (OSCs) helps in improving power conversion efficiency (PCE). In the present study, we demonstrated microwave synthesis of CdS nanoparticles (NPs) for their application in one of most efficient OSCs consisting of poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b']dithiophene-2,6-diyl] [3-fluoro-2-[(2-ethylhexyl)carbonyl] thieno[3,4-b]thiophenediyl]] (PTB7): [6,6]-phenyl C<sub>71</sub>-butyric acid methyl ester (PCBM) photoactive blend. This is crucial to fully explore the promising features of low cost and scalability in organic-inorganic hybrid solar cells. Synthesized CdS NPs are slightly elongated and highly crystalline with their absorption lies in the visible region as confirmed by High resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), UV-Vis absorption spectroscopy studies. Our experimental results for the devices in an inverted geometry having a structure ITO/ZnO/PTB7: CdS: PCBM/MoO<sub>3</sub>/Ag has shown increase in J<sub>sc</sub> and PCE by nearly 10%. However, it was observed that this increase is

only when NPs were added in the low concentration in active layer. UV-Vis absorption spectroscopy, Photoluminescence (PL) and atomic force microscopy (AFM) studies were carried out in order understand the device performance.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Electronics and Communications Engineering, Indian Institute of Technology Bombay, Organic and Nano-electronics Group

Contributors: Sharma, R., Bhalerao, S., Gupta, D.

Number of pages: 7

Pages: 274-280

Publication date: 1 Jun 2016

Peer-reviewed: Yes

#### Publication information

Journal: Organic Electronics: physics, materials, applications

Volume: 33

ISSN (Print): 1566-1199

Ratings:

Scopus rating (2016): CiteScore 3.4 SJR 1.081 SNIP 0.944

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Biomaterials, Chemistry(all), Condensed Matter Physics, Materials Chemistry, Electrical and Electronic Engineering

Keywords: CdS nanoparticles, Microwave synthesis, Organic solar cells, PCBM, PL quenching, PTB7

DOIs:

10.1016/j.orgel.2016.03.030

Source: Scopus

Source ID: 84962355464

Research output: Contribution to journal > Article > Scientific > peer-review

#### Optical Projection Tomography Technique for Image Texture and Mass Transport Studies in Hydrogels Based on Gellan Gum

The microstructure and permeability are crucial factors for the development of hydrogels for tissue engineering, since they influence cell nutrition, penetration, and proliferation. The currently available imaging methods able to characterize hydrogels have many limitations. They often require sample drying and other destructive processing, which can change hydrogel structure, or they have limited imaging penetration depth. In this work, we show for the first time an alternative nondestructive method, based on optical projection tomography (OPT) imaging, to characterize hydrated hydrogels without the need of sample processing. As proof of concept, we used gellan gum (GG) hydrogels obtained by several cross-linking methods. Transmission mode OPT was used to analyze image microtextures, and emission mode OPT to study mass transport. Differences in hydrogel structure related to different types of cross-linking and between modified and native GG were found through the acquired Haralicks image texture features followed by multiple discriminant analysis (MDA). In mass transport studies, the mobility of FITC-dextran (MW 20, 150, 2000 kDa) was analyzed through the macroscopic hydrogel. The FITC-dextran velocities were found to be inversely proportional to the size of the dextran as expected. Furthermore, the threshold size in which the transport is affected by the hydrogel mesh was found to be 150 kDa (Stokes radii between 69 and 95 Å). On the other hand, the mass transport study allowed us to define an index of homogeneity to assess the cross-linking distribution, structure inside the hydrogel, and repeatability of hydrogel production. As a conclusion, we showed that the set of OPT imaging based material characterization methods presented here are useful for screening many characteristics of hydrogel compositions in relatively short time in an inexpensive manner, providing tools for improving the process of designing hydrogels for tissue engineering and drugs/cells delivery applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: BioMediTech, Department of Electronics and Communications Engineering, Research group: Computational Biophysics and Imaging Group, Research group: Biomaterials and Tissue Engineering Group, Faculty of Computing and Electrical Engineering, BioMediTech - Institute of Biosciences and Medical Technology, Heart Group, ICVS/3Bs - PT Government Associ. Laboratory

Contributors: Soto, A. M., Koivisto, J. T., Parraga, J. E., Silva-Correia, J., Oliveira, J. M., Reis, R. L., Kellomäki, M., Hyttinen, J., Figueiras, E.

Number of pages: 10

Pages: 5173-5182

Publication date: 24 May 2016

Peer-reviewed: Yes

## Publication information

Journal: Langmuir

Volume: 32

Issue number: 20

ISSN (Print): 0743-7463

Ratings:

Scopus rating (2016): CiteScore 3.99 SJR 1.559 SNIP 1.178

Original language: English

ASJC Scopus subject areas: Electrochemistry, Condensed Matter Physics, Surfaces and Interfaces, Materials Science(all), Spectroscopy

DOIs:

10.1021/acs.langmuir.6b00554

Source: Scopus

Source ID: 84971278446

Research output: Contribution to journal > Article > Scientific > peer-review

## Lipid-assisted protein transport: A diffusion-reaction model supported by kinetic experiments and molecular dynamics simulations

The protein transport inside a cell is a complex phenomenon that goes through several difficult steps. The facilitated transport requires sophisticated machineries involving protein assemblies. In this work, we developed a diffusion-reaction model to simulate co-transport kinetics of proteins and lipids. We assume the following: (a) there is always a small lipid concentration of order of the Critical Micellar Concentration (CMC) in equilibrium with the membrane; (b) the binding of lipids to proteins modulates the hydrophobicity of the complexes and, therefore, their ability to interact and merge with the bilayer; and (c) some lipids leave the bilayer to replenish those bound to proteins. The model leads to a pair of integral equations for the time-evolution of the adsorbed proteins in the lipid bilayer. Relationships between transport kinetics, CMC, and lipid-protein binding constants were found. Under particular conditions, a perturbation analysis suggests the onset of kinks in the protein adsorption kinetics. To validate our model, we performed leakage measurements of vesicles composed by either high or low CMC lipids interacting with Islet Amyloid PolyPeptide (IAPP) and A $\beta$  (1-40) used as sample proteins. Since the lipid-protein complex stoichiometry is not easily accessible, molecular dynamics simulations were performed using monomeric IAPP interacting with an increasing number of phospholipids. Main results are the following: (a) 1:1 lipid-protein complexes generally show a faster insertion rate proportional to the complex hydrophobicity and inversely related to lipid CMC; (b) on increasing the number of bound lipids, the protein insertion rate decreases; and (c) at slow lipids desorption rate, the lipid-assisted proteins transport might exhibit a discontinuous behavior and does non-linearly depend on protein concentration.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, University of Catania, Università degli Studi di Catania, Department of Chemical Sciences, Department of Physics, University of Helsinki, Carnegie Mellon University

Contributors: La Rosa, C., Scalisi, S., Lolicato, F., Pannuzzo, M., Raudino, A.

Publication date: 14 May 2016

Peer-reviewed: Yes

## Publication information

Journal: Journal of Chemical Physics

Volume: 144

Issue number: 18

Article number: 184901

ISSN (Print): 0021-9606

Ratings:

Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 1.003

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1063/1.4948323

Source: Scopus

Source ID: 84969668014

Research output: Contribution to journal > Article > Scientific > peer-review

## Effect of Hole Transporting Material on Charge Transfer Processes in Zinc Phthalocyanine Sensitized ZnO Nanorods

The photoinduced electron transfer processes were studied for hybrid systems consisting of self-assembled monolayer of zinc phthalocyanine (ZnPc) assembled on ZnO nanorods and a film of organic hole transporting material (HTM) atop. Polythiophene (P3HT) or Spiro-OMeTAD were used as HTM. The study was carried out by ultrafast transient absorption spectroscopy technique with selective excitation of ZnPc at 680 nm or P3HT at 500 nm. Data analysis revealed that

photoexcitation of ZnPc in the structure ZnO|ZnPc|P3HT results in a fast (1.8 ps) electron transfer from ZnPc to ZnO, which is followed by a hole transfer from the ZnPc cation to P3HT roughly in 30 ps. However, in the case of ZnO|ZnPc|Spiro-OMeTAD structure, the primary reaction upon excitation of ZnPc is a fast (0.5 ps) hole transfer from ZnPc to Spiro-OMeTAD, and the second step is electron injection from the ZnPc anion to ZnO in roughly 120 ps. Thus, we demonstrate two structurally very similar hybrid architectures that implement two different mechanisms for photoinduced charge separation found in dye-sensitized or in organic solar cells.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Hakola, H., Sariola-Leikas, E., Efimov, A., Tkachenko, N. V.

Number of pages: 8

Pages: 7044-7051

Publication date: 21 Apr 2016

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 120

Issue number: 13

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.189

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

10.1021/acs.jpcc.6b01583

Source: Scopus

Source ID: 84964529902

Research output: Contribution to journal > Article > Scientific > peer-review

#### Influence of heat treatment on the abrasive wear resistance of a $\text{Cr}_3\text{C}_2\text{NiCr}$ coating deposited by an ethene-fuelled HVOF spray process

This work reveals the influence of heat treatments on the microstructure, mechanical properties and abrasive wear behaviour of a  $\text{Cr}_3\text{C}_2\text{NiCr}$  coating deposited by an ethene-fuelled high-velocity oxygen-fuel spray process using an agglomerated-and-sintered feedstock powder. The wear resistance of an as-sprayed and heat treated (8 h at 800 °C) coating was evaluated in low- and high-stress abrasion regimes, the latter in a temperature range up to 800 °C. Precipitation of secondary carbides from the supersaturated as-sprayed binder matrix is at the core of the observed changes in the coatings wear resistance upon heat treating. This aging process renders the binder matrix softer and more ductile, as was probed by means of nanoindentation, and thereby improves its resistance against micro-cracking which is identified as an important wear mechanism in high-stress abrasion conditions.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, AC2T Research GmbH, Fraunhofer Institut für Werkstoff- und Strahltechnik, Fraunhofer Institut für Keramische Technologien und Systeme

Contributors: Janka, L., Norpoth, J., Trache, R., Berger, L. M.

Number of pages: 8

Pages: 444-451

Publication date: 15 Apr 2016

Peer-reviewed: Yes

#### Publication information

Journal: Surface and Coatings Technology

Volume: 291

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2016): CiteScore 2.56 SJR 0.882 SNIP 1.379

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces

Keywords: Abrasion, CrC, Heat treatment, HVOF, Mechanical properties

DOIs:

10.1016/j.surfcoat.2016.02.066

Source: Scopus

Source ID: 84960192258

Research output: Contribution to journal › Article › Scientific › peer-review

### Coordination networks incorporating halogen-bond donor sites and azobenzene groups

Two Zn coordination networks,  $\{[Zn(1)(Py)_2]_2(2\text{-propanol})\}_n$  (3) and  $\{[Zn(1)_2(Bipy)_2](DMF)_2\}_n$  (4), incorporating halogen-bond (XB) donor sites and azobenzene groups have been synthesized and fully characterized. Obtaining 3 and 4 confirms that it is possible to use a ligand wherein its coordination bond acceptor sites and XB donor sites are on the same molecular scaffold (i.e., an aromatic ring) without interfering with each other. We demonstrate that XBs play a fundamental role in the architectures and properties of the obtained coordination networks. In 3, XBs promote the formation of 2D supramolecular layers, which, by overlapping each other, allow the incorporation of 2-propanol as a guest molecule. In 4, XBs support the connection of the layers and are essential to firmly pin DMF solvent molecules through  $I\cdots O$  contacts, thus increasing the stability of the solvated systems.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Fernandez-Palacio, F., Saccone, M., Priimägi, A., Terraneo, G., Pilati, T., Metrangolo, P., Resnati, G.

Number of pages: 7

Pages: 2251-2257

Publication date: 7 Apr 2016

Peer-reviewed: Yes

#### Publication information

Journal: CrystEngComm

Volume: 18

Issue number: 13

ISSN (Print): 1466-8033

Ratings:

Scopus rating (2016): CiteScore 3.37 SJR 1.053 SNIP 0.905

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics

DOIs:

10.1039/c6ce00059b

Source: Scopus

Source ID: 84962331348

Research output: Contribution to journal › Article › Scientific › peer-review

### Strain rate change tests with the Split Hopkinson Bar method

In this paper, methods to produce rapid strain rate changes for strain rate sensitivity measurements in Split Hopkinson Bar arrangements are presented and discussed. Two different cases are considered: a strain rate change test within the high strain rate region in compression, and a tension test incorporating a large strain rate jump directly from the low strain rate region to high strain rates. The former method is based on the loading wave amplitude manipulation, while the latter method is based on the incorporation of a low strain rate loading device into a Tensile Split Hopkinson Bar apparatus.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Materials Characterization

Contributors: Isakov, M., Kokkonen, J., Östman, K., Kuokkala, V.

Pages: 231-242

Publication date: 1 Apr 2016

Peer-reviewed: Yes

#### Publication information

Journal: European Physical Journal. Special Topics

Volume: 225

Issue number: 2

ISSN (Print): 1951-6355

Ratings:

Scopus rating (2016): CiteScore 1.94 SJR 0.581 SNIP 0.793



Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Materials Science(all), Physical and Theoretical Chemistry

DOIs:

10.1140/epjst/e2015-99999-x

Source: Scopus

Source ID: 84941343460

Research output: Contribution to journal > Article > Scientific > peer-review

### DFT simulations and microkinetic modelling of 1-pentyne hydrogenation on Cu<sub>20</sub> model catalysts

Adsorption and dissociation of H<sub>2</sub> and hydrogenation of 1-pentyne on neutral and anionic Cu<sub>20</sub> clusters have been investigated using the density functional theory and microkinetic modelling. Molecular adsorption of H<sub>2</sub> is found to occur strictly at atop sites. The H<sub>2</sub> dimer is activated upon adsorption, and the dissociation occurs with moderate energy barriers. The dissociated H atoms reside preferentially on 3-fold face and 2-fold edge sites. Based on these results, the reaction paths leading to the partial and total hydrogenation of 1-pentyne have been studied step-by-step. The results suggest that copper clusters can display selective activity on the hydrogenation of alkyne and alkene molecules. The hydrogenated products are more stable than the corresponding initial reactants following an energetic staircase with the number of added H atoms. Stable semi-hydrogenated intermediates are formed before the partial (1-pentene) and total (pentane) hydrogenation stages of 1-pentyne. The microkinetic model analysis shows that C<sub>5</sub>H<sub>10</sub> is the dominant product. Increasing the reactants (C<sub>5</sub>H<sub>8</sub>/H<sub>2</sub>) ratio enhances the formation of products (C<sub>5</sub>H<sub>10</sub> and C<sub>5</sub>H<sub>12</sub>).

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Aalto University, COMP Centre of Excellence, Department of Applied Physics, Aalto University

Contributors: Ma, L., Melander, M., Weckman, T., Lipasti, S., Laasonen, K., Akola, J.

Number of pages: 10

Pages: 61-70

Publication date: 1 Apr 2016

Peer-reviewed: Yes

### Publication information

Journal: Journal of Molecular Graphics and Modelling

Volume: 65

ISSN (Print): 1093-3263

Ratings:

Scopus rating (2016): CiteScore 1.77 SJR 0.524 SNIP 0.731

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Spectroscopy, Computer Graphics and Computer-Aided Design, Materials Chemistry

Keywords: Adsorption and dissociation, Cluster model, Density functional theory, Heterogeneous catalysis, Hydrogenation

DOIs:

10.1016/j.jmglm.2016.02.007

### Bibliographical note

INT=fys,"Ma, Li"

Source: Scopus

Source ID: 84961675623

Research output: Contribution to journal > Article > Scientific > peer-review

### Microwave assisted laser-induced breakdown spectroscopy at ambient conditions

Signal enhancements in laser-induced breakdown spectroscopy (LIBS) using external microwave power are demonstrated in ambient air. Pulsed microwave at 2.45 GHz and of 1 millisecond duration was delivered via a simple near field applicator (NFA), with which an external electric field is generated and coupled into laser induced plasma. The external microwave power can significantly increase the signal lifetime from a few microseconds to hundreds of microseconds, resulting in a great enhancement on LIBS signals with the use of a long integration time. The dependence of signal enhancement on laser energy and microwave power is experimentally assessed. With the assistance of microwave source, a significant enhancement of ~ 100 was achieved at relatively low laser energy that is only slightly above the ablation threshold. A limit of detection (LOD) of 8.1 ppm was estimated for copper detection in Cu/Al<sub>2</sub>O<sub>3</sub> solid samples. This LOD corresponds to a 93-fold improvement compared with conventional single-pulse LIBS. Additionally, in the microwave assisted LIBS, the self-reversal effect was greatly reduced, which is beneficial in measuring elements of high concentration. Temporal measurements have been performed and the results revealed the evolution of the emission process in microwave-enhanced LIBS. The optimal position of the NFA related to the ablation point has also been investigated.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Optics, Research group: Applied Optics, Optics Laboratory, Department of Physics, Tampere University of Technology, University of Adelaide

Contributors: Viljanen, J., Sun, Z., Alwahabi, Z. T.

Number of pages: 8

Pages: 29-36

Publication date: 1 Apr 2016

Peer-reviewed: Yes

### Publication information

Journal: Spectrochimica Acta Part B: Atomic Spectroscopy

Volume: 118

ISSN (Print): 0584-8547

Ratings:

Scopus rating (2016): CiteScore 3.23 SJR 1.095 SNIP 1.351

Original language: English

ASJC Scopus subject areas: Instrumentation, Atomic and Molecular Physics, and Optics, Analytical Chemistry, Spectroscopy

Keywords: Copper Detection, Laser-induced breakdown spectroscopy, Microwave signal enhancement

DOIs:

10.1016/j.sab.2016.02.002

Source: Scopus

Source ID: 84962861465

Research output: Contribution to journal > Article > Scientific > peer-review

### Metal chalcogenide quantum dots: Biotechnological synthesis and applications

Metal chalcogenide (metal sulfide, selenide and telluride) quantum dots (QDs) have attracted considerable attention due to their quantum confinement and size-dependent photoemission characteristics. QDs are one of the earliest products of nanotechnology that were commercialized for tracking macromolecules and imaging cells in life sciences. An array of physical, chemical and biological methods have been developed to synthesize different QDs. Biological production of QDs follow green chemistry principles, thereby use of hazardous chemicals, high temperature, high pressure and production of by-products is either minimized or completely avoided. In the past decade, significant progress has been made wherein a diverse range of living organisms, i.e. viruses, bacteria, fungi, microalgae, plants and animals have been explored for synthesis of all three types of metal chalcogenide QDs. However, better understanding of the biological mechanisms that mediate the synthesis of metal chalcogenides and control the growth of QDs is needed for improving their yield and properties as well as addressing issues that arise during scale-up. In this review, we present the current status of the biological synthesis and applications of metal chalcogenide QDs. Where possible, the role of key biological macromolecules in controlled production of the nanomaterials is highlighted, and also technological bottlenecks limiting widespread implementation are discussed. The future directions for advancing biological metal chalcogenide synthesis are presented.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry

Contributors: Mal, J., Nancharaiah, Y. V., Van Hullebusch, E. D., Lens, P. N. L.

Number of pages: 19

Pages: 41477-41495

Publication date: Apr 2016

Peer-reviewed: Yes

### Publication information

Journal: RSC Advances

Volume: 6

Issue number: 47

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all)

DOIs:

10.1039/c6ra08447h

Source: Scopus

Source ID: 84966421058

Research output: Contribution to journal › Article › Scientific › peer-review

### Long-Lived Triplet Excited States of Bent-Shaped Pentacene Dimers by Intramolecular Singlet Fission

Intramolecular singlet fission (ISF) is a promising photophysical process to construct more efficient light energy conversion systems as one excited singlet state converts into two excited triplet states. Herein we synthesized and evaluated bent-shaped pentacene dimers as a prototype of ISF to reveal intrinsic characters of triplet states (e.g., lifetimes of triplet excited states). In this study, meta-phenylene-bridged TIPS-pentacene dimer (PcD-3Ph) and 2,2'-bipheynyl bridged TIPS-pentacene dimer (PcD-Biph) were newly synthesized as bent-shaped dimers. In the steady-state spectroscopy, absorption and emission bands of these dimers were fully characterized, suggesting the appropriate degree of electronic coupling between pentacene moieties in these dimers. In addition, the electrochemical measurements were also performed to check the electronic interaction between two pentacene moieties. Whereas the successive two oxidation peaks owing to the delocalization were observed in a directly linked-pentacene dimer (PcD) by a single bond, the cyclic voltammograms in PcD-Biph and PcD-3Ph implied the weaker interaction compared to that of p-phenylene-bridged TIPS-pentacene dimer (PcD-4Ph) and PcD. The femtosecond and nanosecond transient absorption spectra clearly revealed the slower ISF process in bent-shaped pentacene dimers (PcD-Biph and PcD-3Ph), more notably, the slower relaxation of the excited triplet states in PcD-Biph and PcD-3Ph. Namely, the quantum yields of triplet states ( $\Phi_T$ ) by ISF approximately remain constant (ca. 180-200%) in all dimer systems, whereas the lifetimes of the triplet excited states became much longer (up to 360 ns) in PcD-Biph as compared to PcD-4Ph (15 ns). Additionally, the lifetimes of the corresponding triplet states in PcD-Biph and PcD-3Ph were sufficiently affected by solvent viscosity. In particular, the lifetimes of PcD-Biph triplet state in THF/paraffin (1.0  $\mu$ s) increased up to approximately three times as compared to that in THF (360 ns), whereas those of PcD-4Ph were quite similar in both solvent.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Sakuma, T., Sakai, H., Araki, Y., Mori, T., Wada, T., Tkachenko, N. V., Hasobe, T.

Number of pages: 9

Pages: 1867-1875

Publication date: 31 Mar 2016

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry A

Volume: 120

Issue number: 11

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.971

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1021/acs.jpca.6b00988

Source: Scopus

Source ID: 84962062610

Research output: Contribution to journal › Article › Scientific › peer-review

### Stability and Function at High Temperature. What Makes a Thermophilic GTPase Different from Its Mesophilic Homologue

Comparing homologous enzymes adapted to different thermal environments AIDS to shed light on their delicate stability/function trade-off. Protein mechanical rigidity was postulated to secure stability and high-temperature functionality of thermophilic proteins. In this work, we challenge the corresponding-state principle for a pair of homologous GTPase domains by performing extensive molecular dynamics simulations, applying conformational and kinetic clustering, as well as exploiting an enhanced sampling technique (REST2). While it was formerly shown that enhanced protein flexibility and high temperature stability can coexist in the apo hyperthermophilic variant, here we focus on the holo states of both homologues by mimicking the enzymatic turnover. We clearly show that the presence of the ligands affects the conformational landscape visited by the proteins, and that the corresponding state principle applies for some functional modes. Namely, in the hyperthermophilic species, the flexibility of the effector region ensuring long-range communication and of the P-loop modulating ligand binding are recovered only at high temperature.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Laboratoire de Biochimie Théorique  
Contributors: Katava, M., Kalimeri, M., Stirnemann, G., Sterpone, F.  
Number of pages: 10  
Pages: 2721-2730  
Publication date: 17 Mar 2016  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 120

Issue number: 10

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2016): CiteScore 3.03 SJR 1.345 SNIP 1.023

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films  
DOIs:

10.1021/acs.jpcc.6b00306

Source: Scopus

Source ID: 84961282502

Research output: Contribution to journal › Article › Scientific › peer-review

#### HPLC-SEC: a new approach to characterise complex wastewater effluents

This work investigates the use of HPLC-SEC to characterise dissolved organic matter (DOM) of complex wastewater effluents. A silica-based column, sodium acetate eluent and multiple detections were employed: UV-254 absorbance for humic-type, and tryptophan-like (Ex/Em = 270/355) and tyrosine-like (Ex/Em = 270/310) fluorescence for protein type compounds. Effects of eluent pH, eluent ionic strength and injection volume on separation efficiency were tested. Humic-type and protein-type fractions were clearly differentiated and eluted within and out of calibration range. Eluent ionic strength had the greatest influence on global resolution; the lowest eluent concentration of 0.01 M produced the best separation for all wastewater effluents tested at any detection. UV-254 absorbance was higher at neutral and basic eluent pH while tryptophan-like fluorescence depended on the sample composition rather than on the eluent pH or ionic strength. Tyrosine-like fluorescence decreased significantly with the increase of eluent ionic strength. Accurate molecular weight measurements could not be done, the separation being influenced by secondary interactions, but could be approximated using separate calibrations with sodium salts of polystyrene-sulfonates and protein standards. The results show that this method is suitable for determining DOM in wastewater at low eluent concentrations (up to 0.03 M), at neutral or slightly basic pH.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Degree Programme in Energy and Environmental Engineering, Tampere University of Applied Sciences, Department of Biological and Environmental Science, University of Jyväskylä

Contributors: Szabo, H. M., Lepistö, R., Tuhkanen, T.

Number of pages: 14

Pages: 257-270

Publication date: 19 Feb 2016

Peer-reviewed: Yes

#### Publication information

Journal: International Journal of Environmental Analytical Chemistry

Volume: 96

Issue number: 3

ISSN (Print): 0306-7319

Ratings:

Scopus rating (2016): CiteScore 1.28 SJR 0.368 SNIP 0.501

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Environmental Chemistry, Soil Science, Health, Toxicology and Mutagenesis, Pollution, Waste Management and Disposal, Water Science and Technology, Public Health, Environmental and Occupational Health

Keywords: DOM, Fluorescence, greywater, humic, ionic strength, proteins, tryptophan, UV-254

DOIs:

10.1080/03067319.2016.1150463

#### Bibliographical note

EXT="Tuhkanen, Tuula"

Source: Scopus

Source ID: 84961206778

Research output: Contribution to journal > Article > Scientific > peer-review

### Phenothiazine and carbazole substituted pyrene based electroluminescent organic semiconductors for OLED devices

Due to their easy availability, low cost and opportunities for exploiting reactions of bromo substituents, 1,3,6,8-tetrabromopyrene has attracted major attention in the organic electronics community for designing and constructing novel classes of pyrene based organic semiconducting functional materials. In the present work, 1,3,6,8-tetrabromo pyrene was transformed into the corresponding tetrasubstituted carbazole and phenothiazine derivatives using the classical Suzuki coupling reaction. These newly synthesized materials with a carbazole substituent (PY-CA) and a phenothiazine substituent (PY-PH) were characterised thoroughly and were successfully used as an active light-emitting layer in organic light emitting diodes which resulted in blue and green emission with promising device performance. PY-CA exhibited the maximum brightness at around  $2500 \text{ cd m}^{-2}$  and the power efficiency of  $1.5 \text{ lm W}^{-1}$  while that of PY-PH exhibited  $2116 \text{ cd m}^{-2}$  and  $0.45 \text{ lm W}^{-1}$  respectively.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Polymer Science and Engineering Division, Council of Scientific and Industrial Research India, University of Hong Kong, CSIRO Energy Centre, National University of Singapore, Queensland University of Technology QUT

Contributors: Salunke, J. K., Wong, F. L., Feron, K., Manzhos, S., Lo, M. F., Shinde, D., Patil, A., Lee, C. S., Roy, V. A. L., Sonar, P., Wadgaonkar, P. P.

Number of pages: 10

Pages: 1009-1018

Publication date: 7 Feb 2016

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Materials Chemistry C

Volume: 4

Issue number: 5

ISSN (Print): 2050-7534

Ratings:

Scopus rating (2016): CiteScore 5.14 SJR 1.825 SNIP 1.265

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Chemistry

DOIs:

10.1039/c5tc03690a

Source: Scopus

Source ID: 84957013671

Research output: Contribution to journal > Article > Scientific > peer-review

### Ambient-Pressure XPS Study of a Ni-Fe Electrocatalyst for the Oxygen Evolution Reaction

Chemical analysis of solid-liquid interfaces under electrochemical conditions has recently become feasible due to the development of new synchrotron radiation techniques. Here we report the use of "tender" X-ray ambient-pressure X-ray photoelectron spectroscopy (APXPS) to characterize a thin film of Ni-Fe oxyhydroxide electrodeposited on Au as the working electrode at different applied potentials in 0.1 M KOH as the electrolyte. Our results show that the as-prepared 7 nm thick Ni-Fe (50% Fe) film contains Fe and Ni in both their metallic as well as oxidized states, and undergoes further oxidation when the sample is subjected to electrochemical oxidation-reduction cycles. Metallic Fe is oxidized to  $\text{Fe}^{3+}$  and metallic Ni to  $\text{Ni}^{2+/3+}$ . This work shows that it is possible to monitor the chemical nature of the Ni-Fe catalyst as a function of potential when the corresponding current densities are small. This allows for operando measurements just above the onset of OER; however, current densities as they are desired in photoelectrochemical devices ( $\sim 1\text{-}10 \text{ mA cm}^{-2}$ ) could not be achieved in this work, due to ohmic losses in the thin electrolyte film. We use a two-dimensional model to describe the spatial distribution of the electrochemical potential, current density, and pH as a function of the position above the electrolyte meniscus, to provide guidance toward enabling the acquisition of operando APXPS at high current density. The shifts in binding energy of water with applied potential predicted by the model are in good agreement with the experimental values.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Surface Science, SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Department of Chemical and Biomolecular Engineering,

Berkeley, Materials Sciences Division, Lawrence Berkeley National Laboratory, Materials and Corrosion Engineering, Exponent, Inc., Polymer Science and Materials Chemistry  
Contributors: Ali-Löyty, H., Louie, M. W., Singh, M. R., Li, L., Sanchez Casalongue, H. G., Ogasawara, H., Crumlin, E. J., Liu, Z., Bell, A. T., Nilsson, A., Friebel, D.

Number of pages: 7

Pages: 2247-2253

Publication date: 4 Feb 2016

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 120

Issue number: 4

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.189

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

Electronic versions:

MS+SI(post-print). Embargo ended: 4/01/17

DOIs:

10.1021/acs.jpcc.5b10931

URLs:

<http://urn.fi/URN:NBN:fi:tty-201606034213>. Embargo ended: 4/01/17

Source: Scopus

Source ID: 84957588014

Research output: Contribution to journal > Article > Scientific > peer-review

#### Guanidinium Pairing Facilitates Membrane Translocation

Ab initio free energy calculations of guanidinium pairing in aqueous solution confirm the counterintuitive conjecture that the like-charge ion pair is thermodynamically stable. Transferring the guanidinium pair to the inside of a POPC lipid bilayer, like-charge ion pairing is found to occur also inside the membrane defect. It is found to contribute to the nonadditivity of ion transfer, thereby facilitating the presence of ions inside the bilayer. The effect is quantified by free energy decomposition and comparison with ammonium ions, which do not form a stable pair. The presence of two charges inside the center of the bilayer leads to the formation of a pore. Potential consequences for cell penetrating peptides and ion conduction are drawn.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Universität Regensburg, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Bijiňička Cesta 54

Contributors: Allolio, C., Baxova, K., Vazdar, M., Jungwirth, P.

Number of pages: 11

Pages: 143-153

Publication date: 14 Jan 2016

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 120

Issue number: 1

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2016): CiteScore 3.03 SJR 1.345 SNIP 1.023

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/acs.jpcc.5b10404

#### Bibliographical note

EXT="Vazdar, Mario"

Source: Scopus

### Physical and Chemical Characterization of Real-World Particle Number and Mass Emissions from City Buses in Finland

Exhaust emissions of 23 individual city buses at Euro III, Euro IV and EEV (Enhanced Environmentally Friendly Vehicle) emission levels were measured by the chasing method under real-world conditions at a depot area and on the normal route of bus line 24 in Helsinki. The buses represented different technologies from the viewpoint of engines, exhaust after-treatment systems (ATS) and fuels. Some of the EEV buses were fueled by diesel, diesel-electric, ethanol (RED95) and compressed natural gas (CNG). At the depot area the emission factors were in the range of  $0.3\text{--}21 \times 10^{14} \text{ \# (kg fuel)}^{-1}$ ,  $6\text{--}40 \text{ g (kg fuel)}^{-1}$ ,  $0.004\text{--}0.88 \text{ g (kg fuel)}^{-1}$ ,  $0.004\text{--}0.56 \text{ g (kg fuel)}^{-1}$ ,  $0.01\text{--}1.2 \text{ g (kg fuel)}^{-1}$ , for particle number ( $EF_N$ ), nitrogen oxides ( $EF_{NO_x}$ ), black carbon ( $EF_{BC}$ ), organics ( $EF_{Org}$ ), and particle mass ( $EF_{PM_{10}}$ ), respectively. The highest particulate emissions were observed from the Euro III and Euro IV buses and the lowest from the ethanol and CNG-fueled buses, which emitted BC only during acceleration. The organics emitted from the CNG-fueled buses were clearly less oxidized compared to the other bus types. The bus line experiments showed that lowest emissions were obtained from the ethanol-fueled buses whereas large variation existed between individual buses of the same type indicating that the operating conditions by drivers had large effect on the emissions.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, University of Helsinki, Univerzita v Liberci, Finnish Meteorological Institute, Aerosol Physics Laboratory, Helsinki Region Environmental Services Authority (HSY)

Contributors: Pirjola, L., Dittrich, A., Niemi, J. V., Saarikoski, S., Timonen, H., Kuuluvainen, H., Järvinen, A., Kousa, A., Rönkkö, T., Hillamo, R.

Number of pages: 11

Pages: 294-304

Publication date: 5 Jan 2016

Peer-reviewed: Yes

#### Publication information

Journal: Environmental Science and Technology

Volume: 50

Issue number: 1

ISSN (Print): 0013-936X

Ratings:

Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.923

Original language: English

ASJC Scopus subject areas: Chemistry(all), Environmental Chemistry

DOIs:

10.1021/acs.est.5b04105

Source: Scopus

Source ID: 84953432299

Research output: Contribution to journal > Article > Scientific > peer-review

### Heat capacities of crystalline and glassy lithium metaphosphate up to the transition region

Heat capacity measurements have been conducted by means of DSC on both crystalline and glassy lithium metaphosphate, from room temperature up to the melting region. The heat capacity of the glass is slightly higher than that of the crystal. Contrary to the crystal, in the neighborhood of  $T_g$ ,  $C_p$  increases rapidly by  $10 \text{ J mol}^{-1} \text{ K}^{-1}$  conferring to this glass a "fragile character." Nevertheless, the passage through  $T_m$  does not show any discontinuity and the values of the glass and of the crystal are identical. The Debye model appears to be realistic to describe the glass heat capacity to temperature dependence. The Debye temperature and frequency were determined by minimizing the  $R_p$  and  $\chi^2$  parameters of the  $C_v$  fitting curve. From the calculation of the entropy of the liquid at  $T > T_m$ , the excess entropy of the glass at  $T_g$  was determined. Using the dependence of the glass transition on the heating rate, we calculated the values of the activation energy for structural relaxation ( $E_{relax}$ ) and of the lower limit of the glass transition temperature ( $T_g$ ) which is a thermodynamic parameter, contrary to  $T_g$  which is a kinetic parameter.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Electronics and Communications Engineering, Research group: Biomaterials and Tissue Engineering Group, Glass and Ceramic Group, ISCR 6226, University of Rennes, 35700 Rennes, France, University of Rennes 1 - IETR, UMR CNRS 6226 Sciences Chimiques de Rennes

Contributors: Rocherullé, J., Massera, J., Oudadesse, H., Calvez, L., Trolès, J., Zhang, X. H.

Number of pages: 7

Pages: 401-407  
Publication date: 2016  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Thermal Analysis and Calorimetry

Volume: 123

Issue number: 1

ISSN (Print): 1388-6150

Ratings:

Scopus rating (2016): CiteScore 1.76 SJR 0.609 SNIP 0.992

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Condensed Matter Physics

Keywords: Crystal, Glass, Glass transition, Heat capacity

DOIs:

10.1007/s10973-015-4938-9

Source: Scopus

Source ID: 84953636195

Research output: Contribution to journal › Article › Scientific › peer-review

#### Thermal desorption of molecular oxygen from SnO<sub>2</sub> (110) surface: Insights from first-principles calculations

First-principles density functional theory calculations in the generalized gradient approximation, with plane wave basis set and pseudopotentials, have been used to investigate the desorption pathways of molecular oxygen species adsorbed on the SnO<sub>2</sub> (110) surface. Energetics of the thermodynamically favored precursors is studied in dependence on the surface charge provided either by surface defects or by donor type impurities from the near-surface region. The resonant desorption modes of O<sub>2</sub> molecules are examined in the framework of ab initio atomic thermodynamics and relationship of these results to experimental observations is discussed.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Research group: Electronic Structure Theory, South-Ukrainian University

Contributors: Golovanov, V., Golovanova, V., Rantala, T. T.

Number of pages: 8

Pages: 15-22

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physics and Chemistry of Solids

Volume: 89

ISSN (Print): 0022-3697

Ratings:

Scopus rating (2016): CiteScore 1.94 SJR 0.596 SNIP 0.948

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Chemistry(all), Materials Science(all)

Keywords: A. oxides, B. ab initio calculations, C. surface properties

DOIs:

10.1016/j.jpics.2015.10.010

Source: Scopus

Source ID: 84945973267

Research output: Contribution to journal › Article › Scientific › peer-review

#### Remarkable Dependence of the Final Charge Separation Efficiency on the Donor-Acceptor Interaction in Photoinduced Electron Transfer

The unprecedented dependence of final charge separation efficiency as a function of donor-acceptor interaction in covalently-linked molecules with a rectilinear rigid oligo-p-xylene bridge has been observed. Optimization of the donor-acceptor electronic coupling remarkably inhibits the undesirable rapid decay of the singlet charge-separated state to the ground state, yielding the final long-lived, triplet charge-separated state with circa 100% efficiency. This finding is extremely useful for the rational design of artificial photosynthesis and organic photovoltaic cells toward efficient solar energy conversion.

#### General information



Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Kyoto Women's University, Tokushima University, Kobe University, Japan Science and Technology Agency, University of Tokyo  
Contributors: Higashino, T., Yamada, T., Yamamoto, M., Furube, A., Tkachenko, N. V., Miura, T., Kobori, Y., Jono, R., Yamashita, K., Imahori, H.

Pages: 629-633

Publication date: 2016

Peer-reviewed: Yes

### Publication information

Journal: *Angewandte Chemie (International Edition)*

Volume: 55

Issue number: 2

ISSN (Print): 1433-7851

Ratings:

Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.182

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis

Keywords: Charge separation, Electron transfer, Electronic coupling, Exciplexes, Marcus theory

DOIs:

10.1002/anie.201509067

Source: Scopus

Source ID: 84958749577

Research output: Contribution to journal > Article > Scientific > peer-review

### Preferential adsorption of Cu in a multi-metal mixture onto biogenic elemental selenium nanoparticles

Preferential adsorption of Cu contained in wastewaters is desirable as the Cu can then be reprocessed and reused more easily. In this study, biogenic elemental selenium nanoparticles (BioSeNPs) were assessed for their ability to preferentially adsorb Cu from an equimolar mixture containing Cu, Cd and Zn. Variations in metal to BioSeNPs ratios and initial metal solution pH improved the preferential adsorption capacity of BioSeNPs toward Cu, with the ratio of Cu adsorbed to combined Cd and Zn adsorbed varying from 2.3 to 6.6. More than 78% of the added Cu was adsorbed at an initial metal solution pH of 5.2 and metal to BioSeNPs ratio of  $0.21 \text{ mg mg}^{-1}$  when the ratio of Cu adsorbed to the sum of Cd and Zn adsorbed was 2.3. Infrared spectroscopy revealed that the Cu, Cd and Zn were interacting with the hydroxyl and carboxyl surface functional groups of the BioSeNPs. The modeling of BioSeNPs' acid-base titration revealed the presence of high concentrations of carboxylic groups ( $C=60.3 \text{ mol kg}^{-1}$ ) with a  $\text{p}K_a$  of 3.9, providing further evidence of their interaction with Cu. The adsorption of Cu resulted in a lower colloidal stability of the BioSeNPs as indicated by more than 99% retention of added BioSeNPs after adsorption of heavy metals and filtration. BioSeNPs showed a good preferential adsorption capacity toward Cu as compared to other adsorbent. This study provides a proof-of-concept for the preferential adsorption of Cu onto BioSeNPs which are present in the effluent of a bioreactor treating selenium oxyanions containing wastewater.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Tampere University of Technology, Research group: Industrial Bioengineering and Applied Organic Chemistry, Université Paris-Est

Contributors: Jain, R., Dominic, D., Jordan, N., Rene, E. R., Weiss, S., van Hullebusch, E. D., Hübner, R., Lens, P. N. L.

Pages: 917-925

Publication date: 2016

Peer-reviewed: Yes

Early online date: 2015

### Publication information

Journal: *Chemical Engineering Journal*

Volume: 284

ISSN (Print): 1385-8947

Ratings:

Scopus rating (2016): CiteScore 6.34 SJR 1.758 SNIP 1.941

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all), Industrial and Manufacturing Engineering, Environmental Chemistry

Keywords: Biogenic, Copper, FT-IR, Heavy metals, Preferential adsorption, Selenium nanoparticles

DOIs:

10.1016/j.cej.2015.08.144

Source: Scopus

Source ID: 84942540702

Research output: Contribution to journal › Article › Scientific › peer-review

### A Three-Component Assembly Promoted by Boronic Acids Delivers a Modular Fluorophore Platform (BASHY Dyes)

A multicomponent reaction, symbolized on the cover by a puzzle, was used to prepare a molecularly diverse series of boron-containing heterocyclic dyes [boronic acid salicylidenehydrazone (BASHY) dyes]. The dyes are strongly fluorescent in the green-yellow spectral range and were applied in cell-staining protocols to visualize lipid droplets (as shown in the background of the picture). More information can be found in the Full Paper by U.Pischel, et al. (DOI: 10.1002/chem.201503943).

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Urban circular bioeconomy (UrCirBio), Faculdade de Farmacia da Universidade de Lisboa, Universidad de Huelva

Contributors: Santos, F. M. F., Rosa, J. N., Candeias, N. R., Carvalho, C. P., Matos, A. I., Ventura, A. E., Florindo, H. F., Silva, L. C., Pischel, U., Gois, P. M. P.

Pages: 1631-1637

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: Chemistry: A European Journal

Volume: 22

Issue number: 5

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.082

Original language: English

ASJC Scopus subject areas: Chemistry(all)

DOIs:

10.1002/chem.201503943

Source: Scopus

Source ID: 84958037809

Research output: Contribution to journal › Article › Scientific › peer-review

### The electrooxidation-induced structural changes of gold di-superatomic molecules: Au<sub>23</sub> vs. Au<sub>25</sub>

The gold cluster compounds Au<sub>38</sub>(SC<sub>2</sub>H<sub>4</sub>Ph)<sub>24</sub> and [Au<sub>25</sub>(PPh<sub>3</sub>)<sub>10</sub>(SC<sub>2</sub>H<sub>4</sub>Ph)<sub>5</sub>Cl<sub>2</sub>]<sup>2+</sup> are known to possess bi-icosahedral Au<sub>23</sub> and Au<sub>25</sub> cores, respectively, inside their ligand shells. These Au cores can be viewed as quasi-molecules composed of two Au<sub>13</sub> superatoms sharing three and one Au<sup>+</sup> atoms, respectively. In the present work, we studied the structural changes of these gold di-superatomic molecules upon electrooxidation via spectroelectrochemical techniques, X-ray absorption fine structure analysis, and density functional theory calculations. The Au<sub>23</sub> core was electrochemically stable, but the Au<sub>25</sub> core underwent irreversible structural change. This marked difference in the stability of the oxidized states is ascribed to differences in the bonding scheme of Au<sub>13</sub> units and/or the bonding nature of the protecting ligands.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Research group: Materials and Molecular Modeling, Department of Chemistry, University of Tokyo, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Aalto University

Contributors: Matsuo, S., Yamazoe, S., Goh, J., Akola, J., Tsukuda, T.

Number of pages: 6

Pages: 4822-4827

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 18

Issue number: 6

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.117

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

Electronic versions:

Matsuo et al. 2016

DOIs:

10.1039/c5cp06969f

URLs:

<http://urn.fi/URN:NBN:fi:tty-201702101112>

Source: Scopus

Source ID: 84957557018

Research output: Contribution to journal › Article › Scientific › peer-review

### **Cholesterol oxidation products and their biological importance**

The main biological cause of oxysterols is the oxidation of cholesterol. They differ from cholesterol by the presence of additional polar groups that are typically hydroxyl, keto, hydroperoxy, epoxy, or carboxyl moieties. Under typical conditions, oxysterol concentration is maintained at a very low and precisely regulated level, with an excess of cholesterol. Like cholesterol, many oxysterols are hydrophobic and hence confined to cell membranes. However, small chemical differences between the sterols can significantly affect how they interact with other membrane components, and this in turn can have a substantial effect on membrane properties. In this spirit, this review describes the biological importance and the roles of oxysterols in the human body. We focus primarily on the effect of oxysterols on lipid membranes, but we also consider other issues such as enzymatic and nonenzymatic synthesis processes of oxysterols as well as pathological conditions induced by oxysterols.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic

Contributors: Kulig, W., Cwiklik, L., Jurkiewicz, P., Rog, T., Vattulainen, I.

Number of pages: 17

Pages: 144-160

Publication date: 2016

Peer-reviewed: Yes

### **Publication information**

Journal: Chemistry and Physics of Lipids

Volume: 199

ISSN (Print): 0009-3084

Ratings:

Scopus rating (2016): CiteScore 2.78 SJR 0.971 SNIP 0.88

Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Biology, Organic Chemistry, Cell Biology

Keywords: Biological membranes, Biophysical properties, Cholesterol, Oxidation, Oxidative stress, Oxysterols, Reactive oxygen species

DOIs:

10.1016/j.chemphyslip.2016.03.001

### **Bibliographical note**

EXT="Cwiklik, Lukasz"

Source: Scopus

Source ID: 84959894259

Research output: Contribution to journal › Article › Scientific › peer-review

### **High-Yield Excited Triplet States in Pentacene Self-Assembled Monolayers on Gold Nanoparticles through Singlet Exciton Fission**

One of the major drawbacks of organic-dye-modified self-assembled monolayers on metal nanoparticles when employed for efficient use of light energy is the fact that singlet excited states on dye molecules can be easily deactivated by means of energy transfer to the metal surface. In this study, a series of 6,13-bis(triisopropylsilylethynyl)pentacene-alkanethiolate monolayer protected gold nanoparticles with different particle sizes and alkane chain lengths were successfully synthesized and were employed for the efficient generation of excited triplet states of the pentacene derivatives by singlet fission. Time-resolved transient absorption measurements revealed the formation of excited triplet states in high yield

(172±26%) by suppressing energy transfer to the gold surface.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Keio University

Contributors: Kato, D., Sakai, H., Tkachenko, N. V., Hasobe, T.

Pages: 5230-5234

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: Angewandte Chemie (International Edition)

Volume: 55

Issue number: 17

ISSN (Print): 1433-7851

Ratings:

Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.182

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis

Keywords: Gold, Nanoparticles, Pentacene, Self-assembled monolayers, Singlet fission

DOIs:

10.1002/anie.201601421

Source: Scopus

Source ID: 84961773531

Research output: Contribution to journal > Article > Scientific > peer-review

#### Superfluorinated Ionic Liquid Crystals Based on Supramolecular, Halogen-Bonded Anions

Unconventional ionic liquid crystals in which the liquid crystallinity is enabled by halogen-bonded supramolecular anions [C<sub>n</sub>F<sub>2n+1</sub>-I...I...I-C<sub>n</sub>F<sub>2n+1</sub>]<sup>-</sup> are reported. The material system is unique in many ways, demonstrating for the first time 1) ionic, halogen-bonded liquid crystals, and 2) imidazolium-based ionic liquid crystals in which the occurrence of liquid crystallinity is not driven by the alkyl chains of the cation.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Cavallo, G., Terraneo, G., Monfredini, A., Saccone, M., Priimägi, A., Pilati, T., Resnati, G., Metrangolo, P., Bruce, D. W.

Pages: 6300-6304

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: Angewandte Chemie (International Edition)

Volume: 55

Issue number: 21

ISSN (Print): 1433-7851

Ratings:

Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.182

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis

Keywords: Fluorophobic effect, Halogen bonding, Ionic liquid crystals, Self-assembly, Supramolecular chemistry

Electronic versions:

Superfluorinated Ionic Liquid Crystals Based on Supramolecular, Halogen-Bonded Anions

DOIs:

10.1002/anie.201601278

URLs:

<http://urn.fi/URN:NBN:fi:tty-201605033937>

Source: Scopus

Source ID: 84979722901

Research output: Contribution to journal > Article > Scientific > peer-review

### Compatibilization of natural rubber/nitrile rubber blends by sol-gel nano-silica generated by in situ method

**Abstract:** Controlled growth of in situ silica, into natural rubber (NR)/nitrile rubber (NBR) blend (40/60 composition by weight) following solution sol-gel method, results in a coherent blend morphology with enhanced composite properties. Similar composites, i.e., in situ silica-filled NR/NBR blend (40/60 by weight), showed better mechanical properties than any other composition that were prepared by soaking sol-gel method in earlier study. However, silica content in the rubber blend was limited to 20 phr (parts per hundred parts of rubber) and could not be increased under experimental condition following soaking sol-gel method. In the present work, silica content is increased (up to 30 phr) beyond that limit for the same blend composition. Accordingly, mechanical properties of the NR/NBR composites are improved. Use of a silane coupling agent, viz., bis-(3-triethoxysilylpropyl)-tetra sulfide, in the reactive sol-gel system during in situ silica generation brings in remarkable effect in silica distribution, rubber-filler interaction and mechanical properties of the composites. TEM micrographs of the selected composites reveal that silica is mostly grown at the interfacial region, when silane is used in particular. This results in further enhancement in mechanical properties and compatibility of the blend at the same silica content as evident from stress-strain and dynamic mechanical analysis studies. The reinforcement of effect in situ silica is assessed by Guth-Gold equation and modified form of Guth equation (with shape factor  $f = 2.53$ ). The results are supported by the detailed studies on rheological, morphological, mechanical and viscoelastic properties of the composites. Graphical Abstract: [Figure not available: see fulltext.]

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Visvesvaraya National Institute of Technology, Indian Rubber Manufacturers Research Association, Department of Elastomers, Leibniz-Institut für Polymerforschung Dresden E.V., University of Kalyani

Contributors: Bansod, N. D., Kapgade, B. P., Das, C., Das, A., Basu, D., Debnath, S. C.

Number of pages: 12

Pages: 548-559

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: JOURNAL OF SOL-GEL SCIENCE AND TECHNOLOGY

Volume: 80

Issue number: 2

ISSN (Print): 0928-0707

Ratings:

Scopus rating (2016): CiteScore 1.53 SJR 0.48 SNIP 0.678

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Biomaterials, Ceramics and Composites, Electronic, Optical and Magnetic Materials, Materials Chemistry

Keywords: In situ silica, Reinforcement, Rubber blend, Rubber-filler interaction, Silane treatment, Sol-gel method  
DOIs:

10.1007/s10971-016-4114-0

Source: Scopus

Source ID: 84974817789

Research output: Contribution to journal > Article > Scientific > peer-review

### Controllable Electronic Structures and Photoinduced Processes of Bay-Linked Perylene-dimide Dimers and a Ferrocene-Linked Triad

A series of perylene-3,4,9,10-bis(dicarboximide) (PDI) dimers linked through the bay regions was systematically synthesized to examine the electronic structures and photophysical properties in dependence on the distance and orientation between the two PDI units. The spectroscopic and electrochemical measurements suggested that the coupling value of a directly linked PDI dimer (PDI)<sub>2</sub> is much larger than those of para- and meta-phenylene-bridged PDI dimers p-(PDI)<sub>2</sub> and m-(PDI)<sub>2</sub>. The width of Davydov splitting was quantitatively evaluated to compare the coupling values between the two PDI units in these dimers by absorption spectroscopy in frozen 2-methyl-THF. Excimer formation of PDI dimers induced the strong fluorescence quenching and large red-shifts. Femtosecond transient absorption revealed a broad absorption derived from an excimer in the range from about 600nm to the near-IR region. The rate constants of formation and decay of the excimer are strongly dependent on the coupling values. Time-resolved measurements on ferrocene-linked p-(PDI)<sub>2</sub> revealed a competition between the photoinduced processes of electron transfer and excimer formation in PhCN, which is in sharp contrast with the sole electron-transfer process in toluene.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry  
Contributors: Horinouchi, H., Sakai, H., Araki, Y., Sakanoue, T., Takenobu, T., Wada, T., Tkachenko, N. V., Hasobe, T.  
Pages: 9631-9641  
Publication date: 2016  
Peer-reviewed: Yes

#### Publication information

Journal: Chemistry: A European Journal

Volume: 22

Issue number: 28

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.082

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Electron transfer, Electronic structure, Excimers, Perylenediimides, Photophysics

DOIs:

10.1002/chem.201601058

Source: Scopus

Source ID: 84973522054

Research output: Contribution to journal > Article > Scientific > peer-review

#### Fire-safe and environmentally friendly nanocomposites based on layered double hydroxides and ethylene propylene diene elastomer

In this work we describe layered double hydroxide (LDH), known as naturally occurring hydrotalcite, based rubber composites that can serve as outstanding fire retardant elastomeric materials. The preparation and detailed characterization of these composites are presented in this study. The inherent slow sulfur cure nature of EPDM rubber is considerably improved by the addition of LDH as realised by the observation of a shortening of the vulcanization time and an improvement of ultimate rheometric torque. This behavior of LDH signifies not only the filler-like character of itself, but also offers vulcanization active surface properties of layered double hydroxide particles. A good rubber-filler interaction was also realised by observing a positive shift of the glass transition temperature of ethylene propylene diene rubber (EPDM) in dynamic mechanical analysis (DMA). The flame retardant property was studied by the cone calorimeter test. The cone calorimeter investigation with sulfur cured gum rubber compounds found a peak heat release rate (PHRR) value of  $654 \text{ kW m}^{-2}$ . However, at a higher phr loading of Zn-Al LDH i.e., at 40 phr and 100 phr, the PHRR is diminished to  $311 \text{ kW m}^{-2}$  and  $161 \text{ kW m}^{-2}$ , respectively. Thus, this present work can pave the way to fabricate environmentally friendly fire retardant elastomeric composites for various applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Institut für Werkstoffwissenschaft, Leibniz-Institut für Polymerforschung Dresden E.V., IMDEA Materials Institute, Cochin University of Science and Technology

Contributors: Basu, D., Das, A., Wang, D. Y., George, J. J., Stöckelhuber, K. W., Boldt, R., Leuteritz, A., Heinrich, G.

Number of pages: 12

Pages: 26425-26436

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: RSC Advances

Volume: 6

Issue number: 31

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all)

DOIs:

10.1039/c5ra27444c

Source: Scopus

Source ID: 84961194468

Research output: Contribution to journal > Article > Scientific > peer-review

### **Alginate microgels created by selective coalescence between core drops paired with an ultrathin shell**

We report a highly biocompatible and practical protocol to create alginate microgels for bioactive encapsulation. Double-emulsion drops composed of dual cores enclosed by an ultrathin shell are prepared in a capillary microfluidic device, which exhibit selective coalescence between the cores. When the cores are laden with alginate precursors and divalent ions, respectively, coalescence leads to the formation of alginate microgels in the fused core of double-emulsion drops. The microgel can be rapidly released into a continuous water phase by rupturing the liquid shell. This method neither involves any toxic chemical cues for gelation nor long-term exposure to oil, thereby providing highly biocompatible encapsulation.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Korea Institute of Energy Research, Chungnam National University

Contributors: Lee, T. Y., Ramasamy, P., Oh, Y. K., Lee, K., Kim, S. H.

Number of pages: 7

Pages: 3232-3238

Publication date: 2016

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Materials Chemistry B

Volume: 4

Issue number: 19

ISSN (Print): 2050-7518

Ratings:

Scopus rating (2016): CiteScore 4.8 SJR 1.468 SNIP 1.007

Original language: English

ASJC Scopus subject areas: Biomedical Engineering, Medicine(all), Chemistry(all), Materials Science(all)

DOIs:

10.1039/c6tb00580b

Source: Scopus

Source ID: 84970955852

Research output: Contribution to journal > Article > Scientific > peer-review

### **Decoding the Morphological Diversity in Two Dimensional Crystalline Porous Polymers by Core Planarity Modulation**

Two new chemically stable triazine- and phenyl-core-based crystalline porous polymers (CPPs) have been synthesized using a single-step template-free solvothermal route. Unique morphological diversities were observed for these CPPs [2,3-DhaTta (ribbon) and 2,3-DhaTab (hollow sphere)] by simply altering the linker planarity. A detailed time-dependent study established a significant correlation between the molecular level structures of building blocks with the morphology of CPPs. Moreover, a DFT study was done for calculating the interlayer stacking energy, which revealed that the extent of stacking efficiency is responsible for governing the morphological diversity in these CPPs.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: CSIR-National Chemical Laboratory, Indian Institute of Technology Kanpur, Indian Institute of Technology Bombay, Jacobs University Bremen, Polymer Science and Engineering Division

Contributors: Halder, A., Kandambeth, S., Biswal, B. P., Kaur, G., Roy, N. C., Addicoat, M., Salunke, J. K., Banerjee, S., Vanka, K., Heine, T., Verma, S., Banerjee, R.

Number of pages: 5

Pages: 7806-7810

Publication date: 2016

Peer-reviewed: Yes

#### **Publication information**

Journal: Angewandte Chemie (International Edition)

Volume: 55

Issue number: 27

ISSN (Print): 1433-7851

Ratings:

Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.182

Original language: English

ASJC Scopus subject areas: Catalysis, Chemistry(all)

Keywords: covalent organic frameworks, density functional calculations, dihedral angles, morphology, stacking interactions

DOIs:

10.1002/anie.201600087

URLs:

<http://www.scopus.com/inward/record.url?scp=84960155135&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84960155135

Research output: Contribution to journal > Article > Scientific > peer-review

### **Photoresponsive liquid-crystalline polymer films bilayered with an inverse opal structure**

An inverse opal film was layered to a photodeformable film, and its photoresponsive behavior was investigated. This bilayer films composed of colorless photonic crystal using inverse opal structures and colored photoresponsive layers with azobenzene-containing CLCP.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tokyo Institute of Technology, Japan Science and Technology Agency

Contributors: Akamatsu, N., Aizawa, M., Tatsumi, R., Hisano, K., Priimägi, A., Shishido, A.

Number of pages: 4

Pages: 145-148

Publication date: 2016

Peer-reviewed: Yes

#### **Publication information**

Journal: JOURNAL OF PHOTOPOLYMER SCIENCE AND TECHNOLOGY

Volume: 29

Issue number: 1

ISSN (Print): 0914-9244

Ratings:

Scopus rating (2016): CiteScore 0.88 SJR 0.3 SNIP 0.558

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Polymers and Plastics, Materials Chemistry

Keywords: Bragg diffraction, Inverse opal structure, Photoresponsive film

DOIs:

10.2494/photopolymer.29.145

Source: Scopus

Source ID: 84981200985

Research output: Contribution to journal > Article > Scientific > peer-review

### **Optical non-contact pH measurement in cell culture with sterilizable, modular parts**

A non-contact real time pH measurement using fully modular optical parts is described for phenol-red medium cell cultures. The modular parts can be sterilized, and once the measurement is started at the beginning of culture, no recalibration or maintenance is needed till the end of the culture. Measurements can be carried out without any special manual attention. The modular assembly of LED and sensor cassettes is unique, robust, reusable and reproducible. pH is measured in an intact closed flow system, without wasting any culture medium. A special pump encapsulation enables the system to be effortlessly functional in extremely humid incubator environments. This avoids lengthy sample tubings in and out of the incubator, associated large temperature changes and CO<sub>2</sub> buffering issues. A new correction model to compensate errors caused e.g. by bilayers in spectrometric pH measurement is put-forward, which improves the accuracy of pH estimation significantly. The method provides resolution down to 0.1 pH unit in physiological pH range with mean absolute error 0.02.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Automation Science and Engineering, Research area: Microsystems, Research area: Dynamic Systems, Research area: Measurement Technology and Process Control, Tampere University Hospital

Contributors: Kattiparambil Rajan, D., Patrikoski, M., Verho, J., Sivula, J., Ihalainen, H., Miettinen, S., Lekkala, J.

Number of pages: 6

Pages: 755-761



Publication date: 2016  
Peer-reviewed: Yes  
Early online date: 1 Dec 2016

#### Publication information

Journal: Talanta  
Volume: 161  
ISSN (Print): 0039-9140  
Ratings:

Scopus rating (2016): CiteScore 4.19 SJR 1.168 SNIP 1.276

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Cell culture non-contact pH measurement, Cell culture optical pH measurement, Cell culture pH measurement, Long term pH measurement, Phenol red medium pH measurement

DOIs:

10.1016/j.talanta.2016.09.021

Source: Scopus

Source ID: 84988421947

Research output: Contribution to journal › Article › Scientific › peer-review

#### On describing the optoelectronic characteristics of poly(benzodithiophene-: Co -quinoxaline)-fullerene complexes: The influence of optimally tuned density functionals

Here, we investigate the effects of both tuning the range-separation parameter of long-range corrected (LRC) density functionals and including dispersion corrections on describing the local optoelectronic properties of polymer-fullerene interfaces that are critical to the performance of polymer solar cells (PSCs). Focusing on recently studied (Chen, et al., Chem. Mater., 2012, 24, 4766-4772) PSC active layers derived from poly(benzodithiophene-co-quinoxaline) and substituted fullerene PC<sub>71</sub>BM, we compare the performance of global hybrid functionals (B3LYP and B3LYP-D) alongside two LRC functionals ( $\omega$ B97X and  $\omega$ B97X-D) and their optimally tuned (OT) analogs (OT- $\omega$ B97X and OT- $\omega$ B97X-D). Our results confirm that OT-LRC functionals generally improve the description of the optical properties of the individual materials with respect to experiment. For electron-donor (eD)-electron-acceptor (eA) complexes used to describe the local optoelectronic properties of the material interface, PC<sub>71</sub>BM is found to preferentially settle near the quinoxaline acceptor units on the copolymer backbone, regardless of the functional, though dispersion corrections have a strong influence on the intermolecular distances and, in turn, the nature of the excited states. All functionals yield very similar descriptions of the transition maxima for the complexes, i.e. predominant local excitations on the copolymer. Importantly, tuning the range-separation parameter of the LRC functional is shown to have a profound effect, as the OT functionals allow for the description of the charge transfer states of the eD-eA complexes, while the non-tuned LRC functionals predict only local intramolecular excitations. These results hold considerable importance for deriving the appropriate physical understanding of the interfacial structure-property-function relationships of PSCs.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Department of Physics, University of Kentucky

Contributors: Kastinen, T., Niskanen, M., Risko, C., Cramariuc, O., Hukka, T. I.

Number of pages: 17

Pages: 27654-27670

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 18

Issue number: 39

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.117

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1039/c6cp04567g

Source: Scopus

Source ID: 84991045177

Research output: Contribution to journal › Article › Scientific › peer-review

### Enhanced adsorption of orthophosphate and copper onto hydrochar derived from sewage sludge by KOH activation

Hydrothermal carbonization producing hydrochar from organic waste is increasingly gaining attention to deal with the challenge of excess waste activated sludge produced during centralized aerobic wastewater treatment. Hydrochar is used as an adsorbent for the removal of organics, metals and biotic contaminants. This study demonstrated the application of KOH activated hydrochar, called enhanced hydrochar (EHC) derived from sewage sludge, for the removal of orthophosphate from wastewater by means of batch adsorption, zetametry and infrared spectroscopy. The maximum  $Q_e$  -  $PO_4^{3-}$  of EHC was  $14.3 \text{ mg orthophosphate adsorbed per g of EHC}$  when the initial orthophosphate concentration was increased to  $150 \text{ mg L}^{-1}$ . The application of orthophosphate removal by EHC from the effluent of a constructed wetland was demonstrated by achieving more than 97% orthophosphate removal at an EHC dosage of  $6.0 \text{ g L}^{-1}$  and an initial orthophosphate concentration of  $13.1 \text{ mg L}^{-1}$ . pH dependent adsorption experiments and infrared spectroscopy showed the orthophosphate removal by EHC was due to the replacement of hydroxyl groups by orthophosphate in the EHC. Acid-base titration showed the KOH washing of the raw hydrochar (RHC) led to a 1.7 times increase in the hydroxyl groups in EHC compared to RHC. This study further confirmed the higher uptake capacity of EHC compared to RHC towards copper as a model divalent cation. EHC can thus be applied for the removal of both anions (orthophosphate) and cations (copper) from wastewater.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education, Zurich University of Applied Sciences

Contributors: Spataru, A., Jain, R., Chung, J. W., Gerner, G., Krebs, R., Lens, P. N. L.

Number of pages: 8

Pages: 101827-101834

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: RSC Advances

Volume: 6

Issue number: 104

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

DOIs:

10.1039/c6ra22327c

URLs:

<http://www.scopus.com/inward/record.url?scp=84994048409&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84994048409

Research output: Contribution to journal > Article > Scientific > peer-review

### Nonlinear transmittance and optical power limiting in magnesium ferrite nanoparticles: effects of laser pulsewidth and particle size

We report comparative measurements of size dependent nonlinear transmission and optical power limiting in nanocrystalline magnesium ferrite ( $MgFe_2O_4$ ) particles excited by short (nanosecond) and ultrashort (femtosecond) laser pulses. A standard sol-gel technique is employed to synthesize particles in the size range of 10-50 nm, using polyvinyl alcohol as the chelating agent. The structure and morphology of the samples are studied using X-ray diffraction, scanning electron microscopy and transmission electron microscopy. Growth of the particles in time is tracked through Fourier transform infrared spectroscopy. Nonlinear transmission measurements have been carried out using the open aperture Z-scan technique employing 532 nm, 5 nanosecond pulses and 800 nm, 100 femtosecond pulses, respectively. The measured optical nonlinearity is primarily of a reverse saturable absorption (RSA) nature, arising mostly from excited state absorption for nanosecond excitation, and two-photon absorption for femtosecond excitation. The optical limiting efficiency is found to increase with particle size for both cases. The calculated nonlinear parameters indicate that these materials are potential candidates for optical limiting applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, National Institute of Technology Karnataka, International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Raman Research Institute

Contributors: Perumbilavil, S., Sridharan, K., Abraham, A. R., Janardhanan, H. P., Kalarikkal, N., Philip, R.  
Number of pages: 8  
Pages: 106754-106761  
Publication date: 2016  
Peer-reviewed: Yes

#### Publication information

Journal: RSC Advances

Volume: 6

Issue number: 108

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

DOIs:

10.1039/c6ra15788b

Source: Scopus

Source ID: 84995977139

Research output: Contribution to journal > Article > Scientific > peer-review

### **Synthesis, crystal structure, physico-chemical characterization and dielectric properties of a new hybrid material, 1-Ethylpiperazine-1,4-dium tetrachlorocadmate**

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Carthage University, Laboratoire de chimie des Matériaux, Faculté des Sciences de Bizerte, Université de Carthage

Contributors: Dhieb, A. C., Valkonen, A., Rzaigui, M., Smirani, W.

Number of pages: 7

Pages: 50-56

Publication date: 15 Dec 2015

Peer-reviewed: Yes

Early online date: 22 Aug 2015

#### Publication information

Journal: Journal of Molecular Structure

Volume: 1102

ISSN (Print): 0022-2860

Ratings:

Scopus rating (2015): CiteScore 1.7 SJR 0.446 SNIP 0.822

Original language: English

ASJC Scopus subject areas: Spectroscopy, Analytical Chemistry, Inorganic Chemistry, Organic Chemistry

Keywords: Dielectric properties, IR-Raman spectroscopies, NMR spectroscopy, Phase transition, Photoluminescence, X-Ray diffraction

DOIs:

10.1016/j.molstruc.2015.08.044

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<http://www.scopus.com/inward/record.url?scp=84940482600&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84940482600

Research output: Contribution to journal > Article > Scientific > peer-review

### **The formation and physical properties of the particle emissions from a natural gas engine**

Natural gas engine particle emissions were studied using an old gasoline engine modified to run with natural gas. The tests were steady-state tests performed on two different low loads in an engine dynamometer. Exhaust particle number concentration, size distribution, volatility and electric charge were measured. Exhaust particles were observed to have peak diameters below 10 nm. To get the full picture of particle emissions from natural gas engines, size range 1-5 nm is relevant and important to take into consideration. A particle size magnifier (PSM) was used in this engine application for measuring particles smaller than 3 nm and it proved to be a useful instrument when measuring natural gas engine exhaust particles. It is concluded that the detected particles probably originated from the engine cylinders or their vicinity and grew to detectable sizes in the sampling process because a small fraction of the particles were observed to carry electric charge

and the particles did not evaporate totally at 265°C.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Aerosol Physics, Research group: The Instrumentation, Emissions, and Atmospheric Aerosols Group, Engineering materials science and solutions (EMASS), Urban circular bioeconomy (UrCirBio), Atmospheric Composition Research, VTT Technical Research Centre of Finland, Finnish Meteorological Institute

Contributors: Alanen, J., Saukko, E., Lehtoranta, K., Murtonen, T., Timonen, H., Hillamo, R., Karjalainen, P., Kuuluvainen, H., Harra, J., Keskinen, J., Rönkkö, T.

Number of pages: 7

Pages: 155-161

Publication date: 15 Dec 2015

Peer-reviewed: Yes

#### Publication information

Journal: Fuel

Volume: 162

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2015): CiteScore 4.46 SJR 1.781 SNIP 2.091

Original language: English

ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

Keywords: Fine particle emission, Internal combustion engine, Natural gas, Particle formation

DOIs:

10.1016/j.fuel.2015.09.003

URLs:

<http://www.scopus.com/inward/record.url?scp=84941782885&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84941782885

Research output: Contribution to journal › Article › Scientific › peer-review

#### Modeling carbon dioxide transport in PDMS-based microfluidic cell culture devices

Maintaining a proper pH level is crucial for successful cell culturing. Mammalian cells are commonly cultured in incubators, where the cell culture medium is saturated with a mixture of air and 5% carbon dioxide (CO<sub>2</sub>). Therefore, to keep cell culture medium pH in an acceptable level outside these incubators, a suitable CO<sub>2</sub> concentration must be dissolved in the medium. However, it can be very difficult to control and measure precisely local concentration levels. Furthermore, possible undesired concentration gradients generated during long-term cell culturing are almost impossible to detect. Therefore, we have developed a computational model to estimate CO<sub>2</sub> transport in silicone-based microfluidic devices. An extensive set of experiments was used to validate the finite element model. The model parameters were obtained using suitable measurement set-ups and the model was validated using a fully functional cell cultivation device. The predictions obtained by the simulations show very good responses to experiments. It is shown in this paper how the model helps to understand the dynamics of CO<sub>2</sub> transport in silicone-based cell culturing devices possessing different geometries, thus providing cost-effective means for studying different device designs under a variety of experimental conditions without the need of actual testing. Finally, based on the results from the computational model, an alternative strategy for feeding CO<sub>2</sub> is proposed to accelerate the system performance such that a faster and more uniform CO<sub>2</sub> concentration response is achieved in the area of interest.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Automation Science and Engineering, Department of Materials Science, Research group: Paper Converting and Packaging, BioMediTech, Integrated Technologies for Tissue Engineering Research (ITTE), BioMediTech

Contributors: Mäki, A. J., Peltokangas, M., Kreutzer, J., Auvinen, S., Kallio, P.

Number of pages: 10

Pages: 515-524

Publication date: 1 Dec 2015

Peer-reviewed: Yes

#### Publication information

Journal: Chemical Engineering Science

Volume: 137

ISSN (Print): 0009-2509

Ratings:

Scopus rating (2015): CiteScore 2.96 SJR 1.022 SNIP 1.55

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all), Applied Mathematics, Industrial and Manufacturing Engineering

Keywords: Carbon dioxide, Finite element method, Mass transport, Microfluidics cell culturing, Numerical simulation, pH

Electronic versions:

Revised\_Manuscript\_AnttiMaki. Embargo ended: 28/07/17

DOIs:

10.1016/j.ces.2015.06.065

URLs:

<http://urn.fi/URN:NBN:fi:tty-201807252020>. Embargo ended: 28/07/17

### Bibliographical note

ORG=ase,0.9

ORG=mol,0.1

Source: Scopus

Source ID: 84938149959

Research output: Contribution to journal > Article > Scientific > peer-review

### Differential basal-to-apical accessibility of lamin A/C epitopes in the nuclear lamina regulated by changes in cytoskeletal tension

Nuclear lamins play central roles at the intersection between cytoplasmic signalling and nuclear events. Here, we show that at least two N- and C-terminal lamin epitopes are not accessible at the basal side of the nuclear envelope under environmental conditions known to upregulate cell contractility. The conformational epitope on the Ig-domain of A-type lamins is more buried in the basal than apical nuclear envelope of human mesenchymal stem cells undergoing osteogenesis (but not adipogenesis), and in fibroblasts adhering to rigid (but not soft) polyacrylamide hydrogels. This structural polarization of the lamina is promoted by compressive forces, emerges during cell spreading, and requires lamin A/C multimerization, intact nucleoskeleton-cytoskeleton linkages (LINC), and apical-actin stress-fibre assembly. Notably, the identified Ig-epitope overlaps with emerin, DNA and histone binding sites, and comprises various laminopathy mutation sites. Our findings should help decipher how the physical properties of cellular microenvironments regulate nuclear events.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Laboratory of Applied Mechanobiology, HCI e 486.1

Contributors: Ihalainen, T. O., Aires, L., Herzog, F. A., Schwartlander, R., Moeller, J., Vogel, V.

Number of pages: 10

Pages: 1252-1261

Publication date: 1 Dec 2015

Peer-reviewed: Yes

### Publication information

Journal: Nature Materials

Volume: 14

Issue number: 12

ISSN (Print): 1476-1122

Ratings:

Scopus rating (2015): CiteScore 25.58 SJR 16.382 SNIP 8.962

Original language: English

ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials, Condensed Matter Physics, Materials Science(all), Chemistry(all)

DOIs:

10.1038/nmat4389

URLs:

<http://www.scopus.com/inward/record.url?scp=84947870719&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84947870719

Research output: Contribution to journal > Article > Scientific > peer-review

### Graphene-intercalated Fe<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> heterojunctions for efficient photoelectrolysis of water

Interfacial modification of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> multilayer photoanodes by intercalating few-layer graphene (FLG) was found to improve water splitting efficiency due to superior transport properties, when compared to individual iron and titanium oxides and heterojunctions thereof. Both metal oxides and graphene sheets were grown by plasma-enhanced chemical vapor deposition. Compared to the onset potential achieved for  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> films (1 V vs. RHE), the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> bilayer structure yielded a better onset potential (0.3 V vs. RHE). Heterojunctioned bilayers exhibited a higher photocurrent density (0.32 mA cm<sup>-2</sup> at 1.23 V vs. RHE) than the single  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> layer (0.22 mA cm<sup>-2</sup> at 1.23 V vs. RHE), indicating more efficient light harvesting and higher concentration of photogenerated charge carriers. For more efficient charge transport at the interface, a few layer graphene sheet was intercalated into the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> interface, which substantially increased the photocurrent density to 0.85 mA cm<sup>-2</sup> (1.23 V vs. RHE) and shifted the onset potential (0.25 V vs. RHE). Ultrafast transient absorption spectroscopy studies indicated that the incorporation of FLG between the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> layers resulted in reduced recombination in the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> layer. The results showed that graphene intercalation improved the charge separation and the photocurrent density of the FTO/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>/FLG/TiO<sub>2</sub> system.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Universitat zu Koln, Institute of Inorganic Chemistry, Ruhr-Universität Bochum

Contributors: Kaouk, A., Ruoko, T. P., Gönüllü, Y., Kaunisto, K., Mettenböcker, A., Gurevich, E., Lemmetyinen, H., Ostendorf, A., Mathur, S.

Number of pages: 7

Pages: 101401-101407

Publication date: 13 Nov 2015

Peer-reviewed: Yes

#### Publication information

Journal: RSC Advances

Volume: 5

Issue number: 123

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2015): CiteScore 3.42 SJR 0.947 SNIP 0.834

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all)

Electronic versions:

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<http://www.scopus.com/inward/record.url?scp=84948652698&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84948652698

Research output: Contribution to journal > Article > Scientific > peer-review

### Tri-functionality of Fe<sub>3</sub>O<sub>4</sub>-embedded carbon microparticles in microalgae harvesting

Microalgae have received significant attention as promising resources for biodiesel. However, the downstream processes for the production of biodiesel, which range from cultivation, harvesting, dewatering, and lipid extraction to oil upgrading, are economically impracticable and can be improved. Therefore, efficient microalgal harvesting and integrated technologies are required to realize microalgae-based biodiesel. Herein, tri-functional (cationic, magnetic, and lipophilic) carbon microparticles filled with magnetite (Fe<sub>3</sub>O<sub>4</sub>) are synthesized through one-step aerosol spray pyrolysis and applied in microalgal harvesting and serial microalgal lipid entrapment. Carbon microparticles are tri-functional in the following respects: (i) the cationic carbon microparticles facilitate flocculation with anionic microalgae due to electrostatic attractions; (ii) the magnetic properties of the carbon microparticles, owing to embedded magnetites, enable the separation of microalgal flocs from low concentration cultures (~2 g L<sup>-1</sup>) with a separation efficiency of 99%; and (iii) the lipophilicity enables the recovery of lipid droplets extracted from oleaginous microalgae. Microalgal lipids are directly separated through adsorption onto magnetic carbon microparticles from concentrated microalgal slurries after harvesting. The tri-functionality may facilitate the integrated use of magnetic carbon microparticles in microalgal biorefineries and the tri-functional microparticles could potentially be applied in various areas such as biomedicine, catalysis, magnetism, energy materials, and environmental remediation.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), KAIST, Korea Institute of Energy Research

Contributors: Seo, J. Y., Lee, K., Ramasamy, P., Kim, B., Lee, S. Y., Oh, Y. K., Park, S. B.

Number of pages: 9

Pages: 206-214

Publication date: 5 Nov 2015

Peer-reviewed: Yes

### Publication information

Journal: Chemical Engineering Journal

Volume: 280

ISSN (Print): 1385-8947

Ratings:

Scopus rating (2015): CiteScore 5.68 SJR 1.676 SNIP 1.895

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all), Industrial and Manufacturing Engineering, Environmental Chemistry

Keywords: Aerosol spray pyrolysis, Cationic functionality, Lipophilicity, Magnetic materials, Microalgae harvesting

DOIs:

10.1016/j.cej.2015.05.122

URLs:

<http://www.scopus.com/inward/record.url?scp=84933567826&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84933567826

Research output: Contribution to journal > Article > Scientific > peer-review

### Effect of rubber polarity on selective wetting of carbon nanotubes in ternary blends

Based on atomic force microscopy (AFM) and Fourier transform infrared spectroscopy (FTIR) analysis of the rubber-filler gel (wetting concept) the kinetics of selective wetting of carbon nanotubes (CNTs) in ternary styrene butadiene rubber (SBR)/butadiene rubber (BR)/natural rubber (NR) blends was qualitatively and quantitatively characterized. Almost all CNTs are found to be wetted by the non-polar NR but not by the other non-polar rubber like BR or weakly polar SBR. It was proposed that phospholipids, which are linked to the  $\alpha$ -terminal of NR can interact with the CNT surface through cation- $\pi$  interactions forming strong bonding between NR and CNTs. Using the corrected surface tension value of NR, which involves the effect of phospholipids found in our previous work the selective wetting of CNTs in ternary rubber blends can be well predicted using the Z-model for a thermodynamic equilibrium state. By replacing the non-polar BR by a polar rubber like nitrile butadiene rubber (NBR) as a blend component CNTs are wetted by NBR slightly more than by NR thanks to the strong interaction between CNTs and nitrile groups of NBR. SBR remains unbound to CNTs in both blends.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Institut für Polymerwerkstoffe E.V., Martin-Luther-University Halle-Wittenberg, Fraunhofer IWM, Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V., Vietnamese Academy of Science and Technology Institute of Chemistry, Polymer Service GmbH Merseburg

Contributors: Le, H. H., Parsaker, M., Sriharish, M. N., Henning, S., Menzel, M., Wießner, S., Das, A., Do, Q. K., Heinrich, G., Radosch, H. J.

Number of pages: 12

Pages: 960-971

Publication date: 1 Nov 2015

Peer-reviewed: Yes

### Publication information

Journal: Express Polymer Letters

Volume: 9

Issue number: 11

ISSN (Print): 1788-618X

Ratings:

Scopus rating (2015): CiteScore 2.88 SJR 0.929 SNIP 1.553

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Physical and Theoretical Chemistry, Polymers and Plastics, Organic Chemistry, Materials Chemistry

Keywords: Carbon nanotubes, Manocomposites, Rubber blends, Selective filler wetting

DOIs:

10.3144/expresspolymlett.2015.87

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Source: Scopus

Source ID: 84940868023

Research output: Contribution to journal › Article › Scientific › peer-review

### Comparison of different cationized proteins as biomaterials for nanoparticle-based ocular gene delivery

Cationized polymers have been proposed as transfection agents for gene therapy. The present work aims to improve the understanding of the potential use of different cationized proteins (atelocollagen, albumin and gelatin) as nanoparticle components and to investigate the possibility of modulating the physicochemical properties of the resulting nanoparticle carriers by selecting specific protein characteristics in an attempt to improve current ocular gene-delivery approaches. The toxicity profiles, as well as internalization and transfection efficiency, of the developed nanoparticles can be modulated by modifying the molecular weight of the selected protein and the amine used for cationization. The most promising systems are nanoparticles based on intermediate molecular weight gelatin cationized with the endogenous amine spermine, which exhibit an adequate toxicological profile, as well as effective association and protection of pDNA or siRNA molecules, thereby resulting in higher transfection efficiency and gene silencing than the other studied formulations.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Federal University of Rio Grande do Sul, University of Santiago de Compostela (USC), University Clinical Hospital of Santiago de Compostela (IDIS)

Contributors: Zorzi, G. K., Párraga, J. E., Seijo, B., Sanchez, A.

Number of pages: 9

Pages: 533-541

Publication date: 1 Nov 2015

Peer-reviewed: Yes

#### Publication information

Journal: Colloids and Surfaces B: Biointerfaces

Volume: 135

ISSN (Print): 0927-7765

Ratings:

Scopus rating (2015): CiteScore 4.26 SJR 1.085 SNIP 1.232

Original language: English

ASJC Scopus subject areas: Biotechnology, Surfaces and Interfaces, Physical and Theoretical Chemistry, Colloid and Surface Chemistry

Keywords: Cationized proteins, Gene therapy, Nanoparticles, pDNA, siRNA

DOIs:

10.1016/j.colsurfb.2015.08.008

URLs:

<http://www.scopus.com/inward/record.url?scp=84939622417&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84939622417

Research output: Contribution to journal › Article › Scientific › peer-review

### Submolecular Plasticization Induced by Photons in Azobenzene Materials

We demonstrate experimentally for the first time that the illumination of azobenzene derivatives leads to changes in molecular environment similar to those observed on heating but that are highly heterogeneous at the submolecular scale. This localized photoplasticization, which can be associated with a free volume gradient, helps to understand the puzzling phenomenon of photoinduced macroscopic material flow and photoexpansion upon illumination far below the glass transition temperature ( $T_g$ ). The findings stem from the correlation of infrared (IR) spectral band shifts measured upon illumination with those measured at controlled temperatures for two amorphous DR1-functionalized azo derivatives, a polymer, pDR1A, and a molecular glass, gDR1. This new approach reveals that IR spectroscopy can be used as an efficient label-free molecular-scale thermometer that allows the assignment of an effective temperature ( $T_{eff}$ ) to each moiety in these compounds when irradiated. While no band shift is observed upon illumination for the vibrational modes assigned to backbone moieties of pDR1A and gDR1 and a small band shift is found for the spacer moiety, dramatic band shifts are recorded for the azo moiety, corresponding to an increase in  $T_{eff}$  of up to nearly 200 °C and a molecular environment that is equivalent to thermal heating well above the bulk  $T_g$  of the material. An irradiated azo-containing material thus combines characteristic properties of amorphous materials both below and above its bulk  $T_g$ . The direct measurement of  $T_{eff}$  is a powerful probe of the local environment at the submolecular scale, paving the way toward better rationalization of photoexpansion and the athermal malleability of azo-containing materials upon illumination below their  $T_g$ .

g



### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Département de Chimie, Succ. Centre-Ville, Royal Military College of Canada

Contributors: Vapaavuori, J., Laventure, A., Bazuin, C. G., Lebel, O., Pellerin, C.

Number of pages: 8

Pages: 13510-13517

Publication date: 28 Oct 2015

Peer-reviewed: Yes

### Publication information

Journal: Journal of the American Chemical Society

Volume: 137

Issue number: 42

ISSN (Print): 0002-7863

Ratings:

Scopus rating (2015): CiteScore 12.81 SJR 6.775 SNIP 2.6

Original language: English

ASJC Scopus subject areas: Catalysis, Chemistry(all), Biochemistry, Colloid and Surface Chemistry

DOIs:

10.1021/jacs.5b06611

URLs:

<http://www.scopus.com/inward/record.url?scp=84946020103&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84946020103

Research output: Contribution to journal > Article > Scientific > peer-review

### Photomechanical Energy Transfer to Photopassive Polymers through Hydrogen and Halogen Bonds

The supramolecular assembly of photoactive azobenzenes with passive polymers via halogen or hydrogen bonding is a cost-effective way to design materials for various photomechanical applications that convert light energy directly into macroscopic motion, for instance, in all-optical surface patterning and photochemical imaging of plasmonic structures. To elucidate the molecular-level origins of this motion, we show, by coupling dynamic infrared spectroscopy to a photo-orientation setup, that supramolecular bonds above a certain interaction strength threshold are photostable under vigorous photoisomerization cycling and capable of translating the photo-orientation of azobenzenes into the orientation of nonabsorbing host polymer side chains. A correlation is found between azobenzene photoinduced molecular orientation and macroscopic all-optical surface patterning efficiency. The improved performance of halogen-bonded systems in photopatterning applications can be related to the absence of a plasticizing effect on the polymer matrix, which may enable the material to retain an optimal glass transition temperature, in contrast to hydrogen-bonded and nonbonded references. Thus, our results provide design guidelines in terms of the nature and strength of the supramolecular interaction and of the degree of azo functionalization needed to optimize the motion transfer to passive polymers.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Département de Chimie, Succ. Centre-Ville, Aalto University, Politecnico di Milano, Royal Military College of Canada

Contributors: Vapaavuori, J., Heikkinen, I. T. S., Dichiarante, V., Resnati, G., Metrangolo, P., Sabat, R. G., Bazuin, C. G., Priimagi, A., Pellerin, C.

Number of pages: 8

Pages: 7535-7542

Publication date: 27 Oct 2015

Peer-reviewed: Yes

### Publication information

Journal: Macromolecules

Volume: 48

Issue number: 20

ISSN (Print): 0024-9297

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Scopus rating (2015): CiteScore 5.82 SJR 2.357 SNIP 1.58

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry

DOIs:

10.1021/acs.macromol.5b01813

URLs:

<http://www.scopus.com/inward/record.url?scp=84945400553&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

EXT="Vapaavuori, Jaana"

Source: Scopus

Source ID: 84945400553

Research output: Contribution to journal > Article > Scientific > peer-review

#### In Situ Photocontrol of Block Copolymer Morphology during Dip-Coating of Thin Films

We demonstrate a unique combination of simultaneous top-down and bottom-up control of the morphology of block copolymer films by application of in situ optical irradiation during dip-coating. A light-addressable and block-selective small molecule, 4-butyl-4'-hydroxyazobenzene (BHAB), is introduced into a diblock copolymer of polystyrene and poly(4-vinylpyridine) (PS-P4VP) of 28.4 wt % P4VP via supramolecular chemistry, notably by hydrogen bonding to P4VP. We show that the spherical morphology of thin films dip-coated from a THF solution at slow withdrawal rates in the dark convert to cylindrical morphology when dip-coated under illumination. This is attributed to volume expansion of the P4VP/BHAB phase due to trans-cis photoisomerization combined with a light-induced increase in BHAB uptake in the film. The demonstrated photocontrol highlights the potential of dip-coating as a scalable film preparation method that can be easily coupled with external stimuli to direct nanostructured self-assembly in the films as solvent evaporates.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Département de Chimie, Succ. Centre-Ville

Contributors: Vapaavuori, J., Grosrenaud, J., Pellerin, C., Bazuin, C. G.

Number of pages: 5

Pages: 1158-1162

Publication date: 20 Oct 2015

Peer-reviewed: Yes

#### Publication information

Journal: ACS Macro Letters

Volume: 4

Issue number: 10

ISSN (Print): 2161-1653

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Scopus rating (2015): CiteScore 5.91 SJR 2.392 SNIP 1.403

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry

DOIs:

10.1021/acsmacrolett.5b00483

URLs:

<http://www.scopus.com/inward/record.url?scp=84946032702&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84946032702

Research output: Contribution to journal > Article > Scientific > peer-review

#### Production of sulfonated polyetheretherketone/polypropylene fibers for photoactive textiles

New photocatalytic fibers made of sulfonated polyetheretherketone (SPEEK)/polypropylene (PP) are melt compounded and melt spun, first on laboratory scale and then on a semi-industrial scale. Fiber spinnability is optimized and the fibers are characterized using mechanical testing, electron paramagnetic resonance (EPR) spectroscopy, and scanning electron microscopy (SEM). According to the results, the fiber spinnability remains at a good level up to 10 wt % SPEEK concentration. Optimal processing temperature is 200°C due to the thermal degradation at higher temperatures. EPR measurements show good and long-lasting photoactivity after the initial irradiation but also decay in the radical intensity during several irradiation cycles. Mechanical tenacity of the SPEEK/PP 5:95 fiber is approximately 20% lower than for otherwise similar PP fiber. The fiber is a potential alternative to compete against TiO<sub>2</sub>-based products but more research needs to be done to verify the real-life performance.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Department of Mechanical Engineering and Industrial Systems, Research area: Sustainable Machine Systems, University College of Borås, Högskolan i Borås, Next Technology Tecnotessile Società Nazionale di Ricerca S.r.l., Department of Biotechnology, Chemistry and Pharmacy, University of Siena

Contributors: Mylläri, V., Fatarella, E., Ruzzante, M., Pogni, R., Baratto, M. C., Skrifvars, M., Syrjälä, S., Järvelä, P.  
Publication date: 1 Oct 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Applied Polymer Science

Volume: 132

Issue number: 39

Article number: 42595

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2015): CiteScore 1.74 SJR 0.587 SNIP 0.846

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)

Keywords: blends, fibers, functionalization of polymers, photochemistry, textiles

DOIs:

10.1002/app.42595

URLs:

<http://www.scopus.com/inward/record.url?scp=84937636904&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

ORG=mol,0.5

ORG=mei,0.5

EXT="Skrifvars, Mikael"

Source: Scopus

Source ID: 84937636904

Research output: Contribution to journal > Article > Scientific > peer-review

#### Atomic-level characterization of transport cycle thermodynamics in the glycerol-3-phosphate: Phosphate antiporter

Membrane transporters actively translocate their substrate by undergoing large-scale structural transitions between inward-(IF) and outward-facing (OF) states ('alternating-access' mechanism). Despite extensive structural studies, atomic-level mechanistic details of such structural transitions, and as importantly, their coupling to chemical events supplying the energy, remain amongst the most elusive aspects of the function of these proteins. Here we present a quantitative, atomic-level description of the functional thermodynamic cycle for the glycerol-3-phosphate:phosphate antiporter GlpT by using a novel approach in reconstructing the free energy landscape governing the IF  $\leftrightarrow$  OF transition along a cyclic transition pathway involving both apo and substrate-bound states. Our results provide a fully atomic description of the complete transport process, offering a structural model for the alternating-access mechanism and substantiating the close coupling between global structural transitions and local chemical events.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Univ Illinois, University of Illinois System, University of Illinois Urbana-Champaign, Frederick Seitz Mat Res Lab, Dept Mat Sci & Engr, Department of Biochemistry

Contributors: Moradi, M., Enkavi, G., Tajkhorshid, E.

Publication date: 29 Sep 2015

Peer-reviewed: Yes

#### Publication information

Journal: Nature Communications

Volume: 6

Article number: 8393

ISSN (Print): 2041-1723

Ratings:

Scopus rating (2015): CiteScore 11.23 SJR 6.287 SNIP 2.815

Original language: English

ASJC Scopus subject areas: Biochemistry, Genetics and Molecular Biology(all), Chemistry(all), Physics and Astronomy(all)

DOIs:

10.1038/ncomms9393

URLs:

<http://www.scopus.com/inward/record.url?scp=84942854331&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84942854331

### PIP2 and Talin Join Forces to Activate Integrin

Integrins are major players in cell adhesion and migration, and malfunctions in controlling their activity are associated with various diseases. Nevertheless, the details of integrin activation are not completely understood, and the role of lipids in the process is largely unknown. Herein, we show using atomistic molecular dynamics simulations that the interplay of phosphatidylinositol 4,5-bisphosphate (PIP2) and talin may directly alter the conformation of integrin  $\alpha 11\beta 3$ . Our results provide a new perspective on the role of PIP2 in integrin activation and indicate that the charged PIP2 lipid headgroup can perturb a clasp at the cytoplasmic face of the integrin heterodimer.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Tampere University of Technology, Research group: Biological Physics and Soft Matter, BioMediTech, Computational Science X (CompX), Multi-scaled biodata analysis and modelling (MultiBAM), BioMediTech, Department of Physics and Chemistry, University of Southern Denmark, Fimlab Laboratories Ltd

Contributors: Orlowski, A., Kukkurainen, S., Pöyry, A., Rissanen, S., Vattulainen, I., Hytönen, V. P., Róg, T.

Number of pages: 9

Pages: 12381-12389

Publication date: 24 Sep 2015

Peer-reviewed: Yes

Early online date: 26 Aug 2015

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 119

Issue number: 38

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/acs.jpcc.5b06457

#### Bibliographical note

AUX=fys,"Pöyry, Annika"

Source: Scopus

Source ID: 84942342622

Research output: Contribution to journal › Article › Scientific › peer-review

### Construction of an Interconnected Nanostructured Carbon Black Network: Development of Highly Stretchable and Robust Elastomeric Conductors

In the present work, a strong filler-filler network of conductive carbon black was strategically established in an elastomer matrix, which leads to a unique combination of electrical and mechanical properties. The novelty of our composites was the development of a strong percolated morphology of nanostructured conducting carbon black particles by the incorporation of relatively large nonreinforcing spherical silica particles, inside the soft elastomer matrix. This technique allowed us to fabricate solution styrene butadiene rubber (S-SBR) composites with outstanding electrical conductivity of 40 S/m, tensile strength  $\sim 10$  MPa, and extensibility up to 200%. Furthermore, the electrical conductivity was strain-independent up to 50% elongation strain. The electrical conductivity was found to be unaltered after 2000 loading-unloading cycles. This is the first ever report of a robust elastomeric system with such high electrical conductivity where all the basic ingredients used were selected from well-known commercially available raw materials of rubber industry. This work directly manifests an industrially viable method for preparing high-performance elastic conductors that can be utilized in robust and flexible applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V., Technische Universität Dresden, Institut für Werkstoffwissenschaft, Institut für Polymerwerkstoffe E.V., Elkem AS, Silicon Materials

Contributors: Bhagavatheswaran, E. S., Parsekar, M., Das, A., Le, H. H., Wiessner, S., Stöckelhuber, K. W., Schmaucks, G., Heinrich, G.

Number of pages: 9

Pages: 21723-21731  
Publication date: 17 Sep 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 119

Issue number: 37

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.24

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

10.1021/acs.jpcc.5b06629

URLs:

<http://www.scopus.com/inward/record.url?scp=84941928016&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84941928016

Research output: Contribution to journal › Article › Scientific › peer-review

#### Effect of spraying parameters on the microstructural and corrosion properties of HVOF-sprayed Fe-Cr-Ni-B-C coatings

Thermally sprayed Fe-based coatings have been extensively studied as future solution in order to replace more expensive, harmful and environmentally dangerous Ni- and WC-based coatings for several industrial applications where high corrosion and wear resistance are required. The aim of the present study is to investigate the effect of spraying parameters on the microstructure and the corrosion resistance of Fe-based coatings manufactured with the High Velocity Air Fuel (HVOF) thermal spray process. Six sets of thermal spraying parameters have been chosen and their effect on the overall quality of coatings was investigated. All HVOF coatings showed comparably dense microstructure with near-zero oxidation, proving the high quality of the deposition process. However, higher anti-corrosion and mechanical properties were achieved by increasing the spraying air pressure and decreasing the particle feeding rate without altering the thickness and the overall deposition rate. Powder feeding rate was reported to have a remarkable effect on microstructure and corrosion properties. Coatings with beneficial compressive residual stresses were successfully obtained by increasing air pressure during spraying which resulted in improved microstructural and corrosion properties.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Surface Engineering, Engineering materials science and solutions (EMASS), University of Modena and Reggio Emilia, Department of Engineering Enzo Ferrari

Contributors: Milanti, A., Matikainen, V., Koivuluoto, H., Bolelli, G., Lusvarghi, L., Vuoristo, P.

Number of pages: 10

Pages: 81-90

Publication date: 15 Sep 2015

Peer-reviewed: Yes

#### Publication information

Journal: Surface and Coatings Technology

Volume: 277

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2015): CiteScore 2.46 SJR 0.852 SNIP 1.37

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces

Keywords: Corrosion behaviour, Fe-based coating, HVOF, Structure

DOIs:

10.1016/j.surfcoat.2015.07.018

URLs:

<http://www.scopus.com/inward/record.url?scp=84939782846&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84939782846

Research output: Contribution to journal › Article › Scientific › peer-review

### Superatom Model for Ag-S Nanocluster with Delocalized Electrons

Several Ag-S nanoclusters where the cluster core comprises mixed metal (main component) and sulfur atoms show superatomic orbitals in the conduction band edge. However, there are no superatomic states, i.e., delocalized electrons, in the valence band, and the clusters in question can be labeled as “zerovalent”. We show here an example of an Ag-S cluster which fulfills the superatom model and has delocalized electrons: The recently synthesized and characterized  $[Ag_62S_{12}(StBu)_{32}]^{2+}$  cluster has four delocalized valence electrons based on a simple counting rule, and we compare it to the zerovalent cluster  $[Ag_62S_{13}(StBu)_{32}]^{4+}$ . Our electronic structure analysis confirms the existence of superatomic states in the valence and conduction bands, but the locations of these states do not agree completely with the conventional prediction based on the spherical Jellium model.  $[Ag_62S_{12}(StBu)_{32}]^{2+}$  displays the 1S2 electronic shell closure at the Fermi energy instead of the 1S21P2 configuration as suggested by its electron count. This shift of energy levels and electron shell closing has been introduced by the core-shell structure of the cluster. Our optical absorption simulation can reproduce the features observed in the experiments, and we assign these features to the transitions involving superatomic states within the conduction band.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research group: Materials and Molecular Modeling, Computational Science X (CompX), COMP Centre of Excellence, Department of Applied Physics, Aalto University

Contributors: Goh, J. Q., Akola, J.

Number of pages: 8

Pages: 21165-21172

Publication date: 10 Sep 2015

Peer-reviewed: Yes

Early online date: 19 Aug 2015

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 119

Issue number: 36

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Ratings:

Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.24

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

10.1021/acs.jpcc.5b05824

URLs:

<http://www.scopus.com/inward/record.url?scp=84941254956&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84941254956

Research output: Contribution to journal > Article > Scientific > peer-review

### Molecular Design of Light-Responsive Hydrogels, for in Situ Generation of Fast and Reversible Valves for Microfluidic Applications

Reversible light-responsive hydrogel valves with response characteristics compatible for microfluidics have been obtained by optimization of molecular design of spiropyran photoswitches and gel composition. Self-protonating gel formulations were exploited, wherein acrylic acid was copolymerized in the hydrogel network as an internal proton donor, to achieve a swollen state of the hydrogel in water at neutral pH. Light-responsive properties were endowed upon the hydrogels by copolymerization of spiropyran chromophores, using electron withdrawing and donating groups to tune the gel-swelling and shrinkage behavior. In all cases, the shrinkage was determined by the water diffusion rate, while for the swelling the isomerization kinetics is the rate-determining step. For one hydrogel, reversible and reproducible volume changes were observed. Finally, gel-valves integrated within microfluidic channels were fabricated, allowing reversible and repeatable operation, with opening and closing of the valve in minutes.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Eindhoven University of Technology, Dublin City University

Contributors: Ter Schiphorst, J., Coleman, S., Stumpel, J. E., Ben Azouz, A., Diamond, D., Schenning, A. P. H. J.

Number of pages: 7

Pages: 5925-5931

Publication date: 8 Sep 2015

Peer-reviewed: Yes

### Publication information

Journal: Chemistry of Materials

Volume: 27

Issue number: 17

ISSN (Print): 0897-4756

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Scopus rating (2015): CiteScore 9.38 SJR 3.958 SNIP 2.038

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Chemical Engineering(all), Chemistry(all)

DOIs:

10.1021/acs.chemmater.5b01860

URLs:

<http://www.scopus.com/inward/record.url?scp=84941088068&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84941088068

Research output: Contribution to journal > Article > Scientific > peer-review

### Measuring synthesis yield in graphene oxide synthesis by modified hummers method

Synthesis of graphene oxide by the modified Hummers method and measuring the synthesis yield were investigated.

Based on the results, a comprehensive method to measure graphene oxide synthesis yield was proposed, which will allow comparison of future literature results. In addition, changes are proposed to the exfoliation procedure to improve the yield of the modified Hummers synthesis. With the proposed method, systematic error of the concentration measurement was calculated to be  $\pm 0.08 \times 10^{-3}$  g mL<sup>-1</sup>. In addition, changes proposed to the graphene oxide exfoliation process can improve the synthesis yield by up to 70%.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Ceramic materials, Tampere University of Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group:

Materials Characterization, Engineering materials science and solutions (EMASS), University of Helsinki

Contributors: Frankberg, E. J., George, L., Efimov, A., Honkanen, M., Pessi, J., Levänen, E.

Number of pages: 5

Pages: 755-759

Publication date: 2 Sep 2015

Peer-reviewed: Yes

### Publication information

Journal: Fullerenes Nanotubes and Carbon Nanostructures

Volume: 23

Issue number: 9

ISSN (Print): 1536-383X

Ratings:

Scopus rating (2015): CiteScore 1.62 SJR 0.278 SNIP 0.596

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Physical and Theoretical Chemistry, Materials Science(all), Atomic and Molecular Physics, and Optics

Keywords: Concentration, Graphene oxide, Hummers method, Synthesis, Yield

Electronic versions:

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DOIs:

10.1080/1536383X.2014.993754

URLs:

<http://urn.fi/URN:NBN:fi:tty-201603173654>

### Bibliographical note

Versio ja lupa ok 26.1.2016 KK

Source: Scopus

Source ID: 84929598253

Research output: Contribution to journal > Article > Scientific > peer-review

### Unintentional boron contamination of MBE-grown GaInP/AlGaInP quantum wells

The effects of unintentional boron contamination on optical properties of GaInP/AlGaInP quantum well structures grown by molecular beam epitaxy (MBE) are reported. Photoluminescence and secondary-ion mass spectrometry (SIMS) measurements revealed that the optical activity of boron-contaminated quantum wells is heavily affected by the amount of boron in GaInP/AlGaInP heterostructures. The boron concentration was found to increase when cracking temperature of the phosphorus source was increased. Boron incorporation was enhanced also when aluminum was present in the material.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications, Frontier Photonics, VTT Technical Research Centre of Finland

Contributors: Tukiainen, A., Likonen, J., Toikkanen, L., Leinonen, T.

Pages: 60-63

Publication date: 1 Sep 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Crystal Growth

Volume: 425

ISSN (Print): 0022-0248

Ratings:

Scopus rating (2015): CiteScore 1.63 SJR 0.686 SNIP 1.051

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Materials Chemistry, Inorganic Chemistry

Keywords: A1. Defects, A1. Impurities, A3. Molecular beam epitaxy, B1. Phosphides, B2. Semiconducting III-V materials

DOIs:

10.1016/j.jcrysgro.2015.02.048

URLs:

<http://www.sciencedirect.com/science/article/pii/S0022024815001384> (Link to paper in Sciencedirect)

Source: Scopus

Source ID: 84951561374

Research output: Contribution to journal > Article > Scientific > peer-review

### Searching for a robust strategy for minimizing alkali chlorides in fluidized bed boilers during burning of high SRF-energy-share fuel

To meet the increasing volume of waste to be treated via energy recovery, high SRF-energy-share fuel is being fired in conventional waste-to-energy facilities. In this work, corrosion related risk during firing of 70 e-% share (target fuel) is studied and compared against the base case fuel containing 50 e-% share. Cl and S concentration is highest in the target fuel as a direct result of increasing the proportion of SRF in the fuel mixture. Br, Zn and Pb showed the same trend. Meanwhile, the concentration of Na, K, Al and Si are highly dependent on the type of the SRF fired. The corrosion risk of the base and target fuels are analyzed using the composition of the fine aerosol fraction and deposit samples measured near the vicinity of the superheater. Surprisingly aerosols for the target fuel are less risky - having less Cl and more S, than that of the base fuel. The effects of sulfur based additives - elemental sulfur and sulfate injection, and fuel substitution on the risk of superheater corrosion are likewise analyzed. All these strategies can reduce the concentration of Cl in the aerosols, however it is concluded that sulfate injection is considered as a robust strategy for mitigating alkali chloride formation. Sulfate injection is able to reduce Cl in the aerosols and deposits regardless of the quality of the fuel mixture. Robust strategies are important in ensuring the boiler performance during high SRF-energy share firing. An attempt of linking the quality of the deposits and the properties of the flue gas and aerosols around the superheater using partial least squares regression is also presented.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), University of Jyväskylä, Valmet Technologies Oy, VTT Technical Research Centre of Finland, Department of Chemistry, Renewable Natural Resources and Chemistry of Living Environment, Stora Enso

Contributors: Bajamundi, C. J. E., Vainikka, P., Hedman, M., Silvennoinen, J., Heinanen, T., Taipale, R., Kontinen, J.

Number of pages: 12

Pages: 25-36

Publication date: 1 Sep 2015

Peer-reviewed: Yes



### Publication information

Journal: Fuel

Volume: 155

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2015): CiteScore 4.46 SJR 1.781 SNIP 2.091

Original language: English

ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

Keywords: Alkali chloride mitigation, Corrosion, SRF, Waste-to-energy

DOIs:

10.1016/j.fuel.2015.03.087

URLs:

<http://www.scopus.com/inward/record.url?scp=84928243284&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84928243284

Research output: Contribution to journal > Article > Scientific > peer-review

### How large are nonadiabatic effects in atomic and diatomic systems?

With recent developments in simulating nonadiabatic systems to high accuracy, it has become possible to determine how much energy is attributed to nuclear quantum effects beyond zero-point energy. In this work, we calculate the non-relativistic ground-state energies of atomic and molecular systems without the Born-Oppenheimer approximation. For this purpose, we utilize the fixed-node diffusion Monte Carlo method, in which the nodes depend on both the electronic and ionic positions. We report ground-state energies for all systems studied, ionization energies for the first-row atoms and atomization energies for the first-row hydrides. We find the ionization energies of the atoms to be nearly independent of the Born-Oppenheimer approximation, within the accuracy of our results. The atomization energies of molecular systems, however, show small effects of the nonadiabatic coupling between electrons and nuclei.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Computational Science X (CompX), University of Illinois at Urbana-Champaign, University of Illinois, Materials Sciences and Technology Division, Oak Ridge National Laboratory

Contributors: Yang, Y., Kylänpää, I., Tubman, N. M., Krogel, J. T., Hammes-Schiffer, S., Ceperley, D. M.

Publication date: Sep 2015

Peer-reviewed: Yes

### Publication information

Journal: Journal of Chemical Physics

Volume: 143

Issue number: 12

Article number: 124308

ISSN (Print): 0021-9606

Ratings:

Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 1.042

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1063/1.4931667

URLs:

<http://www.scopus.com/inward/record.url?scp=84942891339&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84942891339

Research output: Contribution to journal > Article > Scientific > peer-review

### Fe<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> nanosystems by a hybrid PE-CVD/ALD approach: controllable synthesis, growth mechanism, and photocatalytic properties

Supported Fe<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> nanocomposites are fabricated by an original vapor phase synthetic strategy, consisting of the initial growth of Fe<sub>2</sub>O<sub>3</sub> nanosystems on fluorine-doped tin oxide substrates by plasma enhanced-chemical vapor deposition, followed by atomic layer deposition of TiO<sub>2</sub> overlayers with variable thickness, and final thermal treatment in air. A thorough characterization of the target systems is carried out by X-ray diffraction, atomic force microscopy, field emission-scanning electron microscopy, energy dispersive X-ray spectroscopy, transmission electron microscopy, and X-ray photoelectron spectroscopy. High purity nanomaterials characterized by the co-presence of Fe<sub>2</sub>O<sub>3</sub> (hematite) and TiO<sub>2</sub> (anatase), with an intimate Fe<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> contact, are successfully obtained. In addition, photocatalytic tests

demonstrate that, whereas both single-phase oxides do not show appreciable activity, the composite systems are able to degrade methyl orange aqueous solutions under simulated solar light, and even visible light, with an efficiency directly dependent on TiO<sub>2</sub> overlayer thickness. This finding opens attractive perspectives for eventual applications in wastewater treatment.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Padova University, Padova University and INSTM, Department of Physics and Astronomy, University of Turku, Univ Antwerp, University of Antwerp, EMAT, CNR-IENI and INSTM, Department of Chemistry, Department of Chemical and Pharmaceutical Sciences, ICCOM-CNR Trieste Research Unit - INSTM Research Unit, Trieste University

Contributors: Barreca, D., Carraro, G., Warwick, M. E. A., Kaunisto, K., Gasparotto, A., Gombac, V., Sada, C., Turner, S., Van Tendeloo, G., Maccato, C., Fornasiero, P.

Number of pages: 8

Pages: 6219-6226

Publication date: 28 Aug 2015

Peer-reviewed: Yes

#### Publication information

Journal: CrystEngComm

Volume: 17

Issue number: 32

ISSN (Print): 1466-8033

Ratings:

Scopus rating (2015): CiteScore 3.83 SJR 1.04 SNIP 0.98

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics

DOIs:

10.1039/c5ce00883b

URLs:

<http://www.scopus.com/inward/record.url?scp=84938522112&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84938522112

Research output: Contribution to journal › Article › Scientific › peer-review

#### Effects of thinning and heating for TiO<sub>2</sub>/AlInP junctions

TiO<sub>2</sub>/AlInP junctions are used to construct the antireflection coatings for solar cells and to passivate III-V nanostructure surfaces. The thickness of AlInP epilayer affects light absorption and appropriate Al composition determining further the energy barrier for carriers. We report on reducing the AlInP thickness by dry etching down to 10 nm without introducing harmful defect states at TiO<sub>2</sub>/AlInP interface and AlInP/GaInP interface below, according to photoluminescence. Synchrotron-radiation photoelectron spectroscopy reveals that increased oxidation of phosphorus is not harmful to TiO<sub>2</sub>/AlInP and that post heating of the material enhances AlInP oxidation and group III element segregation resulting in decreased material homogeneity.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications, Frontier Photonics, Department of Physics and Astronomy, University of Turku, University of Turku

Contributors: Mäkelä, J., Tuominen, M., Yasir, M., Polojärvi, V., Aho, A., Tukiainen, A., Kuzmin, M., Punkkinen, M. P. J., Laukkanen, P., Kokko, K., Guina, M.

Number of pages: 4

Pages: 6-9

Publication date: 24 Aug 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Electron Spectroscopy and Related Phenomena

Volume: 205

ISSN (Print): 0368-2048

Ratings:

Scopus rating (2015): CiteScore 1.73 SJR 0.817 SNIP 0.813

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Physical and Theoretical Chemistry, Spectroscopy, Condensed Matter Physics, Atomic and Molecular Physics, and Optics, Radiation

Keywords: AllnP, Passivation, Solar cell, TiO<sub>2</sub>

DOIs:

10.1016/j.elspec.2015.08.004

URLs:

<http://www.scopus.com/inward/record.url?scp=84939833093&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

EXT="Laukkanen, P."

EXT="Tuominen, M."

EXT="Kuzmin, M."

Source: Scopus

Source ID: 84939833093

Research output: Contribution to journal › Article › Scientific › peer-review

#### Electrospun Black Titania Nanofibers: Influence of Hydrogen Plasma-Induced Disorder on the Electronic Structure and Photoelectrochemical Performance

This work encompasses a facile method for tailoring surface defects in electrospun TiO<sub>2</sub> nanofibers by employing hydrogen plasma treatments. This amiable processing method was proven with SQUID, EPR, and XPS to be highly effective in generating oxygen vacancies, accompanied by the reduction of Ti<sup>4+</sup> centers to Ti<sup>3+</sup>, resulting in the formation of black titania. The treatment temperature was found to affect the Ti<sup>3+</sup>/Ti<sup>4+</sup> ratios and surface valence, while preserving the original 1D morphology of the titania fibers. Ab initio DFT calculations showed that a high concentration of oxygen vacancies is highly efficient in producing midgap states that enhance the system absorption over the whole visible range, as observed with UV/vis/NIR diffuse reflectance spectroscopy. Pristine TiO<sub>2</sub> nanofibers produced a photocurrent density of similar to 0.02 mA/cm<sup>2</sup> at 1.23 V vs RHE, whereas the hydrogen plasma treatment resulted in up to a 10-fold increase in the photoelectrochemical performance.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Universita degli Studi di Padova, Italy, Univ Cologne, University of Cologne, Dept Chem, Chair Inorgan & Mat Chem, Padova University, INSTM, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Institute of Inorganic Chemistry, Catalonia Institute for Energy Research (IREC), Multiscale Materials Modelling and Tribo Simulation, CNR-IENI

Contributors: Lepcha, A., Maccato, C., Mettenbörger, A., Andreu, T., Mayrhofer, L., Walter, M., Olthof, S., Ruoko, T. P., Klein, A., Moseler, M., Meerholz, K., Morante, J. R., Barreca, D., Mathur, S.

Number of pages: 8

Pages: 18835-18842

Publication date: 20 Aug 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 119

Issue number: 33

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.24

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

Keywords: ROOM-TEMPERATURE, WATER, SURFACE, NANOSTRUCTURES, NANOPARTICLES, PHOTOCATALYSIS, INSULATORS, CONVERSION, DEFECTS, ARRAYS

Electronic versions:

Electrospun\_black\_titania\_nanofibers\_post-print

DOIs:

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URLs:

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Source: Scopus

Source ID: 84939825598

Research output: Contribution to journal › Article › Scientific › peer-review

### **Influence of relative humidity and physical load during storage on dustiness of inorganic nanomaterials: implications for testing and risk assessment**

Dustiness testing using a down-scaled EN15051 rotating drum was used to investigate the effects of storage conditions such as relative humidity and physical loading on the dustiness of five inorganic metal oxide nanostructured powder materials. The tests consisted of measurements of gravimetric respirable dustiness index and particle size distributions. Water uptake of the powders during 7 days of incubation was investigated as an explanatory factor of the changes. Consequences of these varying storage conditions in exposure modelling were tested using the control banding and risk management tool NanoSafer. Drastic material-specific effects on powder respirable dustiness index were observed with the change in  $\text{TiO}_2$  from 30 % RH (639 mg/kg) to 50 % RH (1.5 mg/kg). All five tested materials indicate a decreasing dustiness index with relative humidity increasing from 30 to 70 % RH. Test of powder water uptake showed an apparent link with the decreasing dustiness index. Effects of powder compaction appeared more material specific with both increasing and decreasing dustiness indices observed as an effect of compaction. Tests of control banding exposure models using the measured dustiness indices in three different exposure scenarios showed that in two of the tested materials, one 20 % change in RH changed the exposure banding from the lowest level to the highest. The study shows the importance of powder storage conditions prior to tests for classification of material dustiness indices. It also highlights the importance of correct storage information and relative humidity and expansion of the dustiness test conditions specifically, when using dustiness indices as a primary parameter for source strength in exposure assessment.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Materials Characterization, Engineering materials science and solutions (EMASS), Department of Micro and Nanotechnology, Denmark Technical University DTU, Finnish Institute of Occupational Health, CIC biomaGUNE, National Research Centre for the Working Environment

Contributors: Levin, M., Rojas, E., Vanhala, E., Vippola, M., Liguori, B., Kling, K. I., Koponen, I. K., Mølhave, K., Tuomi, T., Gregurec, D., Moya, S., Jensen, K. A.

Publication date: 14 Aug 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Nanoparticle Research

Volume: 17

Issue number: 8

Article number: 337

ISSN (Print): 1388-0764

Ratings:

Scopus rating (2015): CiteScore 1.97 SJR 0.568 SNIP 0.725

Original language: English

ASJC Scopus subject areas: Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Modelling and Simulation, Chemistry(all), Materials Science(all), Bioengineering

Keywords: Dustiness, Exposure assessment, Nanotechnology, Occupational health, Powder storage, Rotating drum  
DOIs:

10.1007/s11051-015-3139-6

URLs:

<http://www.scopus.com/inward/record.url?scp=84939162642&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84939162642

Research output: Contribution to journal > Article > Scientific > peer-review

### **Effect of Phosphatidic Acid on Biomembrane: Experimental and Molecular Dynamics Simulations Study**

We consider the impact of phosphatidic acid (namely, 1,2-dioleoyl-sn-glycero-3-phosphate, DOPA) on the properties of a zwitterionic (1,2-dipalmitoyl-sn-glycero-3-phosphocholine, DPPC) bilayer used as a model system for protein-free cell membranes. For this purpose, experimental measurements were performed using differential scanning calorimetry and the Langmuir monolayer technique at physiological pH. Moreover, atomistic-scale molecular dynamics (MD) simulations were performed to gain information on the mixed bilayer's molecular organization. The results of the monolayer studies clearly showed that the DPPC/DOPA mixtures are nonideal and the interactions between lipid species change from attractive, at low contents of DOPA, to repulsive, at higher contents of that component. In accordance with these results, the MD simulations demonstrated that both monoanionic and dianionic forms of DOPA have an ordering and condensing effect on the mixed bilayer at low concentrations. For the DOPA monoanions, this is the result of both (i) strong electrostatic interactions between the negatively charged oxygen of DOPA and the positively charged choline groups of DPPC and (ii) conformational changes of the lipid acyl chains, leading to their tight packing according to the so-called umbrella model, in which large headgroups of DPPC shield the hydrophobic part of DOPA (the conical shape lipid) from contact with water. In the case of the DOPA dianions, cation-mediated clustering was observed. Our results provide a detailed molecular-level description of the lipid organization inside the mixed zwitterionic/PA membranes, which is fully supported by the

experimental data.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Computational Science X (CompX), Jagiellonian University, Faculty of Chemistry

Contributors: Kwolek, U., Kulig, W., Wydro, P., Nowakowska, M., Róg, T., Kepczynski, M.

Number of pages: 10

Pages: 10042-10051

Publication date: 6 Aug 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 119

Issue number: 31

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.058

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/acs.jpccb.5b03604

URLs:

<http://www.scopus.com/inward/record.url?scp=84938696964&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84938696964

Research output: Contribution to journal > Article > Scientific > peer-review

#### Formation and stability of carbon nanotube network in natural rubber: Effect of non-rubber components

**Abstract** The formation and stability of carbon nanotube (CNT) network in natural rubber (NR), deproteinized NR (DPNR) and polyisoprene (IR) compound were investigated by means of the method of the online measured electrical conductance in a whole process from processing and rolling over pressing/cross-linking to post-stretching. The kinetics of CNT flocculation was described and explained by taking into consideration the depletion force considered as driving force and the thickness of the bound rubber layer considered as hindering factor. The presence of linked phospholipids in NR and DPNR improves the rubber-filler interaction of CNTs through the cation- $\pi$  bonding that hinders the filler flocculation. The absence of the cation- $\pi$  bonding in CNT/IR compound and the related thin layer of bound rubber are the reason for the strong tendency of flocculation of CNTs in IR even at room temperature. The effect of pressing time, temperature and cross-linking reaction as well as mechanical deformation on the formation and stability of CNT network in NR compounds was also investigated and discussed by taking into consideration the role of the linked phospholipids.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), An-Institut der Hochschule Merseburg, Hochschule

Albstadt-Sigmaringen, Fraunhofer IWM, Vodafone Department of Mobile Communications Systems, Leibniz-Institut für

Polymerforschung Dresden E.V., University of Technology - National University, Vietnamese Academy of Science and

Technology Institute of Chemistry, University of Applied Sciences Osnabrück, Polymer Service Merseburg

Contributors: Le, H. H., Pham, T., Henning, S., Klehm, J., Wießner, S., Stöckelhuber, K. W., Das, A., Hoang, X. T., Do, Q.

K., Wu, M., Vennemann, N., Heinrich, G., Radosch, H. J.

Number of pages: 11

Pages: 111-121

Publication date: 5 Aug 2015

Peer-reviewed: Yes

#### Publication information

Journal: Polymer

Volume: 73

Article number: 18004

ISSN (Print): 0032-3861

Ratings:

Scopus rating (2015): CiteScore 3.72 SJR 1.144 SNIP 1.257

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Polymers and Plastics

Keywords: Carbon nanotubes, Electrical conductivity, Filler network, Nanocomposites, Rubber

DOIs:

10.1016/j.polymer.2015.07.044

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<http://www.scopus.com/inward/record.url?scp=84938566176&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84938566176

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

### Responsive Polymer Photonics

Stimulus-responsive materials: This thesis describes the development of stimulus-responsive polymeric materials based on liquid crystalline polymers and hydrogels. Novel responsive molecular building blocks were designed and synthesised. Specific monomer mixtures were crosslinked by UV-photopolymerisation methods, and the response of the obtained (structured) material was analysed.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Eindhoven University of Technology

Contributors: Stumpel, J. E.

Number of pages: 3

Pages: 533-535

Publication date: 1 Aug 2015

Peer-reviewed: Yes

### Publication information

Journal: Chemistryopen

Volume: 4

Issue number: 4

ISSN (Print): 2191-1363

Ratings:

Scopus rating (2015): CiteScore 3.23 SJR 1.266 SNIP 0.73

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: cholesteric liquid crystals, hydrogels, optical sensors, polymer coatings, responsive materials

DOIs:

10.1002/open.201500104

URLs:

<http://www.scopus.com/inward/record.url?scp=84942363185&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84942363185

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

### Nonlinear Optical Properties of Fluorescent Dyes Allow for Accurate Determination of Their Molecular Orientations in Phospholipid Membranes

Several methods based on single- and two-photon fluorescence detected linear dichroism have recently been used to determine the orientational distributions of fluorescent dyes in lipid membranes. However, these determinations relied on simplified descriptions of nonlinear anisotropic properties of the dye molecules, using a transition dipole-moment-like vector instead of an absorptivity tensor. To investigate the validity of the vector approximation, we have now carried out a combination of computer simulations and polarization microscopy experiments on two representative fluorescent dyes (DiI and F2N12S) embedded in aqueous phosphatidylcholine bilayers. Our results indicate that a simplified vector-like treatment of the two-photon transition tensor is applicable for molecular geometries sampled in the membrane at ambient conditions. Furthermore, our results allow evaluation of several distinct polarization microscopy techniques. In combination, our results point to a robust and accurate experimental and computational treatment of orientational distributions of DiI, F2N12S, and related dyes (including Cy3, Cy5, and others), with implications to monitoring physiologically relevant processes in cellular membranes in a novel way.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Lawrence Berkeley National Laboratory, Department of Cybernetics, Faculty of Applied Sciences, University of West Bohemia, Institute of Nanobiology and Structural Biology GCRC, V.v.i., Academy of Sciences of the Czech Republic, University of South Bohemia

Contributors: Timr, Š., Brabec, J., Bondar, A., Ryba, T., Železný, M., Lazar, J., Jungwirth, P.

Number of pages: 11  
Pages: 9706-9716  
Publication date: 30 Jul 2015  
Peer-reviewed: Yes  
Early online date: 21 Jul 2015

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 119

Issue number: 30

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.058

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/acs.jpcc.5b05123

URLs:

<http://www.scopus.com/inward/record.url?scp=84938277609&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

EXT="Bondar, Alexey"

Source: Scopus

Source ID: 84938277609

Research output: Contribution to journal > Article > Scientific > peer-review

#### High quality sub-10 nm graphene nanoribbons by on-chip PS-b-PDMS block copolymer lithography

A block copolymer self-assembly holds great promise as a rapid, cheap and scalable approach to nanolithography. We present a straightforward method for fabrication of sub-10 nm line patterns from a lamellar polystyrene-b-polydimethylsiloxane (SD) block copolymer with a total average molecular weight of  $10.5 \text{ kg mol}^{-1}$ . Thin SD films directly spin cast onto silicon substrates and on graphene, form regular line patterns of sub-10 nm pitch on the substrates after a few minutes of annealing at  $45 \text{ }^\circ\text{C}$  in the presence of toluene vapour. Perfect pattern alignment was achieved by confining the films inside the trenches of graphoepitaxial substrates. The SD template was furthermore used as a lithographic mask to fabricate high-quality sub-10 nm graphene nanoribbons. This was realized by one step oxygen plasma treatment, which accomplishes three tasks: hardening the PDMS block by oxidation, and etching both the PS block and the graphene under PS. Raman analysis supports the formation of graphene nanoribbons with an average distance between defects corresponding to the oxidized PDMS pitch, with no sign of defects generated in the ribbon channel. This suggests a high degree of protection of the nanoribbons by the hard oxidized PDMS mask formed in situ during oxygen plasma etching.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Micro and Nanotechnology, Danmarks Tekniske Universitet, DTU Informatik, Center for Nanostructured Graphene, Trinity College Dublin

Contributors: Rasappa, S., Caridad, J. M., Schulte, L., Cagliani, A., Borah, D., Morris, M. A., Bøggild, P., Ndoni, S.

Number of pages: 7

Pages: 66711-66717

Publication date: 29 Jul 2015

Peer-reviewed: Yes

#### Publication information

Journal: RSC Advances

Volume: 5

Issue number: 82

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2015): CiteScore 3.42 SJR 0.947 SNIP 0.834

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

DOIs:

10.1039/c5ra11735f

URLs:

<http://www.scopus.com/inward/record.url?scp=84938940393&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84938940393

Research output: Contribution to journal › Article › Scientific › peer-review

### Quantifying non-ergodic dynamics of force-free granular gases

Brownian motion is ergodic in the Boltzmann-Khinchin sense that long time averages of physical observables such as the mean squared displacement provide the same information as the corresponding ensemble average, even at out-of-equilibrium conditions. This property is the fundamental prerequisite for single particle tracking and its analysis in simple liquids. We study analytically and by event-driven molecular dynamics simulations the dynamics of force-free cooling granular gases and reveal a violation of ergodicity in this Boltzmann-Khinchin sense as well as distinct ageing of the system. Such granular gases comprise materials such as dilute gases of stones, sand, various types of powders, or large molecules, and their mixtures are ubiquitous in Nature and technology, in particular in Space. We treat - depending on the physical-chemical properties of the inter-particle interaction upon their pair collisions - both a constant and a velocity-dependent (viscoelastic) restitution coefficient  $\epsilon$ . Moreover we compare the granular gas dynamics with an effective single particle stochastic model based on an underdamped Langevin equation with time dependent diffusivity. We find that both models share the same behaviour of the ensemble mean squared displacement (MSD) and the velocity correlations in the limit of weak dissipation. Qualitatively, the reported non-ergodic behaviour is generic for granular gases with any realistic dependence of  $\epsilon$  on the impact velocity of particles.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Max-Planck Institute for the Physics of Complex Systems, Institute for Physics and Astronomy, University of Potsdam, Babes-Bolyai University, Faculty of Physics, Cluj-Napoca, Romania, Akhiezer Institute for Theoretical Physics, Kharkov Institute of Physics and Technology, M.V. Lomonosov Moscow State University

Contributors: Bodrova, A., Chechkin, A. V., Cherstvy, A. G., Metzler, R.

Number of pages: 8

Pages: 21791-21798

Publication date: 27 Jul 2015

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 17

Issue number: 34

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.188

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1039/c5cp02824h

Source: Scopus

Source ID: 84939865265

Research output: Contribution to journal › Article › Scientific › peer-review

### Photoinduced Electron Transfer in CdSe/ZnS Quantum Dot-Fullerene Hybrids

Photoinduced electron transfer (ET) in CdSe/ZnS core-shell quantum dot (QD) - fullerene (COOH-C<sub>60</sub>) hybrids was studied by the means of time-resolved emission and absorption spectroscopy techniques. A series of four QDs with emission in the range 540-630 nm was employed to investigate the dependence of the electron transfer rate on the QD size. Emission of the QDs is quenched upon hybrid formation, and the quenching mechanism is identified as photoinduced electron transfer from the QD to the fullerene moiety due to the fullerene anion signature observed in transient absorption. In order to obtain quantitative information on the ET reaction, several kinetic data analysis techniques were used, including a conventional multiexponential fitting and a maximum entropy method for emission decay analysis, as well as a distributed decay model based on the Poisson distribution of fullerenes in the hybrids. The latter gradually simplifies the interpretation of the transient absorption spectra and indicates that the spectra of QD cations are essentially similar to those of neutral QDs, differing only by a minor decrease in the intensity and broadening. Furthermore, only a minor decrease in the ET rate with the increasing QD size was observed, the time constants being in the range 100-200 ps for all studied QDs. The charge recombination is extended to 10 ns or longer for all hybrids.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry



Contributors: Virkki, K., Demir, S., Lemmetyinen, H., Tkachenko, N. V.  
Number of pages: 12  
Pages: 17561-17572  
Publication date: 23 Jul 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 119

Issue number: 31

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.24

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

10.1021/acs.jpcc.5b04251

#### Bibliographical note

INT=keb,"Demir, Sinem"

Source: Scopus

Source ID: 84938703282

Research output: Contribution to journal > Article > Scientific > peer-review

#### Role of Internal Water on Protein Thermal Stability: The Case of Homologous G Domains

In this work, we address the question of whether the enhanced stability of thermophilic proteins has a direct connection with internal hydration. Our model systems are two homologous G domains of different stability: the mesophilic G domain of the elongation factor thermal unstable protein from *E. coli* and the hyperthermophilic G domain of the EF-1 $\alpha$  protein from *S. solfataricus*. Using molecular dynamics simulation at the microsecond time scale, we show that both proteins host water molecules in internal cavities and that these molecules exchange with the external solution in the nanosecond time scale. The hydration free energy of these sites evaluated via extensive calculations is found to be favorable for both systems, with the hyperthermophilic protein offering a slightly more favorable environment to host water molecules. We estimate that, under ambient conditions, the free energy gain due to internal hydration is about 1.3 kcal/mol in favor of the hyperthermophilic variant. However, we also find that, at the high working temperature of the hyperthermophile, the cavities are rather dehydrated, meaning that under extreme conditions other molecular factors secure the stability of the protein. Interestingly, we detect a clear correlation between the hydration of internal cavities and the protein conformational landscape. The emerging picture is that internal hydration is an effective observable to probe the conformational landscape of proteins. In the specific context of our investigation, the analysis confirms that the hyperthermophilic G domain is characterized by multiple states and it has a more flexible structure than its mesophilic homologue. (Figure Presented).

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Université Paris Diderot, Laboratoire de Biochimie Théorique, Sapienza University

Contributors: Rahaman, O., Kalimeri, M., Melchionna, S., Hénin, J., Sterpone, F.

Number of pages: 11

Pages: 8939-8949

Publication date: 23 Jul 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 119

Issue number: 29

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.058

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/jp507571u

URLs:

<http://www.scopus.com/inward/record.url?scp=84937843946&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84937843946

Research output: Contribution to journal › Article › Scientific › peer-review

### **Electricity production by a microbial fuel cell fueled by brewery wastewater and the factors in its membrane deterioration**

Electricity production from brewery wastewater using dual-chamber microbial fuel cells (MFCs) with a tin-coated copper mesh in the anode was investigated by changing the hydraulic retention time (HRT). The MFCs were fed with wastewater samples from the inlet (inflow, MFC-1) and outlet (outflow, MFC-2) of an anaerobic digester of a brewery wastewater treatment plant. Both chemical oxygen demand removal and current density were improved by decreasing HRT. The best MFC performance was with an HRT of 0.5 d. The maximum power densities of 8.001 and 1.843  $\mu\text{W}/\text{cm}^2$  were obtained from reactors MFC-1 and MFC-2, respectively. Microbial diversity at different conditions was studied using PCR-DGGE profiling of 16S rRNA fragments of the microorganisms from the biofilm on the anode electrode. The MFC reactor had mainly *Geobacter*, *Shewanella*, and *Clostridium* species, and some bacteria were easily washed out at lower HRTs. The fouling characteristics of the MFC Nafion membrane and the resulting degradation of MFC performance were examined. The ion exchange capacity, conductivity, and diffusivity of the membrane decreased significantly after fouling. The morphology of the Nafion membrane and MFC degradation were studied using scanning electron microscopy and attenuated total reflection-Fourier transform infrared spectroscopy.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Portland State University, Department of Civil and Environmental Engineering, Yildiz Technical University

Contributors: Çetinkaya, A. Y., Koroğlu, E. O., Demir, N. M., Baysoy, D. Y., Özkaya, B., Çakmakçı, M.

Number of pages: 9

Pages: 1068-1076

Publication date: 20 Jul 2015

Peer-reviewed: Yes

### **Publication information**

Journal: Chinese Journal of Catalysis

Volume: 36

Issue number: 7

ISSN (Print): 0253-9837

Ratings:

Scopus rating (2015): CiteScore 2.24 SJR 0.579 SNIP 0.772

Original language: English

ASJC Scopus subject areas: Catalysis, Chemistry(all)

Keywords: Anaerobic processes, Biofilm, Microbial community, Microbial fuel cell, Wastewater treatment

DOIs:

10.1016/S1872-2067(15)60833-6

URLs:

<http://www.scopus.com/inward/record.url?scp=84934932934&partnerID=8YFLogxK> (Link to publication in Scopus)

### **Bibliographical note**

EXT="Çakmakçı, Mehmet"

Source: Scopus

Source ID: 84934932934

Research output: Contribution to journal › Article › Scientific › peer-review

### **Lithography-free oxide patterns as templates for self-catalyzed growth of highly uniform GaAs nanowires on Si(111)**

We report self-catalyzed growth of GaAs nanowires (NWs) on Si/SiO<sub>x</sub> patterns fabricated by a lithography-free method. The patterns are defined using droplet epitaxy of GaAs nanocrystals, spontaneous oxidation, and thermal annealing. We investigate the influence of the size and density of the nucleation sites on the NW growth process and show that this approach enables the fabrication of highly uniform GaAs NWs with controllable density. The pattern fabrication and NW growth process are studied and discussed in relation to the surface morphology and chemical properties of the Si/SiO<sub>x</sub> patterns. Furthermore, the optical quality of the NWs is investigated by photoluminescence experiments performed for GaAs-AlGaAs core-shell NWs.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications, Augmented Human Activities (AHA), Frontier Photonics, Department of Physics and Astronomy, University of Turku, University of Turku

Contributors: Hakkarainen, T. V., Schramm, A., Mäkelä, J., Laukkanen, P., Guina, M.

Publication date: 18 Jul 2015

Peer-reviewed: Yes

#### Publication information

Journal: Nanotechnology

Volume: 26

Issue number: 27

Article number: 275301

ISSN (Print): 0957-4484

Ratings:

Scopus rating (2015): CiteScore 3.07 SJR 1.257 SNIP 1.117

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Electrical and Electronic Engineering, Mechanical Engineering, Mechanics of Materials, Materials Science(all)

Keywords: droplet epitaxy, GaAs, nanowires, self-catalyzed

DOIs:

10.1088/0957-4484/26/27/275301

URLs:

<http://www.scopus.com/inward/record.url?scp=84934916555&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

EXT="Laukkanen, P."

Source: Scopus

Source ID: 84934916555

Research output: Contribution to journal > Article > Scientific > peer-review

#### Measuring optical anisotropy in poly(3,4-ethylene dioxythiophene): poly(styrene sulfonate) films with added graphene

Abstract Graphene is a 2D nanomaterial having a great potential for applications in electronics and optoelectronics. Composites of graphene with conducting polymers have shown high performance in practical devices and their solution-processability enables low-cost and high-throughput mass manufacturing using printing techniques. Here we measure the effect of incorporation of graphene into poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) to the optical anisotropy, absorbance and conductivity of the film. Uniaxial anisotropy in PEDOT:PSS films has been thought to be caused by the spin-coating process used in fabrication. We have characterized spray- and spin-coated films using ellipsometry and total internal reflection spectroscopy, the latter especially for films too thick and uneven for ellipsometry, and show that spray-coating, similar to inkjet printing, also produces consistently anisotropic properties even in very thick and uneven films. Possible plasmonic excitations related to graphene are not seen in the films. The optical and electrical anisotropy of graphene/PEDOT:PSS enables routes to high performance devices for electronics, photonics and optoelectronics.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Automation Science and Engineering, Research area: Microsystems, Research area: Measurement Technology and Process Control, Integrated Technologies for Tissue Engineering Research (ITTE), Miktech Oy, University of Jyväskylä

Contributors: Isoniemi, T., Tuukkanen, S., Cameron, D. C., Simonen, J., Toppari, J. J.

Number of pages: 7

Pages: 317-323

Publication date: 9 Jul 2015

Peer-reviewed: Yes

#### Publication information

Journal: Organic Electronics

Volume: 25

ISSN (Print): 1566-1199

Ratings:

Scopus rating (2015): CiteScore 3.6 SJR 1.135 SNIP 1.082

Original language: English

ASJC Scopus subject areas: Biomaterials, Electronic, Optical and Magnetic Materials, Materials Chemistry, Electrical and Electronic Engineering, Chemistry(all), Condensed Matter Physics

Keywords: PEDOT: PSS, Graphene, Anisotropy, Spectroscopy, Conducting polymer, CARBON-NANOTUBE, ELECTRONICS, OPTOELECTRONICS, CONDUCTIVITY, TRANSPARENT, PHOTONICS, GROWTH, CELLS

Electronic versions:

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DOIs:

10.1016/j.orgel.2015.06.037

10.1016/j.orgel.2015.06.037

URLs:

<http://urn.fi/URN:NBN:fi:tty-201601293493>

### Bibliographical note

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EXT="Simonen, Janne"

Source: Scopus

Source ID: 84936759109

Research output: Contribution to journal › Article › Scientific › peer-review

### Synthesis and study of electrochemical and optical properties of substituted perylenemonoimides in solutions and on solid surfaces

A new and efficient methodology towards the synthesis of 7-pyrrolidinyl and 7,12-bispyrrolidinyl perylenemonoimide monoanhydrides (PMI monoanhydrides) and their corresponding dicarboxylic acids is devised. The high yields (70-96%) and facile synthesis of PMI monoanhydrides, as compared to traditional methodologies, make the method attractive and versatile. The reported 7,12-bispyrrolidinyl PMI monoanhydrides are a new family of peryleneimides, where both the bay-substituents are located towards the anhydride cycle. The electrochemical and optical properties of target molecules and their precursors were investigated using UV-Vis spectroscopy and differential pulse voltammetry. Atomic charges and electronic properties were calculated using density functional theory (DFT). In addition, self-assembling monolayers of the PMI monoanhydrides and their corresponding diacids were successfully formed over ZnO and TiO<sub>2</sub> films. The results of the current study indicate that these molecules are potentially good candidates for various applications in the fields of organic electronics and solar cells.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Ahmed, Z., George, L., Hiltunen, A., Lemmetyinen, H., Hukka, T., Efimov, A.

Number of pages: 8

Pages: 13332-13339

Publication date: 7 Jul 2015

Peer-reviewed: Yes

### Publication information

Journal: Journal of Materials Chemistry A

Volume: 3

Issue number: 25

ISSN (Print): 2050-7488

Ratings:

Scopus rating (2015): CiteScore 8.36 SJR 2.62 SNIP 1.63

Original language: English

ASJC Scopus subject areas: Chemistry(all), Renewable Energy, Sustainability and the Environment, Materials Science(all)

DOIs:

10.1039/c5ta02241j

URLs:

<http://www.scopus.com/inward/record.url?scp=84934958229&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84934958229

Research output: Contribution to journal › Article › Scientific › peer-review

### Optimal emission enhancement in orthogonal double-pulse laser-induced breakdown spectroscopy

Abstract Orthogonal double-pulse (DP) laser-induced breakdown spectroscopy (LIBS) was performed using reheating and pre-ablative configurations. The ablation pulse power density was varied by two orders of magnitude and the DP experiments were carried out for a wide range of interpulse delays. For both DP-LIBS schemes, the signal enhancement was evaluated with respect to the corresponding single-pulse (SP) LIBS as a function of the interpulse delay. The reheating scheme shows a sharp maximum signal enhancement of up to 200-fold for low ablative power densities (0.4 GW cm<sup>-2</sup>); however, for power densities larger than 10 GW cm<sup>-2</sup> this configuration did not

improve the SP outcome. On the other hand, a more uniform signal enhancement of about 4-6 was obtained for the pre-ablative scheme nearly independently of the used ablative power density. In terms of the signal-to-noise ratio (SNR) the pre-ablative scheme shows a monotonic increment with the ablative power density. Whereas the reheating configuration reaches a maximum at 2.2 GW cm<sup>-2</sup>, its enhancement effect collapses markedly for fluencies above 10 GW cm<sup>-2</sup>.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Optics, Research group: Applied Optics, Centro de Ciencias Aplicadas y Desarrollo Tecnológico, Universidad Nacional Autónoma de México (CCADET-UNAM), Cátedra CONACyT, Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Universidad Autónoma Metropolitana-Unidad Azcapotzalco

Contributors: Sanginés, R., Contreras, V., Sobral, H., Robledo-Martinez, A.

Number of pages: 7

Pages: 139-145

Publication date: 6 Jul 2015

Peer-reviewed: Yes

#### Publication information

Journal: Spectrochimica Acta Part B: Atomic Spectroscopy

Volume: 110

Article number: 4935

ISSN (Print): 0584-8547

Ratings:

Scopus rating (2015): CiteScore 2.94 SJR 0.999 SNIP 1.414

Original language: English

ASJC Scopus subject areas: Instrumentation, Atomic and Molecular Physics, and Optics, Analytical Chemistry, Spectroscopy

Keywords: Double-pulse, Emission enhancement, LIBS

DOIs:

10.1016/j.sab.2015.06.012

URLs:

<http://www.scopus.com/inward/record.url?scp=84934759672&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84934759672

Research output: Contribution to journal › Article › Scientific › peer-review

#### A comparison of rheology and FTIR in the study of polypropylene and polystyrene photodegradation

Rheology and FTIR spectroscopy are compared as methods to study the degree of photodegradation in polypropylene (PP) and polystyrene (PS) sheets. The materials are hot pressed, artificially photo-aged with fluorescent lights for 4-2048 h and then measured with a rotational rheometer and FTIR. Both materials show a tendency for chain scission which can be seen as a reduction in viscosity. Changes in PP can be observed with both methods after 256 h of irradiation. Changes in PS become significant in rheology after 64 h but in FTIR only after 1024 h of irradiation. Due to the different chemical nature of the materials, the degradation of PS is rather linear with exposure, whereas the degradation of PP is more exponential. Using the zero shear viscosities obtained through extrapolations of the Cole-Cole and Carreau-Yasuda models, relative molecular weights are estimated with the aid of the power-law relationship between these two. These results are compared with the carbonyl indices determined from the FTIR spectra. Rheology is found to be a viable alternative for FTIR in certain situations.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research area: Sustainable Machine Systems, Department of Mechanical Engineering and Industrial Systems, Tampere Univ Technol, Tampere University of Technology, Dept Chem & Bioengn

Contributors: Mylläri, V., Ruoko, T., Syrjälä, S.

Number of pages: 6

Publication date: 1 Jul 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Applied Polymer Science

Volume: 132

Issue number: 28  
Article number: 42246  
ISSN (Print): 0021-8995  
Ratings:

Scopus rating (2015): CiteScore 1.74 SJR 0.587 SNIP 0.846

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)

Keywords: aging, degradation, rheology, thermoplastics, PHOTOOXIDATION, FILMS, PHOTOLYSIS

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10.1002/app.42246

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<http://urn.fi/URN:NBN:fi:tty-201612024837>

URLs:

<http://www.scopus.com/inward/record.url?scp=84928363110&partnerID=8YFLogxK> (Link to publication in Scopus)

### **Bibliographical note**

ORG=mol,0.7

ORG=keb,0.2

ORG=mei,0.1

Source: Scopus

Source ID: 84928363110

Research output: Contribution to journal › Article › Scientific › peer-review

### **On the biomaterials for nanostructured ocular therapeutics**

Due to its unique anatomy, drug delivery to eye structures has always been problematic. Many efforts have been addressed to enhance ocular bioavailability by lowering non-specific interactions between drug and tissue, increasing drug stability or increasing the residence time in the case of topical drugs. In this context, nanotechnology has been a very helpful tool for developing suitable drug delivery systems. More specifically, different kinds of strategies in this field have been proposed to overcome the problems related to ocular administration. However, the success of a nanoparticulated system relies on the correct choice of the material which it is made of. Based on these statements, the present article offers a review of the most important biomaterials employed in nanostructured systems for ocular drug delivery, especially those designated to delivery to the ocular surface and their impact on the final activity of such systems.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Federal University of Rio Grande do Sul, University of Santiago de Compostela (USC), University Clinical Hospital of Santiago de Compostela (IDIS)

Contributors: Zorzi, G. K., Párraga, J. E., Seijo, B., Sánchez, A.

Number of pages: 17

Pages: 1443-1459

Publication date: 1 Jul 2015

Peer-reviewed: Yes

### **Publication information**

Journal: Current Organic Chemistry

Volume: 19

Issue number: 15

ISSN (Print): 1385-2728

Ratings:

Scopus rating (2015): CiteScore 2.01 SJR 0.46 SNIP 0.589

Original language: English

ASJC Scopus subject areas: Organic Chemistry

Keywords: Biomaterial, Drug delivery, Eye, Nanoparticles, Nanotechnology

URLs:

<http://www.scopus.com/inward/record.url?scp=84937231030&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84937231030

Research output: Contribution to journal › Article › Scientific › peer-review

## Synthesis and Photophysical Properties of Two Diazaporphyrin-Porphyrin Hetero Dimers in Polar and Nonpolar Solutions

Two diazaporphyrin (DAP)-porphyrin hetero dimers, in  $\beta$ -meso and  $\beta$ - $\beta$  configurations, were prepared to study their photoinduced intramolecular electron transfer properties. The two meso nitrogen atoms in the porphyrin ring of DAP change its redox potential, making DAP more easily reduced, compared to its porphyrin counterpart. A charge-transfer from porphyrin to DAP in both hetero dimers was verified by versatile optical spectroscopic methods. The steady-state fluorescence spectra indicated an efficient intramolecular exciplex formation for both dimers. For the  $\beta$ -meso dimer, ultrafast time-resolved spectroscopic methods revealed the subpicosecond formation of two types of primary short-living (1-18 ps) intramolecular exciplexes, which relaxed in toluene to form a long-living final exciplex (1.4 ns) followed by a longer-living charge transfer complex (>5 ns). However, in benzonitrile, the lifetime of the final exciplex was longer (660 ps) as was that of the charge transfer complex (180 ps). The  $\beta$ - $\beta$  analogue formed similar short-living exciplexes in both solvents, but the final exciplex and the charge transfer state had significantly shorter lifetimes. The electrochemical redox potential measurements and density functional theory calculations supported the proposed mechanism.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Tampere Graduate School in Information Science and Engineering (TISE), Kyoto Women's University, Department of Molecular Engineering, Graduate School of Engineering, Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto University, Kyushu University, Niigata University

Contributors: Abou-Chahine, F., Fujii, D., Imahori, H., Nakano, H., Tkachenko, N. V., Matano, Y., Lemmetyinen, H.

Number of pages: 10

Pages: 7328-7337

Publication date: 18 Jun 2015

Peer-reviewed: Yes

Early online date: 30 Jan 2015

### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 119

Issue number: 24

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/jp510903a

URLs:

<http://www.scopus.com/inward/record.url?scp=84934905262&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84934905262

Research output: Contribution to journal > Article > Scientific > peer-review

## Catalytic effect of Ca and K on CO<sub>2</sub> gasification of spruce wood char

Gasification is one route to produce chemicals and liquid fuels from biomass. The gasification of the char is catalyzed by alkali and alkaline earth metals in the biomass. In this work the catalytic effect of calcium (Ca) and potassium (K) on CO<sub>2</sub> gasification of spruce wood was studied using a thermo gravimetric analyzer (TGA). The ash-forming elements were first removed from the wood using an acid leaching method. Then, various concentrations of K and Ca were absorbed to the wood by ion-exchange to carboxylic and phenolic groups, impregnation of K<sub>2</sub>CO<sub>3</sub> or physically mixing of CaC<sub>2</sub>O<sub>4</sub>. The prepared spruce samples were placed in a mesh holder and gasified in the TGA at 850 °C in 100% CO<sub>2</sub>. The results demonstrate that the gasification rate of the char increased linearly with an increase in the concentration of Ca or K. Crystalline CaC<sub>2</sub>O<sub>4</sub> distributed only at the surface of the wood particles resulted in low catalytic activity. The catalytic activity of Ca was higher than K in the beginning of char gasification but the catalytic effect of Ca decreased earlier than the catalytic effect of potassium. Further, the char structure was investigated by SEM-EDX. The SEM analysis from interrupted gasification experiments showed the formation of CaCO<sub>3</sub> and K<sub>2</sub>CO<sub>3</sub> layer on the char surface. By adding corresponding levels of Ca and K as the original spruce to the acid washed sample, a similar gasification reactivity was obtained at 850 °C.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), Abo Akademi University, Åbo Akademi University, University of Jyväskylä, Process Chemistry Center, VTT Technical Research Centre of Finland

Contributors: Perander, M., DeMartini, N., Brink, A., Kramb, J., Karlström, O., Hemming, J., Moilanen, A., Konttinen, J., Hupa, M.  
Number of pages: 9  
Pages: 464-472  
Publication date: 15 Jun 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Fuel  
Volume: 150  
ISSN (Print): 0016-2361  
Ratings:

Scopus rating (2015): CiteScore 4.46 SJR 1.781 SNIP 2.091

Original language: English

ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

Keywords: Biomass, Calcium, Char reactivity, CO, Gasification, Potassium

DOIs:

10.1016/j.fuel.2015.02.062

URLs:

<http://www.scopus.com/inward/record.url?scp=84924100908&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

EXT="Kramb, J."

Source: Scopus

Source ID: 84924100908

Research output: Contribution to journal > Article > Scientific > peer-review

#### Inverted critical adsorption of polyelectrolytes in confinement

What are the fundamental laws for the adsorption of charged polymers onto oppositely charged surfaces, for convex, planar, and concave geometries? This question is at the heart of surface coating applications, various complex formation phenomena, as well as in the context of cellular and viral biophysics. It has been a long-standing challenge in theoretical polymer physics; for realistic systems the quantitative understanding is however often achievable only by computer simulations. In this study, we present the findings of such extensive Monte-Carlo in silico experiments for polymer-surface adsorption in confined domains. We study the inverted critical adsorption of finite-length polyelectrolytes in three fundamental geometries: planar slit, cylindrical pore, and spherical cavity. The scaling relations extracted from simulations for the critical surface charge density  $\sigma_{c<inf>c</inf>}$  - defining the adsorption-desorption transition - are in excellent agreement with our analytical calculations based on the ground-state analysis of the Edwards equation. In particular, we confirm the magnitude and scaling of  $\sigma_{c<inf>c</inf>}$  for the concave interfaces versus the Debye screening length  $1/\kappa$  and the extent of confinement  $a$  for these three interfaces for small  $ka$  values. For large  $ka$  the critical adsorption condition approaches the known planar limit. The transition between the two regimes takes place when the radius of surface curvature or half of the slit thickness  $a$  is of the order of  $1/\kappa$ . We also rationalize how  $\sigma_{c<inf>c</inf>}(\kappa)$  dependence gets modified for semi-flexible versus flexible chains under external confinement. We examine the implications of the chain length for critical adsorption - the effect often hard to tackle theoretically - putting an emphasis on polymers inside attractive spherical cavities. The applications of our findings to some biological systems are discussed, for instance the adsorption of nucleic acids onto the inner surfaces of cylindrical and spherical viral capsids.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, Sao Paulo State University

Contributors: De Carvalho, S. J., Metzler, R., Cherstvy, A. G.

Number of pages: 14

Pages: 4430-4443

Publication date: 14 Jun 2015

Peer-reviewed: Yes

#### Publication information

Journal: Soft Matter  
Volume: 11  
Issue number: 22  
ISSN (Print): 1744-683X  
Ratings:

Scopus rating (2015): CiteScore 3.97 SJR 1.634 SNIP 1.24



Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics

DOIs:

10.1039/c5sm00635j

URLs:

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Source: Scopus

Source ID: 84930640692

Research output: Contribution to journal › Article › Scientific › peer-review

### **PEGylated liposomes as carriers of hydrophobic porphyrins**

Sterically stabilized liposomes (SSLs) (PEGylated liposomes) are applied as effective drug delivery vehicles.

Understanding the interactions between hydrophobic compounds and PEGylated membranes is therefore important to determine the effectiveness of PEGylated liposomes for delivery of drugs or other bioactive substances. In this study, we have combined fluorescence quenching analysis (FQA) experiments and all-atom molecular dynamics (MD) simulations to study the effect of membrane PEGylation on the location and orientation of 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin (p-THPP) that has been used in our study as a model hydrophobic compound. First, we consider the properties of p-THPP in the presence of different fluid phosphatidylcholine bilayers that we use as model systems for protein-free cell membranes. Next, we studied the interaction between PEGylated membranes and p-THPP. Our MD simulation results indicated that the arrangement of p-THPP within zwitterionic membranes is dependent on their free volume, and p-THPP solubilized in PEGylated liposomes is localized in two preferred positions: deep within the membrane (close to the center of the bilayer) and in the outer PEG corona (p-THPP molecules being wrapped with the polymer chains). Fluorescence quenching methods confirmed the results of atomistic MD simulations and showed two populations of p-THPP molecules as in MD simulations. Our results provide both an explanation for the experimental observation that PEGylation improves the drug-loading efficiency of membranes and also a more detailed molecular-level description of the interactions between porphyrins and lipid membranes.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Cambridge, Faculty of Physics and Chemistry, Helsinki University, University of Southern Denmark, Jagiellonian University, Centre for Drug Research, Faculty of Pharmacy  
Contributors: Dzieciuch, M., Rissanen, S., Szydłowska, N., Bunker, A., Kumorek, M., Jamróz, D., Vattulainen, I., Nowakowska, M., Róg, T., Kepczynski, M.

Number of pages: 12

Pages: 6646-6657

Publication date: 4 Jun 2015

Peer-reviewed: Yes

### **Publication information**

Journal: Journal of Physical Chemistry Part B

Volume: 119

Issue number: 22

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Ratings:

Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.058

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/acs.jpccb.5b01351

URLs:

<http://www.scopus.com/inward/record.url?scp=84930960276&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84930960276

Research output: Contribution to journal › Article › Scientific › peer-review

### **Equipment for obtaining polymeric nanofibres by electrospinning technology: II. The obtaining of polymeric nanofibers**

The computerized technologies and equipment for obtaining nanofibers impose high training, a large interdisciplinary substantiation, capacity for data storage, memorizing, easy usage, selectivity, fiability, stability, reduced time for analyzing/processing of the technological parameters. That is why the computerized electrospinning equipment and technologies for obtaining nanofibers are possible candidates to carry out these requirements owing to the fact that they present both the proper selectivity/sensibility and the increased processing/determining/intervening speed by using the computerized control. This paper aims to present the operation and application of equipment for obtaining polymeric nanofibers by electrospinning technology. The designing and accomplishing of the suggested electrospinning equipment

has been aimed to obtain a modular system which should allow the control of the technological parameters by means of the computer. Thus, the multitude of the parameters which influence the process of electrospinning, can be independently and automatically varied. The obtained nanofibers were studied by scanning electron microscope.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Computational Science X (CompX), Gheorghe Asachi Technical University Iasi, Faculty of Textile and Leather Engineering and Industrial Management, Centre of Competence in Electrostatics and Electrotechnologies, Alexandru Ioan Cuza University of Iasi, ARHEOINVEST Interdisciplinary Platform, Romanian Inventors Forum, IT Center for Science and Technology, 25 Av. Radu Beller, Bucharest, Romania

Contributors: Manea, L. R., Cramariuc, B., Popescu, V., Cramariuc, R., Sandu, I., Cramariuc, O.

Number of pages: 6

Pages: 180-185

Publication date: 1 Jun 2015

Peer-reviewed: Yes

#### Publication information

Journal: Materiale Plastice

Volume: 52

Issue number: 2

ISSN (Print): 0025-5289

Ratings:

Scopus rating (2015): CiteScore 0.82 SJR 0.28 SNIP 0.778

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Chemistry(all), Mechanics of Materials

Keywords: Electrospinning, Equipment, Modular conception, Nanofibers, Technology

URLs:

<http://www.scopus.com/inward/record.url?scp=84931827044&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

EXT="Cramariuc, Bogdan"

Source: Scopus

Source ID: 84931827044

Research output: Contribution to journal > Article > Scientific > peer-review

#### Polymorph crystal packing effects on charge transfer emission in the solid state

Condensation of 1,8-naphthalic anhydride with N,N-(dimethylamino)aniline produced the donor-acceptor compound DMIM, which crystallised from a chloroform-diethyl ether mixture to afford two different coloured crystal polymorphs. Crystals for one polymorph are small and green, whereas the other crystals are orange and needle-like. X-ray crystal structures for both polymorphs were determined. The donor N,N-dimethylaniline and acceptor naphthalimide groups are twisted with respect to each other; the degree of twist is marginally different for the two structures. The orange crystal polymorph crystallises in the monoclinic space group C2/c and contains two slightly different molecular conformers in the unit cell (calculated density is 1.410 g cm<sup>-3</sup>). The green crystal polymorph crystallises in the triclinic space group P1 and contains only one type of molecule in the unit cell (calculated density is 1.401 g cm<sup>-3</sup>). The crystal packing motifs for the two polymorphs are subtly different, explaining the small variance in the observed densities. Very weak room temperature emission was observed for DMIM in a CHCl<sub>3</sub> solution, but crystals deposited on a glass slide glowed when irradiated at 488 nm using a fluorescence microscope. Disparate solid-state emission spectra and lifetimes for the two polymorphic crystal forms are observed for the dyad. The emission is assigned to charge recombination fluorescence from a charge transfer state. This journal is

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Molecular Photonics Laboratory, School of Chemistry, Newcastle University, United Kingdom, University of Malta

Contributors: He, X., Benniston, A. C., Saarenpää, H., Lemmetyinen, H., Tkachenko, N. V., Baisch, U.

Number of pages: 8

Pages: 3525-3532

Publication date: 1 Jun 2015

Peer-reviewed: Yes

#### Publication information

Journal: Chemical Science

Volume: 6

Issue number: 6

ISSN (Print): 2041-6520

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Scopus rating (2015): CiteScore 9.13 SJR 4.647 SNIP 1.718

Original language: English

ASJC Scopus subject areas: Chemistry(all)

DOIs:

10.1039/c5sc01151e

URLs:

<http://www.scopus.com/inward/record.url?scp=84929589670&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84929589670

Research output: Contribution to journal > Article > Scientific > peer-review

### **Photodiagnostic et chirurgie guidés par la fluorescence**

For many cancers, earlier diagnosis makes treatments less heavy and increases the chances of recovery. Fluorescence diagnosis has become an important method of investigation in clinical practice. It is used to distinguish tumor tissue from healthy tissue, thanks to differences in autofluorescence of specific proteins or in distribution of a fluorescent marker between normal and cancerous lesions. Similarly, complete surgical removal of the tumor is one of the most important prognostic factors for survival of the patient. Fluorescence-guided surgery is now proposed to perform the most complete macroscopic resection of tumors while preserving healthy tissue.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Société Francophone des Lasers Médicaux

Contributors: Mordon, S., Bourg-Heckly, G.

Number of pages: 5

Pages: 41-45

Publication date: 1 Jun 2015

Peer-reviewed: Yes

### **Publication information**

Journal: ACTUALITE CHIMIQUE

Issue number: 397-398

ISSN (Print): 0151-9093

Ratings:

Scopus rating (2015): CiteScore 0.04 SJR 0.102 SNIP 0.003

Original language: French

ASJC Scopus subject areas: Chemistry(all)

Keywords: Cancer, Diagnosis, Fluorescence, Laser, Light, Surgery

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<http://www.scopus.com/inward/record.url?scp=84973474062&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84973474062

Research output: Contribution to journal > Article > Scientific > peer-review

### **Soft graphoepitaxy for large area directed self-assembly of polystyrene-block-poly(dimethylsiloxane) block copolymer on nanopatterned POSS substrates fabricated by nanoimprint lithography**

Polyhedral oligomeric silsesquioxane (POSS) derivatives have been successfully employed as substrates for graphoepitaxial directed self-assembly (DSA) of block copolymers (BCPs). Tailored POSS materials of tuned surface chemistry are subject to nanoimprint lithography (NIL) resulting in topographically patterned substrates with dimensions commensurate with the BCP block length. A cylinder forming polystyrene-block-polydimethylsiloxane (PS-b-PDMS) BCP is synthesized by sequential living anionic polymerization of styrene and hexamethylcyclotrisiloxane. The patterned POSS materials provide a surface chemistry and topography for DSA of this BCP and after solvent annealing the BCP shows well-ordered microphase segregation. The orientation of the PDMS cylinders to the substrate plane could be controlled within the trench walls by the choice of the POSS materials. The BCP patterns are successfully used as on-chip etch mask to transfer the pattern to underlying silicon substrate. This soft graphoepitaxy method shows highly promising results as a means to generate lithographic quality patterns by nonconventional methods and could be applied to both hard and soft substrates. The methodology might have application in several fields including device and interconnect fabrication, nanoimprint lithography stamp production, nanofluidic devices, lab-on-chip, or in other technologies requiring simple nanodimensional patterns. A methodology for fabricating highly ordered silicon nanostructures at a substrate is reported using nanoimprint lithography imprinted polyhedral oligomeric silsesquioxane (POSS) substrates for graphoepitaxial directed self-assembly (DSA) of block copolymer (BCP). The patterned POSS materials provide a surface chemistry and topography for DSA of a cylinder forming polystyrene-block-polydimethylsiloxane BCP with well-ordered microphase

segregation upon solvent annealing.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Trinity College Dublin, University College Cork, Tyndall National Institute at National University of Ireland, Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Laboratoire des Technologies de la Microelectronique (CNRS), Profactor GmbH, University Campus-Dourouti

Contributors: Borah, D., Rasappa, S., Salaun, M., Zellsman, M., Lorret, O., Lontos, G., Ntetsikas, K., Avgeropoulos, A., Morris, M. A.

Number of pages: 8

Pages: 3425-3432

Publication date: 1 Jun 2015

Peer-reviewed: Yes

#### Publication information

Journal: Advanced Functional Materials

Volume: 25

Issue number: 22

ISSN (Print): 1616-301X

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Scopus rating (2015): CiteScore 11.93 SJR 4.859 SNIP 2.439

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Biomaterials, Condensed Matter Physics, Electrochemistry

Keywords: block copolymer, directed self-assembly, nanoimprint lithography, pattern transfer, polyhedral oligomeric silsesquioxane (POSS)

DOIs:

10.1002/adfm.201500100

URLs:

<http://www.scopus.com/inward/record.url?scp=84930932614&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84930932614

Research output: Contribution to journal > Article > Scientific > peer-review

#### La thérapie photodynamique: État de l'art et perspectives

Photodynamic therapy (PDT) is a method of medical treatment using the concomitant action of a photoactivatable molecule called the photosensitizer (PS), light, and oxygen naturally present in the biological medium. After light excitation of the photosensitizer, an energy transfer to oxygen allows to generate the formation of reactive oxygen species, especially singlet oxygen reactive leading to cell death. This technique proves to be very efficient for certain types of cancer (especially in dermatology) and is promising in other pathologies (prostate, brain). This article briefly describes the principle of PDT and then analyzes the latest advances in PDT in terms of clinical applications (actinic keratoses, prostate, brain cancer, retinoblastoma) and the use of PDT for antibacterial applications. Finally, the prospects of this technique with among others the development of new vesicles or the use of X-rays as a source of energy to overcome the problems of light penetration in tissues are presented.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Université de Lorraine, ISLM, Université Pierre et Marie Curie, Sorbonne, France, 13.12.2011, Université de Montpellier 2, Université Reims Champagne Ardenne, Univ Paris 06, Centre National de la Recherche Scientifique (CNRS), Pierre & Marie Curie University - Paris 6, Institut de Recherche pour le Développement (IRD), Inria, Institut National de la Santé et de la Recherche Médicale (Inserm), Univ Sorbonne, CNRS, ICM, UMR S 1127, UMR 7225, U1127, INSERM, Inria Paris Rocquencourt, Inst Cerveau & Mo, Institut Curie, Groupement de Recherche Eau Sol Environnement, Université Paul Sabatier

Contributors: Frochot, C., Barberi-Heyob, M., Blanchard-Desce, M., Bolotine, L., Bonneau, S., Jimenez, C. M., Durand, J. O., Lassalle, H. P., Lemerrier, G., Mordon, S., Maillard, P., Sol, V., Vever-Bizet, C., Vicendo, P.

Number of pages: 5

Pages: 46-50

Publication date: 1 Jun 2015

Peer-reviewed: Yes

#### Publication information

Journal: ACTUALITE CHIMIQUE

Issue number: 397-398

ISSN (Print): 0151-9093

Ratings:

Scopus rating (2015): CiteScore 0.04 SJR 0.102 SNIP 0.003

Original language: French

ASJC Scopus subject areas: Chemistry(all)

Keywords: Cancer, Photodynamic therapy, Photosensitizer

URLs:

<http://www.scopus.com/inward/record.url?scp=84973500613&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84973500613

Research output: Contribution to journal > Article > Scientific > peer-review

### **A facile route to synthesis of S-doped TiO<sub>2</sub> nanoparticles for photocatalytic activity**

There is always a market for cost effective methods of pollution degradation and one of the best areas to keep costs down is through synthesis techniques. This paper provides a simple technique to synthesise porous TiO<sub>2</sub> nanoparticles with increased surface area through a scaffold template technique. Their photocatalytic activity is enhanced by incorporating sulphur as a dopant and were validated by analysing the degradation of malachite green (MG). The materials were doped at a molar ratio of 100:1 (Ti:S) and calcined at different temperatures to adjust the anatase/rutile content. Detailed characterisation of the materials was undertaken using XRD, BET, XPS, TEM and FTIR. The nanoparticles displayed a microporous structure and had an increased surface area of 115 m<sup>2</sup> g<sup>-1</sup> which was reduced by doping and temperature induced phase transformation. Photocatalytic testing showed that the doped materials calcined at 700 °C performed the best in. It was observed that 20 mg l<sup>-1</sup> of MG was decomposed in 30 min using a 40 W UV bulb at pH 9 and the results surpassed those achieved by the commercial catalyst P25 which was also tested for comparison.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Trinity College Dublin, University College Cork, Materials Chemistry and Analysis Group, Centre for Research on Adaptive Nanostructures and Nanodevices

Contributors: McManamon, C., O'Connell, J., Delaney, P., Rasappa, S., Holmes, J. D., Morris, M. A.

Pages: 51-57!

Publication date: 30 May 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Molecular Catalysis A: Chemical

Volume: 406

ISSN (Print): 1381-1169

Ratings:

Scopus rating (2015): CiteScore 3.93 SJR 1.052 SNIP 1.262

Original language: English

ASJC Scopus subject areas: Catalysis, Physical and Theoretical Chemistry, Process Chemistry and Technology

Keywords: Band gap, Photocatalysis, S-doped, TiO<sub>2</sub>

DOIs:

10.1016/j.molcata.2015.05.002

URLs:

<http://www.scopus.com/inward/record.url?scp=84930210395&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84930210395

Research output: Contribution to journal > Article > Scientific > peer-review

### **Hydration of hydroxyl and amino groups examined by molecular dynamics and neutron scattering**

Neutron diffraction with isotopic substitution was performed on aqueous solutions of isopropyl alcohol and isopropylamine. The difference between these two measurements primarily contains information about the different hydration of the alcohol and amino group. This data is used as a test of the accuracy of molecular dynamic simulations of the same systems. Having established the level of accuracy of the modeling, it is employed as an interpretive tool for the experimental data. Even though the alcohol and the amine possess comparable hydrogen bonding capabilities, consisting respectively of either two hydrogen bond acceptors and one donor, or two hydrogen bond donors and one acceptor, we find significant differences in the hydration of the hydroxyl and amino groups.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Institut Laue-Langevin

Contributors: Hladílková, J., Fischer, H. E., Jungwirth, P., Mason, P. E.  
Number of pages: 9  
Pages: 6357-6365  
Publication date: 28 May 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 119

Issue number: 21

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.058

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films  
DOIs:

10.1021/jp510528u

URLs:

<http://www.scopus.com/inward/record.url?scp=84930682015&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84930682015

Research output: Contribution to journal > Article > Scientific > peer-review

### Spectral and kinetic characteristics of indotricarbocyanine complexation with albumin

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Emanuel' Institute of Biochemical Physics, Russian Academy of Sciences, Moscow State University

Contributors: Kuz'min, V. A., Durandin, N. A., Lisitsyna, E. S., Nekipelova, T. D., Podrugina, T. A., Matveeva, E. D., Proskurnina, M. V., Zefirov, N. S.

Number of pages: 3

Pages: 107-109

Publication date: 28 May 2015

Peer-reviewed: Yes

#### Publication information

Journal: DOKLADY PHYSICAL CHEMISTRY

Volume: 462

Issue number: 1

ISSN (Print): 0012-5016

Ratings:

Scopus rating (2015): CiteScore 0.55 SJR 0.295 SNIP 0.705

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1134/S0012501615050036

URLs:

<http://www.scopus.com/inward/record.url?scp=84938328246&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84938328246

Research output: Contribution to journal > Article > Scientific > peer-review

### Effect of melting state on the thermal shock resistance and thermal conductivity of APS ZrO<sub>2</sub>-7.5wt.% Y<sub>2</sub>O<sub>3</sub> coatings

The microstructures of two types of ZrO<sub>2</sub>-7.5wt.% Y<sub>2</sub>O<sub>3</sub> (YSZ) coatings fabricated by air plasma spraying (APS) but containing different amounts of columnar grains were investigated through scanning electron microscopy and electron backscatter diffraction analysis. Differences in the formation mechanisms of columnar and equiaxed grains were characterized using particles collected in a water container, from which it was found that these mechanisms are closely related to the melted state of the in-flight particles. Furthermore, it was found that the higher the columnar grain concentration of an as-sprayed coating, the higher its thermal shock resistance. This means that it is possible to improve the thermal shock resistance of APS YSZ coatings simply by introducing more columnar grains, as this increases their thermal conductivity. Using this knowledge, YSZ coatings with good thermal shock resistance and a thermal conductivity of 0.81W·(m·K)<sup>-1</sup> at 1100°C were successfully prepared.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Shanghai Institute of Ceramics Chinese Academy of Sciences, VTT Technical Research Centre of Finland

Contributors: Song, X., Liu, Z., Suhonen, T., Varis, T., Huang, L., Zheng, X., Zeng, Y.

Number of pages: 7

Pages: 132-138

Publication date: 25 May 2015

Peer-reviewed: Yes

## Publication information

Journal: Surface and Coatings Technology

Volume: 270

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2015): CiteScore 2.46 SJR 0.852 SNIP 1.37

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry

Keywords: Air plasma spraying, Columnar grains, Thermal conductivity, Thermal shock resistance, YSZ coatings

DOIs:

10.1016/j.surfcoat.2015.03.011

URLs:

<http://www.scopus.com/inward/record.url?scp=84927174189&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84927174189

Research output: Contribution to journal > Article > Scientific > peer-review

## Modeling photoionization of aqueous DNA and its components

Conspicuous radiation damage to DNA is usually considered in terms of UVA and UVB radiation. These ultraviolet rays, which are part of the solar spectrum, can indeed cause chemical lesions in DNA, triggered by photoexcitation particularly in the UVB range. Damage can, however, be also caused by higher energy radiation, which can ionize directly the DNA or its immediate surroundings, leading to indirect damage. Thanks to absorption in the atmosphere, the intensity of such ionizing radiation is negligible in the solar spectrum at the surface of Earth. Nevertheless, such an ionizing scenario can become dangerously plausible for astronauts or flight personnel, as well as for persons present at nuclear power plant accidents. On the beneficial side, ionizing radiation is employed as means for destroying the DNA of cancer cells during radiation therapy. Quantitative information about ionization of DNA and its components is important not only for DNA radiation damage, but also for understanding redox properties of DNA in redox sensing or labeling, as well as charge migration along the double helix in nanoelectronics applications. Until recently, the vast majority of experimental and computational data on DNA ionization was pertinent to its components in the gas phase, which is far from its native aqueous environment. The situation has, however, changed for the better due to the advent of photoelectron spectroscopy in liquid microjets and its most recent application to photoionization of aqueous nucleosides, nucleotides, and larger DNA fragments. Here, we present a consistent and efficient computational methodology, which allows to accurately evaluate ionization energies and model photoelectron spectra of aqueous DNA and its individual components. After careful benchmarking, the method based on density functional theory and its time-dependent variant with properly chosen hybrid functionals and polarizable continuum solvent model provides ionization energies with accuracy of 0.2-0.3 eV, allowing for faithful modeling and interpretation of DNA photoionization. The key finding is that the aqueous medium is remarkably efficient in screening the interactions within DNA such that, unlike in the gas phase, ionization of a base, nucleoside, or nucleotide depends only very weakly on the particular DNA context. An exception is the electronic interaction between neighboring bases which can lead to sequence-specific effects, such as a partial delocalization of the cationic hole upon ionization enabled by presence of adjacent bases of the same type.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), UMR ENS-CNRS-UPMC 8640, Department of Physical Chemistry, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Pluhařová, E., Slavíček, P., Jungwirth, P.

Number of pages: 9

Pages: 1209-1217

Publication date: 19 May 2015

Peer-reviewed: Yes

## Publication information

Journal: Accounts of Chemical Research

Volume: 48

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Scopus rating (2015): CiteScore 22.77 SJR 10.775 SNIP 4.504

Original language: English

ASJC Scopus subject areas: Chemistry(all)

DOIs:

10.1021/ar500366z

URLs:

<http://www.scopus.com/inward/record.url?scp=84929590219&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84929590219

Research output: Contribution to journal > Article > Scientific > peer-review

### **Multistep reactions of water with small Pd<sub>n</sub> clusters: A first principles study**

Multistep dissociative chemisorption reactions of water with Pd<sub>4</sub> and Pd<sub>7</sub> clusters were studied using density functional theory. The adsorption energies and referred adsorption sites from water molecule (H<sub>2</sub>O) to partially dissociative (H<sub>2</sub>+O and OH+H), then to fully dissociative (O+H+H) configurations are carefully determined. It is found that the adsorption energies of three dissociative reactions are 5-6 times larger than that of water molecule. Atop sites of Pd<sub>4</sub> and Pd<sub>7</sub> clusters are found to be the most stable sites for the adsorbed H<sub>2</sub>O molecule. For the coadsorption cases of partially and fully dissociated products, H<sub>2</sub> and OH molecules preferably tend to bind at the low coordination (atop or bridge) sites, and O and H atoms prefer to adsorb on the high coordination (hollow) sites. It is also found that the most favorable adsorption sites for the molecular adsorbates (H<sub>2</sub>O, H<sub>2</sub> and OH) are adjacent to the Pd atoms with the largest site-specific polarizabilities. Therefore, site-specific polarizability is a good predictor of the favorable adsorption sites for the weakly bound molecules. The different directions of charge transfer between the Pd clusters and the adsorbate(s) is observed. Furthermore, the processes of the adsorption, dissociation, and the dissociative products diffusion of H<sub>2</sub>O are analyzed.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Northwest University China, Nanjing University

Contributors: Liang, Y., Ma, L., Wang, J., Wang, G.

Publication date: 1 May 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Theoretical and Computational Chemistry

Volume: 14

Issue number: 3

Article number: 1550017

ISSN (Print): 0219-6336

Ratings:

Scopus rating (2015): CiteScore 0.57 SJR 0.249 SNIP 0.321

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Computational Theory and Mathematics, Computer Science Applications

Keywords: Chemisorption, cluster, density functional theory, transition state

DOIs:

10.1142/S0219633615500170

URLs:

<http://www.scopus.com/inward/record.url?scp=84930178634&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84930178634

Research output: Contribution to journal > Article > Scientific > peer-review

### **Energy degradation in photoexcited complexes of indocarbocyanine with albumin**

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Emanuel' Institute of Biochemical Physics, Russian Academy of Sciences, Moscow State University



Contributors: Kuzmin, V. A., Durandin, N. A., Lisitsyna, E. S., Litvinkova, L. V., Nekipelova, T. D., Podrugina, T. A., Matveeva, E. D., Proskurnina, M. V., Zefirov, N. S.  
Number of pages: 2  
Pages: 211-212  
Publication date: 1 May 2015  
Peer-reviewed: Yes

#### Publication information

Journal: HIGH ENERGY CHEMISTRY

Volume: 49

Issue number: 3

ISSN (Print): 0018-1439

Ratings:

Scopus rating (2015): CiteScore 0.59 SJR 0.258 SNIP 0.541

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1134/S0018143915030108

URLs:

<http://www.scopus.com/inward/record.url?scp=84929171887&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84929171887

Research output: Contribution to journal > Article > Scientific > peer-review

#### Ergodicity breaking and particle spreading in noisy heterogeneous diffusion processes

We study noisy heterogeneous diffusion processes with a position dependent diffusivity of the form  $D(x) \sim D_0 |x|^\alpha$  in the presence of annealed and quenched disorder of the environment, corresponding to an effective variation of the exponent  $\alpha$  in time and space. In the case of annealed disorder, for which effectively  $\alpha = \alpha(t)$ , we show how the long time scaling of the ensemble mean squared displacement (MSD) and the amplitude variation of individual realizations of the time averaged MSD are affected by the disorder strength. For the case of quenched disorder, the long time behavior becomes effectively Brownian after a number of jumps between the domains of a stratified medium. In the latter situation, the averages are taken over both an ensemble of particles and different realizations of the disorder. As physical observables, we analyze in detail the ensemble and time averaged MSDs, the ergodicity breaking parameter, and higher order moments of the time averages.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam

Contributors: Cherstvy, A. G., Metzler, R.

Publication date: 14 Apr 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chemical Physics

Volume: 142

Issue number: 14

Article number: 144105

ISSN (Print): 0021-9606

Ratings:

Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 1.042

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1063/1.4917077

URLs:

<http://www.scopus.com/inward/record.url?scp=84927611195&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84927611195

Research output: Contribution to journal > Article > Scientific > peer-review

#### Workplace performance of a loose-fitting powered air purifying respirator during nanoparticle synthesis

Nanoparticle (particles with diameter  $\leq 100$  nm) exposure is recognized as a potentially harmful size fraction for pulmonary particle exposure. During nanoparticle synthesis, the number concentrations in the process room may exceed

$10 \times 10^{6-3}$  cm<sup>-3</sup>. During such conditions, it is essential that the occupants in the room wear highly reliable high-performance respirators to prevent inhalation exposure. Here we have studied the in-use program protection factor (PPF) of loose-fitting powered air purifying respirators, while workers were coating components with TiO<sub>2</sub> or Cu<sub>x</sub>O<sub>y</sub> nanoparticles under a hood using a liquid flame spray process. The PPF was measured using condensation particle counters, an electrical low pressure impactor, and diffusion chargers. The room particle concentrations varied from  $4 \times 10^{6-3}$  to  $40 \times 10^{6-3}$  cm<sup>-3</sup>, and the count median aerodynamic diameter ranged from 32 to 180 nm. Concentrations inside the respirator varied from 0.7 to 7.2 cm<sup>-3</sup>. However, on average, tidal breathing was assumed to increase the respirator concentration by 2.3 cm<sup>-3</sup>. The derived PPF exceeded  $1.1 \times 10^{6-3}$ , which is more than  $40 \times 10^{3-3}$  times the respirator assigned protection factor. We were unable to measure clear differences in the PPF of respirators with old and new filters, among two male and one female user, or assess most penetrating particle size. This study shows that the loose-fitting powered air purifying respirator provides very efficient protection against nanoparticle inhalation exposure if used properly.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research group: Aerosol Synthesis, National Research Centre for the Working Environment, Finnish Institute of Occupational Health, Helsinki University, TNO

Contributors: Koivisto, A. J., Aromaa, M., Koponen, I. K., Fransman, W., Jensen, K. A., Mäkelä, J. M., Hämeri, K. J.

Publication date: 9 Apr 2015

Peer-reviewed: Yes

### Publication information

Journal: Journal of Nanoparticle Research

Volume: 17

Issue number: 4

ISSN (Print): 1388-0764

Ratings:

Scopus rating (2015): CiteScore 1.97 SJR 0.568 SNIP 0.725

Original language: English

ASJC Scopus subject areas: Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Modelling and Simulation, Chemistry(all), Materials Science(all), Bioengineering

Keywords: Aerosol, Air purifying respirator, Filtration, Occupational safety, Protection factor, Respirator performance

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### Bibliographical note

EXT="Koivisto, Antti J."

Source: Scopus

Source ID: 84927730047

Research output: Contribution to journal › Article › Scientific › peer-review

## Rate constant and thermochemistry for $K + O_2 + N_2 = KO_2 + N_2$

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research group: Applied Optics, Frontier Photonics, Department of Chemistry and Center for Advanced Scientific Computing and Modeling (CASCaM), University of North Texas, Department of Chemical and Biochemical Engineering, Technical University of Denmark

Contributors: Sorvajärvi, T., Viljanen, J., Toivonen, J., Marshall, P., Glarborg, P.

Number of pages: 8

Pages: 3329-3336

Publication date: 9 Apr 2015

Peer-reviewed: Yes

Early online date: 31 Mar 2015

### Publication information

Journal: Journal of Physical Chemistry A

Volume: 119

Issue number: 14

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1021/acs.jpca.5b00755

URLs:

<http://www.scopus.com/inward/record.url?scp=84927144088&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84927144088

Research output: Contribution to journal › Article › Scientific › peer-review

### **Oxidation of cholesterol does not alter significantly its uptake into high-density lipoprotein particles**

Using replica exchange umbrella sampling we calculated free energy profiles for uptake of cholesterol and one of its oxysterols (7-ketocholesterol) from an aqueous solution into a high-density lipoprotein particle. These atomistic molecular dynamics simulations show that both sterols are readily taken up from the aqueous solution with comparable free energy minima at the surface of the particle of -17 kcal/mol for cholesterol and -14 kcal/mol for 7-ketocholesterol. Moreover, given its preferred position at the particle surface, 7-ketocholesterol is expected to be able to participate directly in biological signaling processes.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Southern Denmark, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Karilainen, T., Timr, Š., Vattulainen, I., Jungwirth, P.

Number of pages: 7

Pages: 4594-4600

Publication date: 2 Apr 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry Part B

Volume: 119

Issue number: 13

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.058

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

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URLs:

<http://www.scopus.com/inward/record.url?scp=84926433475&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84926433475

Research output: Contribution to journal › Article › Scientific › peer-review

### **Effect of rheological properties of dissolved cellulose/microfibrillated cellulose blend suspensions on film forming**

Enzymatically treated cellulose was dissolved in a NaOH/ZnO solvent system and mixed together with microfibrillated cellulose (MFC) in order to find the threshold in which MFC fibers form a percolation network within the dissolved cellulose solution and in order to improve the properties of regenerated cellulose films. In the aqueous state, correlations between the rheological properties of dissolved cellulose/MFC blend suspensions and MFC fiber concentrations were investigated and rationalized. In addition, rheological properties of diluted MFC suspensions were characterized and a correlation with NaOH concentration was found, thus partly explaining the flow properties of dissolved cellulose/MFC blend suspensions. Finally, based on results from Dynamic Mechanical Analysis (DMA), MFC addition had strengthening/plasticizing effect on regenerated cellulose films if low concentrations of MFC, below the percolation threshold (5.5-6 wt%, corresponding to 0.16-0.18 wt% of MFC in the blend suspensions), were used.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Fibre Materials, Polymer Technology, Department of Biotechnology and Chemical Technology, Aalto University

Contributors: Saarikoski, E., Rissanen, M., Seppälä, J.

Number of pages: 9

Pages: 62-70

Publication date: 30 Mar 2015

Peer-reviewed: Yes

#### Publication information

Journal: Carbohydrate Polymers

Volume: 119

ISSN (Print): 0144-8617

Ratings:

Scopus rating (2015): CiteScore 4.86 SJR 1.44 SNIP 1.808

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics

Keywords: Blend, Dissolved cellulose, Microfibrillated cellulose, Rheology, Suspension

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10.1016/j.carbpol.2014.11.033

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Source: Scopus

Source ID: 84916613635

Research output: Contribution to journal > Article > Scientific > peer-review

#### Effects of fresh lubricant oils on particle emissions emitted by a modern gasoline direct injection passenger car

Particle emissions from a modern turbocharged gasoline direct injection passenger car equipped with a three-way catalyst and an exhaust gas recirculation system were studied while the vehicle was running on low-sulfur gasoline and, consecutively, with five different lubrication oils. Exhaust particle number concentration, size distribution, and volatility were determined both at laboratory and on-road conditions. The results indicated that the choice of lubricant affected particle emissions both during the cold start and warm driving cycles. However, the contribution of engine oil depended on driving conditions being higher during acceleration and steady state driving than during deceleration. The highest emission factors were found with two oils that had the highest metal content. The results indicate that a 10% decrease in the Zn content of engine oils is linked with an 11-13% decrease to the nonvolatile particle number emissions in steady driving conditions and a 5% decrease over the New European Driving Cycle. The effect of lubricant on volatile particles was even higher, on the order of 20%.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Aerosol Physics, Urban circular bioeconomy (UrCirBio), Helsinki University, Aristotle University of Thessaloniki, Department of Informatics, Metropolia University of Applied Sciences, Laboratory of Applied Thermodynamics, Neste Oil Oyj

Contributors: Pirjola, L., Karjalainen, P., Heikkilä, J., Saari, S., Tzamkiozis, T., Ntziachristos, L., Kulmala, K., Keskinen, J., Rönkkö, T.

Number of pages: 9

Pages: 3644-3652

Publication date: 17 Mar 2015

Peer-reviewed: Yes

#### Publication information

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Volume: 49

Issue number: 6

ISSN (Print): 0013-936X

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Original language: English

ASJC Scopus subject areas: Chemistry(all), Environmental Chemistry

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10.1021/es505109u

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## Bibliographical note

EXT="Ntziachristos, Leonidas"

Source: Scopus

Source ID: 84924939595

Research output: Contribution to journal › Article › Scientific › peer-review

## Tribology of HVOF- and HVAF-sprayed WC-10Co4Cr hardmetal coatings: A comparative assessment

This paper provides a comprehensive assessment of the sliding and abrasive wear behaviour of WC-10Co4Cr hardmetal coatings, representative of the existing state-of-the-art. A commercial feedstock powder with two different particle size distributions was sprayed onto carbon steel substrates using two HVOF and two HVAF spray processes. Mild wear rates of  $<10^{-7}$  mm<sup>3</sup>/(Nm) and friction coefficients of  $\approx 0.5$  were obtained for all samples in ball-on-disk sliding wear tests at room temperature against Al<sub>2</sub>O<sub>3</sub> counterparts. WC-10Co4Cr coatings definitely outperform a reference electrolytic hard chromium coating under these test conditions. Their wear mechanisms include extrusion and removal of the binder matrix, with the formation of a wavy surface morphology, and brittle cracking. The balance of such phenomena is closely related to intra-lamellar features, and rather independent of those properties (e.g. indentation fracture toughness, elastic modulus) which mainly reflect large-scale inter-lamellar cohesion, as quantitatively confirmed by a principal component analysis. Intra-lamellar dissolution of WC into the matrix indeed increases the incidence of brittle cracking, resulting in slightly higher wear rates. At 400°C, some of the hardmetal coatings fail because of the superposition between tensile residual stresses and thermal expansion mismatch stresses (due to the difference between the thermal expansion coefficients of the steel substrate and of the hardmetal coating). Those which do not fail, on account of lower residual stresses, exhibit higher wear rates than at room temperature, due to oxidation of the WC grains. The resistance of the coatings against abrasive wear, assessed by dry sand-rubber wheel testing, is related to inter-lamellar cohesion, as proven by a principal component analysis of the collected dataset. Therefore, coatings deposited from coarse feedstock powders suffer higher wear loss than those obtained from fine powders, as brittle inter-lamellar detachment is caused by their weaker interparticle cohesion, witnessed by their systematically lower fracture toughness as well.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Surface Engineering, Engineering materials science and solutions (EMASS), University West, Dipartimento di Ingegneria Enzo Ferrari, University of Modena and Reggio Emilia, Fraunhofer-Institut für Werkstoff- und Strahltechnik (IWS), Fraunhofer-Institut für Keramische Technologien und Systeme (IKTS), Institut für Korrosionsschutz Dresden GmbH

Contributors: Bolelli, G., Berger, L. M., Börner, T., Koivuluoto, H., Lusvarghi, L., Lyphout, C., Markocsan, N., Matikainen, V., Nylén, P., Sassatelli, P., Trache, R., Vuoristo, P.

Number of pages: 20

Pages: 125-144

Publication date: 15 Mar 2015

Peer-reviewed: Yes

## Publication information

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Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces

Keywords: Abrasive wear, Hardmetal, High velocity air-fuel (HVAF), High velocity oxy-fuel (HVOF), Sliding wear, WC-10Co4Cr

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Source: Scopus

Source ID: 84925299473

Research output: Contribution to journal › Article › Scientific › peer-review

## High temperature corrosion of thermally sprayed NiCr and FeCr coatings covered with a KCl-K<sub>2</sub>SO<sub>4</sub> salt mixture

Current boiler tube materials and designs are sensitive to changes in process conditions. The desire to increase efficiency through the increase in process temperature and the use of high-chlorine and alkali containing fuels such as biomass is challenging. The alloying of steel to increase the corrosion resistance leads to a significant increase in cost. Thermally sprayed coatings offer promising, effective, flexible and cost efficient solution to fulfil the material needs for the future. However, some heat exchanger design alterations have to be overcome before global commercialization. High

temperature corrosion in combustion plants can occur by a variety of mechanisms, including passive scale degradation with subsequent rapid scaling, loss of adhesion and scale detachment, attack by molten or partly molten deposits via fluxing reactions and intergranular/interlamellar corrosion. The activated chlorine corrosion mechanism plays a key role in the thermally sprayed coatings due to their unique lamellar structure. In this study, the corrosion behaviour of NiCr and FeCr (HVOF and wire arc) thermally sprayed coatings was tested under simplified biomass combustion conditions. The tests were carried out by using a KCl-K<sub>2</sub>SO<sub>4</sub> salt mixture as a synthetic biomass ash, which was placed on the coated materials and then heat treated for one week (168h) at two different temperatures (550°C and 600°C) and in two different gas atmospheres (air and air+30% H<sub>2</sub>O). After exposure, the metallographic cross sections of the coatings were studied with SEM/EDX. The results showed that the coatings behaved relatively well at the lower test temperature while critical interlamellar corrosion was observed in some cases at the higher test temperature. A few coatings (HVOF Ni49Cr, HVOF Ni21Cr, and wire arc sprayed Fe30Cr) showed promising performance even at 600°C in both atmospheres (dry and wet).

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland, Abo Akad Univ, Abo Akademi University, Dept Phys

Contributors: Varis, T., Bankiewicz, D., Yrjas, P., Oksa, M., Suhonen, T., Tuurna, S., Ruusuvoori, K., Holmström, S.

Number of pages: 9

Pages: 235-243

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Peer-reviewed: Yes

#### Publication information

Journal: Surface and Coatings Technology

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ISSN (Print): 0257-8972

Ratings:

Scopus rating (2015): CiteScore 2.46 SJR 0.852 SNIP 1.37

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry

Keywords: Biomass, Corrosion protection, High temperature corrosion, HVOF, Thermal spray coating, Wire arc

DOIs:

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Source: Scopus

Source ID: 84925343339

Research output: Contribution to journal › Article › Scientific › peer-review

#### Oxidation of the GaAs semiconductor at the Al<sub>2</sub>O<sub>3</sub>/GaAs junction

Atomic-scale understanding and processing of the oxidation of III-V compound-semiconductor surfaces are essential for developing materials for various devices (e.g., transistors, solar cells, and light emitting diodes). The oxidation-induced defect-rich phases at the interfaces of oxide/III-V junctions significantly affect the electrical performance of devices. In this study, a method to control the GaAs oxidation and interfacial defect density at the prototypical Al<sub>2</sub>O<sub>3</sub>/GaAs junction grown via atomic layer deposition (ALD) is demonstrated. Namely, pre-oxidation of GaAs(100) with an In-induced c(8 × 2) surface reconstruction, leading to a crystalline c(4 × 2)-O interface oxide before ALD of Al<sub>2</sub>O<sub>3</sub>, decreases band-gap defect density at the Al<sub>2</sub>O<sub>3</sub>/GaAs interface. Concomitantly, X-ray photoelectron spectroscopy (XPS) from these Al<sub>2</sub>O<sub>3</sub>/GaAs interfaces shows that the high oxidation state of Ga (Ga<sub>2</sub>O<sub>3</sub> type) decreases, and the corresponding In<sub>2</sub>O<sub>3</sub> type phase forms when employing the c(4 × 2)-O interface layer. Detailed synchrotron-radiation XPS of the counterpart c(4 × 2)-O oxide of InAs(100) has been utilized to elucidate the atomic structure of the useful c(4 × 2)-O interface layer and its oxidation process. The spectral analysis reveals that three different oxygen sites, five oxidation-induced group-III atomic sites with core-level shifts between -0.2 eV and +1.0 eV, and hardly any oxygen-induced changes at the As sites form during the oxidation. These results, discussed within the current atomic model of the c(4 × 2)-O interface, provide insight into the atomic structures of oxide/III-V interfaces and a way to control the semiconductor oxidation.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications, Frontier Photonics, Department of Physics and Astronomy, University of Turku, MAX IV Laboratory, Lund University, University of Turku

Contributors: Tuominen, M., Yasir, M., Lång, J., Dahl, J., Kuzmin, M., Mäkelä, J., Punkkinen, M., Laukkanen, P., Kokko, K., Schulte, K., Punkkinen, R., Korpijärvi, V., Polojärvi, V., Guina, M.

Number of pages: 7  
Pages: 7060-7066  
Publication date: 14 Mar 2015  
Peer-reviewed: Yes

#### Publication information

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Volume: 17

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ISSN (Print): 1463-9076

Ratings:

Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.188

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

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#### Bibliographical note

EXT="Kuzmin, Mikhail"

EXT="Mäkelä, Jaakko"

EXT="Laukkanen, Pekka"

Source: Scopus

Source ID: 84923878513

Research output: Contribution to journal > Article > Scientific > peer-review

#### CO oxidation catalyzed by neutral and anionic Cu<sub>20</sub> clusters: Relationship between charge and activity

Reactions of CO and O<sub>2</sub> on neutral and anionic Cu<sub>20</sub> clusters have been investigated by spin-polarized density functional theory. Three reaction mechanisms of CO oxidation are explored: reactions with atomic oxygen (dissociated O<sub>2</sub>) as well as reactions with molecular oxygen, including Langmuir-Hinshelwood (LH) and Eley-Rideal (ER) mechanisms. The adsorption energies, reaction pathways, and reaction barriers for CO oxidation are calculated systematically. The anionic Cu<sub>20</sub><sup>-</sup> cluster can adsorb CO and O<sub>2</sub> more strongly than the neutral counterpart due to the superatomic shell closing of 20 valence electrons which leaves one electron above the band gap. The activation of O<sub>2</sub> molecule upon adsorption is crucial to determine the rate of CO oxidation. The CO oxidation proceeds efficiently on both Cu<sub>20</sub> and Cu<sub>20</sub><sup>-</sup> clusters, when O<sub>2</sub> is pre-adsorbed dissociatively. The ER mechanism has a lower reaction barrier than the LH mechanism on the neutral Cu<sub>20</sub>. In general, CO oxidation occurs more readily on the anionic Cu<sub>20</sub><sup>-</sup> (effective reaction barriers 0.1-0.3 eV) than on the neutral Cu<sub>20</sub> cluster (0.3-0.5 eV). Moreover, Cu<sub>20</sub><sup>-</sup> exhibits enhanced binding for CO<sub>2</sub>. From the analysis of the reverse direction of CO oxidation, it is observed that the transition of CO<sub>2</sub> to CO + O can occur on the Cu<sub>20</sub><sup>-</sup> cluster, which demonstrates that Cu clusters may serve as good catalyst for CO<sub>2</sub> chemistry.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research group: Materials and Molecular Modeling, Computational Science X (CompX), COMP Centre of Excellence, Department of Applied Physics, Aalto University, Department of Physics, Tampere University of Technology, COMP Centre of Excellence, Department of Chemistry, Aalto University

Contributors: Ma, L., Melander, M., Laasonen, K., Akola, J.

Number of pages: 10

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Publication date: 14 Mar 2015

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 17

Issue number: 10

ISSN (Print): 1463-9076

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1039/c5cp00365b

Source: Scopus

Source ID: 84923914179

Research output: Contribution to journal > Article > Scientific > peer-review

## Synthesis, characterization and solid-state photoluminescence studies of six alkoxy phenylene ethynylene dinuclear palladium(II) rods

A rare family of six discrete binuclear  $[\text{PdCl}(\text{PEt}_3)_2]$  phenylene ethynylene rods with alkoxy side chains (methoxy, ethoxy and heptoxy) have been developed, and their solid-state photoluminescence results have been presented and discussed. The shorter bridging ligands are of the general formula  $\text{H}-\text{CC}-\text{C}_6\text{H}_2(\text{R})_2-\text{CC}-\text{H}$ , where  $\text{R} = \text{H}, \text{OCH}_3, \text{OC}_2\text{H}_5,$  and  $\text{OC}_7\text{H}_{15}$ , whereas the longer ones are based on  $\text{H}-\text{CC}-\text{C}_6\text{H}_4-\text{CC}-\text{C}_6\text{H}_2(\text{R})_2-\text{CC}-\text{C}_6\text{H}_4-\text{CC}-\text{H}$ , where  $\text{R} = \text{OCH}_3, \text{OC}_2\text{H}_5$ . These ligands display increasing length in both the main dimension (backbone length) as well as the number of carbons in the side chains (R, alkoxy side chain) that stem from the central phenylene moiety. The X-ray crystal structures of two of the prepared complexes are reported: one corresponds to a shorter rod, 1,4-bis[trans-(PEt<sub>3</sub>)<sub>2</sub>ClPd-CC]-2,5-diethoxybenzene (6c), while the second one is associated with a longer rod, the binuclear complex 1,4-bis[trans-(PEt<sub>3</sub>)<sub>2</sub>ClPd-4-( $-\text{CC}-\text{C}_6\text{H}_4-\text{CC}-$ )]-2,5-diethoxybenzene (7c). All new compounds were characterized by NMR spectroscopy (<sup>1</sup>H, <sup>13</sup>C{<sup>1</sup>H} and <sup>31</sup>P{<sup>1</sup>H}) as well as ESI-MS(TOF), EA, FTIR, UV-Vis, cyclic voltammetry and solid-state photoluminescence. Our work shows the influence of the alkoxy side chains on the electronic structure of the family of binuclear Pd rods by lowering its oxidation potential. In addition to this, the increase of the length of the bridge results in a higher oxidation potential. Solid state photoluminescence results indicate that Pd complexes are characterized by a marked decrease in both the emission intensity and the fluorescence lifetime values as compared to their ligands. This behaviour could be due to some degree of ligand-to-metal charge transfer. This journal is

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Jyväskylä, CQM-Centro de Química da Madeira, Universidade da Madeira Campus Universitário da Penteada, MMRG, Departamento de Física Fundamental y Experimental, Facultad de Física, Universidad de la Laguna

Contributors: Figueira, J., Czardybon, W., Mesquita, J. C., Rodrigues, J., Lahoz, F., Russo, L., Valkonen, A., Rissanen, K.

Number of pages: 13

Pages: 4003-4015

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Peer-reviewed: Yes

### Publication information

Journal: DALTON TRANSACTIONS

Volume: 44

Issue number: 9

ISSN (Print): 1477-9226

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Original language: English

ASJC Scopus subject areas: Inorganic Chemistry

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Source: Scopus

Source ID: 84923350178

Research output: Contribution to journal > Article > Scientific > peer-review

## Resveratrol interferes with the aggregation of membrane-bound human-IAPP: A molecular dynamics study

Amyloid aggregation of islet amyloid polypeptide (IAPP) in pancreatic tissues is a typical feature of type 2 diabetes mellitus. Resveratrol, a natural product extensively studied for its wide range of biological effects, has been shown to inhibit IAPP aggregation. However, the mechanism by which resveratrol inhibits IAPP aggregation is still far from complete elucidation. Now, an increasing knowledge of the mechanism of amyloid toxicity shifts the target of research towards the development of compounds which can prevent amyloid-mediated membrane damage rather than merely inhibit fiber formation. In this study we used all atom molecular dynamics to investigate the interaction of resveratrol with full-length human IAPP in a negatively charged membrane environment. Our results show that the presence of resveratrol induces the formation of secondary structures (sheets and helices) by inserting in a hydrophobic pocket between the interaction surface of two IAPP molecules in aqueous solution. On the other hand, resveratrol significantly perturbs the interaction of IAPP with negatively charged membranes by anchoring specific hydrophobic regions (23FGA25 and 32VGS34) of the peptide and forming a stable 1:2 IAPP:resveratrol complex at the water/membrane interphase.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed



Organisations: Department of Physics, NEST Istituto Nanoscienze-CNR, Department of Chemical Sciences, University of Catania, Unità Organizzativa e di Supporto di Catania, Istituto di Biostrutture e Bioimmagini  
Contributors: Lolicato, F., Raudino, A., Milardi, D., La Rosa, C.  
Number of pages: 6  
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Peer-reviewed: Yes

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Journal: European Journal of Medicinal Chemistry

Volume: 92

ISSN (Print): 0223-5234

Ratings:

Scopus rating (2015): CiteScore 3.87 SJR 1.143 SNIP 1.47

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Keywords: Atomistic simulation, Membrane, Molecular dynamics, Resveratrol, Type II diabetes

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Source: Scopus

Source ID: 84922216978

Research output: Contribution to journal > Article > Scientific > peer-review

#### Crystal structure of 2-methylpiperazine-1,4-dium bis(hydrogen maleate)

In the title salt,

$C_5H_{14}N_2^{2+} \cdot 2C_4H_3O_4^{-}$ , the asymmetric unit contains two independent 2-methylpiperazinium dications, which comprise a racemic pair, and four hydrogen maleate monoanions. In the roughly planar hydrogen maleate anions, intramolecular O - H $\cdots$ O hydrogen bonds generate S(7) rings. In the crystal, the four independent anions are linked to the 2-methylpiperazinium cations through N - H $\cdots$ O hydrogen bonds, forming two-dimensional layered structures lying parallel to (001).

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Laboratoire de chimie des Matériaux, Faculté des Sciences de Bizerte, Université de Carthage, Queensland University of Technology QUT

Contributors: Wecharine, I., Valkonen, A., Rzaigui, M., Sta, W. S., Smith, G.

Pages: o193-o194

Publication date: 1 Mar 2015

Peer-reviewed: Yes

#### Publication information

Journal: Acta Crystallographica Section E : Structure Reports Online

Volume: 71

Issue number: 3

ISSN (Print): 1600-5368

Ratings:

Scopus rating (2015): CiteScore 0.17 SJR 0.186 SNIP 0.118

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Materials Science(all), Chemistry(all)

Keywords: 2-methylpiperazine-1,4-dium, Crystal structure, Hydrogen bonding, Hydrogen maleate

DOIs:

10.1107/S2056989015003102

URLs:

<http://www.scopus.com/inward/record.url?scp=84928116257&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84928116257

Research output: Contribution to journal > Article > Scientific > peer-review

#### Exploring the role of stearic acid in modified zinc aluminum layered double hydroxides and their acrylonitrile butadiene rubber nanocomposites

The proposed study attempted to explore the role of stearic acid modification on the properties of zinc-aluminum based layered double hydroxides (LDH) and their composites with acrylonitrile butadiene rubber (NBR). Three distinctive LDH systems were adapted for such comparison; an unmodified LDH and two stearic acid modified LDH. The use of zinc oxide and stearic acid in the rubber formulation was avoided as the modified LDH would be able to deliver the necessary activators for the vulcanization process. Emphasis was predominantly given to reconnoiter the merits of stearic acid modification on the increase in interlayer distance of the LDH. X-ray diffraction studies and transmission electron microscope morphological investigations of LDH powders indicated that modification with stearic acid increased the interlayer spacing which would favor the intercalation of NBR polymer chains into the layered space. However, stress-strain studies indicated better mechanical properties for composites with unmodified LDH. Composites with LDH showed higher crosslinking densities than conventionally sulfur cured control compounds using zinc oxide/stearic acid as activators. This was evident from equilibrium swelling method as well as statistical theory of rubber elasticity.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V., Technische Universität Dresden, Rubber Technology Centre, Indian Institute of Technology Kharagpur

Contributors: Eshwaran, S. B., Basu, D., Vaikuntam, S. R., Kutlu, B., Wiessner, S., Das, A., Naskar, K., Heinrich, G.

Publication date: 1 Mar 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Applied Polymer Science

Volume: 132

Issue number: 9

Article number: 41539

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2015): CiteScore 1.74 SJR 0.587 SNIP 0.846

Original language: English

ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry

Keywords: crosslinking, elastomers, mechanical properties, properties and characterization, rubber

DOIs:

10.1002/app.41539

URLs:

<http://www.scopus.com/inward/record.url?scp=84913616731&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84913616731

Research output: Contribution to journal › Article › Scientific › peer-review

#### Polymer looping is controlled by macromolecular crowding, spatial confinement, and chain stiffness

We study by extensive computer simulations the looping characteristics of linear polymers with varying persistence length inside a spherical cavity in the presence of macromolecular crowding. For stiff chains, the looping probability and looping time reveal wildly oscillating patterns as functions of the chain length. The effects of crowding differ dramatically for flexible versus stiff polymers. While for flexible chains the looping kinetics is slowed down by the crowders, for stiffer chains the kinetics turns out to be either decreased or facilitated, depending on the polymer length. For severe confinement, the looping kinetics may become strongly facilitated by crowding. Our findings are of broad impact for DNA looping in the crowded and compartmentalized interior of living biological cells.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, Max-Planck Institute for the Physics of Complex Systems

Contributors: Shin, J., Cherstvy, A. G., Metzler, R.

Number of pages: 5

Pages: 202-206

Publication date: 17 Feb 2015

Peer-reviewed: Yes

#### Publication information

Journal: ACS Macro Letters

Volume: 4

Issue number: 2

ISSN (Print): 2161-1653

Ratings:

Scopus rating (2015): CiteScore 5.91 SJR 2.392 SNIP 1.403

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry

DOIs:

10.1021/mz500709w

URLs:

<http://www.scopus.com/inward/record.url?scp=84923204435&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84923204435

Research output: Contribution to journal › Article › Scientific › peer-review

### Neutralized chimeric avidin binding at a reference biosensor surface

We describe the development of a reference biosensor surface, based upon a binary mixture of oligo-ethylene glycol thiols, one of which has biotin at the terminus, adsorbed onto gold as self-assembled monolayers (SAMs). These surfaces were analyzed in detail by X-ray photoelectron spectroscopy (XPS) and secondary ion mass spectrometry (SIMS) to establish the relationship between the thiol solution composition and the surface composition and structure. We report the use of argon cluster primary ions for the analysis of PEG-thiols, establishing that the different thiols are intimately mixed and that SIMS may be used to measure surface composition of thiol SAMs on gold with a detection limit better than 1% fractional coverage. The adsorption of neutralized chimeric avidin to these surfaces was measured simultaneously using ellipsometry and QCM-D. Comparison of the two measurements demonstrates the expected nonlinearity of the frequency response of the QCM but also reveals a strong variation in the dissipation signal that correlates with the surface density of biotin. These variations are most likely due to the difference in mechanical response of neutralized chimeric avidin bound by just one biotin moiety at low biotin density and two biotin moieties at high density. The transition between the two modes of binding occurs when the average spacing of biotin ligands approaches the diameter of the avidin molecule.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), National Physical Laboratory, Chalmers University of Technology, School of Management (JKK)

Contributors: Ray, S., Steven, R. T., Green, F. M., Höök, F., Taskinen, B., Hytönen, V. P., Shard, A. G.

Number of pages: 10

Pages: 1921-1930

Publication date: 17 Feb 2015

Peer-reviewed: Yes

### Publication information

Journal: Langmuir

Volume: 31

Issue number: 6

ISSN (Print): 0743-7463

Ratings:

Scopus rating (2015): CiteScore 4.33 SJR 1.65 SNIP 1.271

Original language: English

ASJC Scopus subject areas: Electrochemistry, Condensed Matter Physics, Surfaces and Interfaces, Materials Science(all), Spectroscopy, Medicine(all)

DOIs:

10.1021/la503213f

URLs:

<http://www.scopus.com/inward/record.url?scp=84923165750&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84923165750

Research output: Contribution to journal › Article › Scientific › peer-review

### Encapsulation of secondary and tertiary ammonium salts by resorcinarenes and pyrogallarenes: The effect of size and charge concentration

The binding of different categories of alkyl ammonium (secondary and tertiary mono- and di-ammonium) salts with resorcinarenes and a pyrogallarene through weak interactions was analysed in all phases.  $^1\text{H}$  NMR spectroscopy and electrospray ionisation mass spectrometry were utilized in analysing the complexes in solution and in the gas phase, respectively. The  $^1\text{H}$  NMR titration studies in methanol- $d_4$  reveal that the association constants for the 1:1 complexes vary according to the electronic properties of the hosts as well as the size, geometric orientation and charge concentration of the guest cations with binding constants of up to  $950\text{ M}^{-1}$  in some cases. Mass spectrometry reveals 1:1 monomeric and

1:2 dimeric complexes in the gas phase. Six co-crystals, three of which are dimeric host-guest capsular assemblies, two open inclusion complexes and a pseudocapsular methanol solvate, were analysed in the solid state through single-crystal X-ray diffraction. The crystal structures confirm that the complexes are held together by multiple cation $\cdots\pi$ , CH $\cdots\pi$  and hydrogen bond interactions.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, University of Jyväskylä

Contributors: Beyeh, N. K., Pan, F., Valkonen, A., Rissanen, K.

Number of pages: 7

Pages: 1182-1188

Publication date: 7 Feb 2015

Peer-reviewed: Yes

#### Publication information

Journal: CrystEngComm

Volume: 17

Issue number: 5

ISSN (Print): 1466-8033

Ratings:

Scopus rating (2015): CiteScore 3.83 SJR 1.04 SNIP 0.98

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics

DOIs:

10.1039/c4ce01927j

URLs:

<http://www.scopus.com/inward/record.url?scp=84921648549&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84921648549

Research output: Contribution to journal > Article > Scientific > peer-review

#### Second-harmonic generation imaging of semiconductor nanowires with focused vector beams

We use second-harmonic generation (SHG) with focused vector beams to investigate individual vertically aligned GaAs nanowires. Our results provide direct evidence that SHG from oriented nanowires is mainly driven by the longitudinal field along the nanowire growth axis. Consequently, focused radial polarization provides a superior tool to characterize such nanowires compared to linear polarization, also allowing this possibility in the native growth environment. We model our experiments by describing the SHG process for zinc-blende structure and dipolar bulk nonlinearity.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Optics, Research group: Nonlinear Optics, Tampere University of Technology, Frontier Photonics, Aalto University, Department of Micro- and Nanosciences, Aalto University, Department of Applied Physics and Nanomicroscopy Center

Contributors: Bautista, G., Mäkitalo, J., Chen, Y., Dhaka, V., Grasso, M., Karvonen, L., Jiang, H., Huttunen, M. J., Huhtio, T., Lipsanen, H., Kauranen, M.

Number of pages: 6

Pages: 1564-1569

Publication date: 6 Feb 2015

Peer-reviewed: Yes

#### Publication information

Journal: Nano Letters

Volume: 15

Issue number: 3

ISSN (Print): 1530-6984

Ratings:

Scopus rating (2015): CiteScore 14.76 SJR 8.359 SNIP 3.064

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Bioengineering, Chemistry(all), Materials Science(all), Mechanical Engineering

Keywords: modeling, nonlinear imaging, radial polarization, Second-harmonic generation, semiconductor

DOIs:

10.1021/nl503984b

URLs:

<http://www.scopus.com/inward/record.url?scp=84924595561&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

AUX=fys,"Grasso, Marco"

EXT="Dhaka, Veer"

EXT="Huttunen, Mikko J."

Source: Scopus

Source ID: 84924595561

Research output: Contribution to journal › Article › Scientific › peer-review

#### Sulfonated polyetheretherketone/polypropylene polymer blends for the production of photoactive materials

Sulfonated polyetheretherketone (SPEEK) was synthesized via a mono-substitution reaction of PEEK in concentrated sulphuric acid and was blended with polypropylene (PP) in 2-10%w/w concentration to be used for the production of photoactive thermoplastic products. SPEEK and SPEEK/PP blends were characterized using FTIR, DSC, TGA, NMR, rheology, SEM, and EPR. Under UV-Vis irradiation, stable benzophenone ketyl (BPK) radicals were generated by hydrogen extraction from PP. By increasing the amount of SPEEK in the polymer blend a linear increase in the BPK radicals was achieved according to the EPR data. DSC and TGA tests indicated weaknesses in the thermal stability of SPEEK but according to the rheological tests this should not have a major effect on processability. The optimal amount of SPEEK in the blend was obtained at 5%w/w. This concentration provided a good compromise between radical concentration, material processability, and cost.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science

Contributors: Fatarelle, E., Mylläri, V., Ruzzante, M., Pogni, R., Baratto, M. C., Skrifvars, M., Syrjälä, S., Järvelä, P.

Publication date: 1 Feb 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Applied Polymer Science

Volume: 132

Issue number: 8

Article number: 41509

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2015): CiteScore 1.74 SJR 0.587 SNIP 0.846

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)

Keywords: Blends, Photochemistry, Polyolefins

DOIs:

10.1002/app.41509

URLs:

<http://www.scopus.com/inward/record.url?scp=84911985923&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

Article first published online: 1 OCT 2014 ;(Volume 132, Issue 8, February 20, 2015)<br/>Contribution:

organisation=mol,FACT1=1<br/>Portfolio EDEND: 2014-12-30<br/>Publisher name: JohnWiley & Sons, Inc.

Source: researchoutputwizard

Source ID: 296

Research output: Contribution to journal › Article › Scientific › peer-review

#### Supramolecular hierarchy among halogen and hydrogen bond donors in light-induced surface patterning

Halogen bonding, a noncovalent interaction possessing several unique features compared to the more familiar hydrogen bonding, is emerging as a powerful tool in functional materials design. Herein, we unambiguously show that one of these characteristic features, namely high directionality, renders halogen bonding the interaction of choice when developing azobenzene-containing supramolecular polymers for light-induced surface patterning. The study is conducted by using an extensive library of azobenzene molecules that differ only in terms of the bond-donor unit. We introduce a new tetrafluorophenol-containing azobenzene photoswitch capable of forming strong hydrogen bonds, and show that an iodoethynyl-containing azobenzene comes out on top of the supramolecular hierarchy to provide unprecedented photoinduced surface patterning efficiency. Specifically, the iodoethynyl motif seems highly promising in future development of polymeric optical and photoactive materials driven by halogen bonding.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Aalto University, VTT Technical Research Centre of Finland, Politecn Milan, Polytechnic University of Milan, NFMLab, DCMIC Giulio Natta, ISTM-CNR, Institute of Molecular Sciences and Technologies of CNR, Università Degli Studi di Milano, McGill University, Politecnico di Milano

Contributors: Saccone, M., Dichiarante, V., Forni, A., Goulet-Hanssens, A., Cavallo, G., Vapaavuori, J., Terraneo, G., Barrett, C. J., Resnati, G., Metrangolo, P., Priimägi, A.

Number of pages: 10

Pages: 759-768

Publication date: 28 Jan 2015

Peer-reviewed: Yes

## Publication information

Journal: Journal of Materials Chemistry C

Volume: 3

ISSN (Print): 2050-7534

Ratings:

Scopus rating (2015): CiteScore 5.32 SJR 1.713 SNIP 1.477

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Chemistry

DOIs:

10.1039/c4tc02315c

URLs:

<http://www.scopus.com/inward/record.url?scp=84925407935&partnerID=8YFLogxK> (Link to publication in Scopus)

## Bibliographical note

EXT="Saccone, Marco"

EXT="Vapaavuori, Jaana"

Source: Scopus

Source ID: 84925407935

Research output: Contribution to journal > Article > Scientific > peer-review

## Silver sulfide nanoclusters and the superatom model

The superatom model of electron-shell closings has been widely used to explain the stability of noble-metal nanoclusters of few nanometers, including thiolate-protected Au and Ag nanoclusters. The presence of core sulfur atoms in silver sulfide (Ag-S) nanoclusters renders them a class of clusters with distinctive properties as compared to typical noble-metal clusters. Here, it is natural to ask whether the superatom model is still applicable for the Ag-S nanoclusters with mixed metal and nonmetal core atoms. To address this question, we applied density functional simulations to analyze a series of Ag-S nanoclusters:  $\text{Ag}_{14}\text{S}(\text{SPh})_{12}(\text{PPh}_3)_8$ ,  $\text{Ag}_{14}(\text{SC}_6\text{H}_3\text{F}_2)_{12}(\text{PPh}_3)_8$ ,  $\text{Ag}_{70}\text{S}_{16}(\text{SPh})_{34}(\text{PhCO}_2)_4(\text{triphos})_4$ , and  $[\text{Ag}_{123}\text{S}_{35}(\text{StBu})_{50}]^{3+}$ . We observed that superatomic orbitals are still present in the conduction band of these Ag-S clusters where the cluster cores comprise mostly silver atoms. Our Bader charge analysis illustrates that thiolates play a significant role in withdrawing charge (electron density) from the core Ag atoms. The simulated optical absorption properties of the selected Ag-S clusters reflect the substantial band gaps associated with typical molecular orbitals on both sides. Apart from  $\text{Ag}_{14}\text{S}(\text{SPh})_{12}(\text{PPh}_3)_8$ , which has a central sulfur atom in the cluster core, superatomic orbitals of the Ag-S clusters can have contributions for individual transitions in the conduction band.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research group: Materials and Molecular Modeling, Computational Science X (CompX), University of Jyväskylä, Departments of Physics and Chemistry

Contributors: Goh, J., Malola, S., Häkkinen, H., Akola, J.

Number of pages: 8

Pages: 1583-1590

Publication date: 22 Jan 2015

Peer-reviewed: Yes

## Publication information

Journal: Journal of Physical Chemistry C

Volume: 119

Issue number: 3

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.24

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

10.1021/jp511037x

URLs:

<http://www.scopus.com/inward/record.url?scp=84921476515&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84921476515

Research output: Contribution to journal › Article › Scientific › peer-review

### **Kinetics of polymer looping with macromolecular crowding: Effects of volume fraction and crowder size**

The looping of polymers such as DNA is a fundamental process in the molecular biology of living cells, whose interior is characterised by a high degree of molecular crowding. We here investigate in detail the looping dynamics of flexible polymer chains in the presence of different degrees of crowding. From the analysis of the looping-unlooping rates and the looping probabilities of the chain ends we show that the presence of small crowders typically slows down the chain dynamics but larger crowders may in fact facilitate the looping. We rationalise these non-trivial and often counterintuitive effects of the crowder size on the looping kinetics in terms of an effective solution viscosity and standard excluded volume. It is shown that for small crowders the effect of an increased viscosity dominates, while for big crowders we argue that confinement effects (caging) prevail. The tradeoff between both trends can thus result in the impediment or facilitation of polymer looping, depending on the crowder size. We also examine how the crowding volume fraction, chain length, and the attraction strength of the contact groups of the polymer chain affect the looping kinetics and hairpin formation dynamics. Our results are relevant for DNA looping in the absence and presence of protein mediation, DNA hairpin formation, RNA folding, and the folding of polypeptide chains under biologically relevant high-crowding conditions.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam

Contributors: Shin, J., Cherstvy, A. G., Metzler, R.

Number of pages: 17

Pages: 472-488

Publication date: 21 Jan 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Soft Matter

Volume: 11

Issue number: 3

ISSN (Print): 1744-683X

Ratings:

Scopus rating (2015): CiteScore 3.97 SJR 1.634 SNIP 1.24

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Medicine(all)

DOIs:

10.1039/c4sm02007c

URLs:

<http://www.scopus.com/inward/record.url?scp=84919341015&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84919341015

Research output: Contribution to journal › Article › Scientific › peer-review

### **Non-universal tracer diffusion in crowded media of non-inert obstacles**

We study the diffusion of a tracer particle, which moves in continuum space between a lattice of excluded volume, immobile non-inert obstacles. In particular, we analyse how the strength of the tracer-obstacle interactions and the volume occupancy of the crowders alter the diffusive motion of the tracer. From the details of partitioning of the tracer diffusion modes between trapping states when bound to obstacles and bulk diffusion, we examine the degree of localisation of the tracer in the lattice of crowders. We study the properties of the tracer diffusion in terms of the ensemble and time averaged mean squared displacements, the trapping time distributions, the amplitude variation of the time averaged mean squared displacements, and the non-Gaussianity parameter of the diffusing tracer. We conclude that tracer-obstacle adsorption and binding triggers a transient anomalous diffusion. From a very narrow spread of recorded individual time averaged trajectories we exclude continuous type random walk processes as the underlying physical model of the tracer diffusion in our system. For moderate tracer-crowder attraction the motion is found to be fully ergodic, while at stronger attraction

strength a transient disparity between ensemble and time averaged mean squared displacements occurs. We also put our results into perspective with findings from experimental single-particle tracking and simulations of the diffusion of tagged tracers in dense crowded suspensions. Our results have implications for the diffusion, transport, and spreading of chemical components in highly crowded environments inside living cells and other structured liquids.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam

Contributors: Ghosh, S. K., Cherstvy, A. G., Metzler, R.

Number of pages: 12

Pages: 1847-1858

Publication date: 21 Jan 2015

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 17

Issue number: 3

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.188

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1039/c4cp03599b

URLs:

<http://www.scopus.com/inward/record.url?scp=84919346836&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84919346836

Research output: Contribution to journal > Article > Scientific > peer-review

#### Rational design of a printable, highly conductive silicone-based electrically conductive adhesive for stretchable radio-frequency antennas

Stretchable radio-frequency electronics are gaining popularity as a result of the increased functionality they gain through their flexible nature, impossible within the confines of rigid and planar substrates. One approach to fabricating stretchable antennas is to embed stretchable or flowable conductive materials, such as conductive polymers, conductive polymer composites, and liquid metal alloys as stretchable conduction lines. However, these conductive materials face many challenges, such as low electrical conductivity under mechanical deformation and delamination from substrates. In the present study, a silicone-based electrically conductive adhesive (silo-ECA) is developed that have a conductivity of  $1.51 \times 10^4 \text{ S cm}^{-1}$  and can maintain conductivity above  $1.11 \times 10^3 \text{ S cm}^{-1}$ , even at a large stain of 240%. By using the stretchable silo- ECAs as a conductor pattern and pure silicone elastomers as a base substrate, stretchable antennas can be fabricated by stencil printing or soft-lithography. The resulting antenna's resonant frequency is tunable over a wide range by mechanical modulation. This fabrication method is low-cost, can support large-scale production, has high reliability over a wide temperature range, and eliminates the concerns of leaking or delamination between conductor and substrate experienced in previously reported micro-fluidic antennas.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Sensing Systems for Wireless Medicine (MediSense), Georgia Institute of Technology, Chinese University of Hong Kong

Contributors: Li, Z., Le, T., Wu, Z., Yao, Y., Li, L., Tentzeris, M., Moon, K. S., Wong, C. P.

Number of pages: 7

Pages: 464-470

Publication date: 21 Jan 2015

Peer-reviewed: Yes

#### Publication information

Journal: Advanced Functional Materials

Volume: 25

Issue number: 3

ISSN (Print): 1616-301X

Ratings:

Scopus rating (2015): CiteScore 11.93 SJR 4.859 SNIP 2.439



Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Biomaterials, Condensed Matter Physics, Electrochemistry

DOIs:

10.1002/adfm.201403275

URLs:

<http://www.scopus.com/inward/record.url?scp=84920994935&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84920994935

Research output: Contribution to journal › Article › Scientific › peer-review

### **Second-Harmonic Generation from Metal Nanoparticles: Resonance Enhancement versus Particle Geometry**

We demonstrate that optical second-harmonic generation (SHG) from arrays of noncentrosymmetric gold nanoparticles depends essentially on particle geometry. We prepare nanoparticles with different geometrical shapes (L and T) but similar wavelengths for the polarization-dependent plasmon resonances. In contrast to recent interpretations emphasizing resonances at the fundamental frequency, the T shape leads to stronger SHG when only one, instead of both, polarization component of the fundamental field is resonant. This is explained by the character of plasmon oscillations supported by the two shapes. Our numerical simulations for both linear and second-order responses display unprecedented agreement with measurements.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Optics, Research group: Nonlinear Optics, Frontier Photonics, Institute of Photonics, Univ Eastern Finland, University of Eastern Finland, Sch Pharm

Contributors: Czaplicki, R., Mäkitalo, J., Siikanen, R., Husu, H., Lehtolahti, J., Kuittinen, M., Kauranen, M.

Number of pages: 5

Pages: 530-534

Publication date: 14 Jan 2015

Peer-reviewed: Yes

Early online date: 18 Dec 2014

#### **Publication information**

Journal: Nano Letters

Volume: 15

Issue number: 1

ISSN (Print): 1530-6984

Ratings:

Scopus rating (2015): CiteScore 14.76 SJR 8.359 SNIP 3.064

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Bioengineering, Chemistry(all), Materials Science(all), Mechanical Engineering

Keywords: Metal nanoparticles, nonlinear optics, plasmonic resonances, second-harmonic generation

DOIs:

10.1021/nl503901e

Additional files:

[Supplementary\\_info\\_to\\_Nano\\_Lett.\\_15\\_\(2015\)\\_530-534\\_R.Czaplicki\\_open](#)

URLs:

<http://www.scopus.com/inward/record.url?scp=84921059491&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: WOS

Source ID: 000348086100083

Research output: Contribution to journal › Article › Scientific › peer-review

### **Oxidation half-reaction of aqueous nucleosides and nucleotides via photoelectron spectroscopy augmented by ab initio calculations**

Oxidative damage to DNA and hole transport between nucleobases in oxidized DNA are important processes in lesion formation for which surprisingly poor thermodynamic data exist, the relative ease of oxidizing the four nucleobases being one such example. Theoretical simulations of radiation damage and charge transport in DNA depend on accurate values for vertical ionization energies (VIEs), reorganization energies, and standard reduction potentials. Liquid-jet photoelectron spectroscopy can be used to directly study the oxidation half-reaction. The VIEs of nucleic acid building blocks are measured in their native buffered aqueous environment. The experimental investigation of purine and pyrimidine nucleotides, nucleosides, pentose sugars, and inorganic phosphate demonstrates that photoelectron spectra of nucleotides arise as a spectral sum over their individual chemical components; that is, the electronic interactions between each component are effectively screened from one another by water. Electronic structure theory affords the assignment of

the lowest energy photoelectron band in all investigated nucleosides and nucleotides to a single ionizing transition centered solely on the nucleobase. Thus, combining the measured VIEs with theoretically determined reorganization energies allows for the spectroscopic determination of the one-electron redox potentials that have been difficult to establish via electrochemistry.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Southern California, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Max-Planck-Institut für Dynamik und Selbstorganisation, Department of Physical Chemistry, Helmholtz Center Berlin

Contributors: Schroeder, C. A., Pluharová, E., Seidel, R., Schroeder, W. P., Faubel, M., Slaviček, P., Winter, B., Jungwirth, P., Bradforth, S. E.

Number of pages: 9

Pages: 201-209

Publication date: 14 Jan 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of the American Chemical Society

Volume: 137

Issue number: 1

ISSN (Print): 0002-7863

Ratings:

Scopus rating (2015): CiteScore 12.81 SJR 6.775 SNIP 2.6

Original language: English

ASJC Scopus subject areas: Catalysis, Chemistry(all), Biochemistry, Colloid and Surface Chemistry

DOIs:

10.1021/ja508149e

URLs:

<http://www.scopus.com/inward/record.url?scp=84921038760&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84921038760

Research output: Contribution to journal > Article > Scientific > peer-review

#### Manipulation of polycarbonate urethane bulk properties via incorporated zwitterionic polynorbornene for tissue engineering application

Elastomeric crosslinked materials based on polycarbonate urethane (PCU) and zwitterionic polynorbornene were designed by thiol-ene click-chemistry and crosslinking reaction. The zwitterionic polynorbornene poly(NSulfoZI) with functionalisable double bonds was first treated with L-cysteine via thiol-ene click-reaction and subsequently formed a crosslinked structure upon treatment with PCU in the presence of a small amount of hexamethylene-1,6-diisocyanate as a crosslinking agent. The obtained materials possessed improved tensile strength (14–20 MPa) and initial modulus (8–14 MPa). All of these materials showed high breaking strain (ε<sub>b</sub> 740–900%) except the material with a high poly(NSulfoZI) content of 28% (ε<sub>b</sub> 470 ± 80%). The biodegradability of these materials was enhanced compared to blank PCU, as demonstrated by testing in PBS for five weeks. Moreover, the cytocompatibility was studied by MTT assay. The adhesion and proliferation of endothelial cells (EA.hy926) over a one-week period indicated that cell growth on these designed material surfaces was enhanced. Therefore, these zwitterionic polynorbornene-modified PCU-based materials could be suitable candidates for tissue engineering applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Tianjin University

Contributors: Khan, M., Yang, J., Shi, C., Feng, Y., Zhang, W., Gibney, K., Tew, G. N.

Pages: 11284-11292

Publication date: 6 Jan 2015

Peer-reviewed: Yes

#### Publication information

Journal: RSC Advances

Volume: 5

Issue number: 15

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2015): CiteScore 3.42 SJR 0.947 SNIP 0.834

Original language: English

ASJC Scopus subject areas: Materials Science(all), Pharmacology, Toxicology and Pharmaceutics(all), Chemistry(all)

DOIs:

10.1039/C4RA14608E

URLs:

<http://pubs.rsc.org/en/Content/ArticleLanding/2015/RA/C4RA14608E#ldivAbstract>

Research output: Contribution to journal › Article › Scientific › peer-review

### Photophysical properties of Sn (IV)tetraphenylporphyrin-pyrene dyad with a $\beta$ -vinyl linker

A Sn(IV)tetraphenylporphyrin (T) has been functionalized with a  $\beta$ -vinyl pyrene (P) and the photophysical properties of the formed dyad (T-P) with its corresponding precursors were studied in three solvents with different polarities using steady-state and time-resolved measurements in ps and fs timescales. When the pyrene moiety is excited at  $\lambda_{\text{exc}} = 340$  nm, the fluorescence spectroscopy experiments indicate in all the studied solvents, an efficient quenching of the pyrene emission. When excited at either  $\lambda_{\text{exc}} = 340$  nm or  $\lambda_{\text{exc}} = 405$  nm, where porphyrin absorbs, a new emissive excited state complex (T-P)\* is observed at wavelengths close to the parent porphyrin emission. The emission is more pronounced in nonpolar hexane showing a mono-exponential decay, but bi-exponential decays are observed in more polar dichloromethane and acetonitrile. When the porphyrin moiety is excited at  $\lambda_{\text{exc}} = 425$  nm, the fs transient absorption analysis shows two different intermediate species ( $\sim 7$ -11 ps and 80-100 ps) with broad absorption in the near-IR region. This implies either the existence of two different excited conformers (T-P)\*, which decay to the ground state via a charge separated state (CSS), or the formation of the (T-P)\* state via the second excited state of the porphyrin moiety, yielding first an excited emissive  $\nu$ (T-P)\* state, with a lifetime of 80-100 ps.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology, Inorganic and Physical Chemistry Division, CSIR-Indian Institute of Chemical Technology

Contributors: Reeta, P. S., Khetubol, A., Jella, T., Chukharev, V., Abou-Chahine, F., Tkachenko, N. V., Giribabu, L., Lemmetyinen, H.

Number of pages: 13

Pages: 288-300

Publication date: 1 Jan 2015

Peer-reviewed: Yes

### Publication information

Journal: Journal of Porphyrins and Phthalocyanines

Volume: 19

Issue number: 1-3

ISSN (Print): 1088-4246

Ratings:

Scopus rating (2015): CiteScore 1.17 SJR 0.413 SNIP 0.457

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: fs transient absorption, kinetics, optical properties, Sn (IV)tetraphenylporphyrin,  $\beta$ -vinyl pyrene donor

DOIs:

10.1142/S1088424615500108

URLs:

<http://www.scopus.com/inward/record.url?scp=84928483683&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84928483683

Research output: Contribution to journal › Article › Scientific › peer-review

### Perfluoro-1,1'-biphenyl and perfluoronaphthalene and their derivatives as $\pi$ -acceptors for anions

Addition of anions to perfluorinated 1,1'-biphenyl 1 or naphthalene 2 results in a shift of the  $^{19}\text{F}$  NMR signals. However, any specific interaction cannot be assigned to this effect. In order to study the interaction in more detail, the salt derivatives 3 and 4 were prepared and studied by single crystal X-ray diffraction revealing weak anion- $\pi$  interactions in the solid state.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, University of Jyväskylä, Institut für Organische Chemie, RWTH Aachen

Contributors: Yi, H., Albrecht, M., Valkonen, A., Rissanen, K.  
Number of pages: 4  
Pages: 746-749  
Publication date: 1 Jan 2015  
Peer-reviewed: Yes

#### Publication information

Journal: New Journal of Chemistry

Volume: 39

Issue number: 1

ISSN (Print): 1144-0546

Ratings:

Scopus rating (2015): CiteScore 3.27 SJR 0.935 SNIP 0.822

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis, Materials Chemistry

DOIs:

10.1039/c4nj01654h

URLs:

<http://www.scopus.com/inward/record.url?scp=84919782132&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84919782132

Research output: Contribution to journal > Article > Scientific > peer-review

#### A comparison of five optical surface topography measurement methods

The results of optical surface topography measurement techniques have been questioned in the past because of possible measurement artifacts due to light penetration into the paper. We compared the topography measurement results from five optical techniques: laser profilometry, shape-from-focus, stripe projection, chromatic sensing, and photometric stereo. These techniques were tested on coated and uncoated papers with a PPS roughness range from 0.7  $\mu\text{m}$  to 7.7  $\mu\text{m}$ . We made the measurement results directly comparable by measuring exactly the same regions on the paper samples and registering the resulting topography maps. We then calculated the point-wise Pearson correlation between the maps at different wavelength bands to obtain quantitative values for the similarity of the measurement results at different structure sizes. The correspondences between the measured topography maps were also examined through multivariate linear regression and roughness indices evaluated at two different structure sizes. For rougher grades like office paper or sack paper, the topography measurements from the five measurement techniques showed corresponding results. For a moderately smooth lightweight coated (LWC) paper, the measured topographies agreed to some degree, and for smooth supercalendered (SC) and woodfree coated (WFC) papers, the agreement was poor. From the available data, it is impossible to tell which of the measurement techniques delivers the true surface topography of smooth papers.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Automation Science and Engineering, Field robotics for efficient work sites (FIRE), Graz University of Technology

Contributors: Mettänen, M., Hirn, U.

Number of pages: 12

Pages: 27-38

Publication date: 1 Jan 2015

Peer-reviewed: Yes

#### Publication information

Journal: TAPPI Journal

Volume: 14

Issue number: 1

ISSN (Print): 0734-1415

Ratings:

Scopus rating (2015): SJR 0.44 SNIP 0.705

Original language: English

ASJC Scopus subject areas: Media Technology, Chemical Engineering(all), Chemistry(all), Mechanical Engineering, Materials Science(all)

Electronic versions:

Mettanen\_Hirn\_TAPPI\_2015\_preprint

URLs:

<http://urn.fi/URN:NBN:fi:tty-201701241070>

URLs:

<http://www.scopus.com/inward/record.url?scp=84923164333&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84923164333

Research output: Contribution to journal › Article › Scientific › peer-review

### **Appropriate pricing policy needed worldwide for improving water services infrastructure**

This article highlights the enormous and growing gap between the projected and required financing of water services infrastructure, which is caused by unviable pricing and/or costrecovery regimes. Globally there is a growing funding gap in rehabilitation, renewal, and replacement of aging water infrastructure and the need for future greenfield investments. Underpricing of water services and the need for rehabilitation seem to be worldwide phenomena. There are diverse constraints in OECD (Organisation for Economic Co-Operation and Development) and non-OECD countries contributing to underpriced water services; however, the message is clear: the global water industry must stop underpricing precious water resources. Future enjoyment of sustainable water services will require customers to bear all or at least a major part of the costs. Better awareness of broader economic and social benefits of water supply, and particularly of sanitation, also will be needed.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Life Cycle Effectiveness of the Built Environment (LCE@BE)

Contributors: Hukka, J. J., Katko, T. S.

Pages: E37-E46

Publication date: 1 Jan 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal American Water Works Association

Volume: 107

Issue number: 1

ISSN (Print): 0003-150X

Ratings:

Scopus rating (2015): CiteScore 0.41 SJR 0.401 SNIP 0.641

Original language: English

ASJC Scopus subject areas: Water Science and Technology, Chemistry(all)

Keywords: Aging and deteriorating infrastructure, Pricing, Sustainability, Sustainable cost recovery, Underpricing, Water services infrastructure

DOIs:

10.5942/jawwa.2015.107.0007

URLs:

<http://www.scopus.com/inward/record.url?scp=84920619765&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84920619765

Research output: Contribution to journal › Article › Scientific › peer-review

### **$\pi$ -Expanded $\alpha,\beta$ -unsaturated ketones: Synthesis, optical properties, and two-photon-induced polymerization**

A library of  $\pi$ -expanded  $\alpha,\beta$ -unsaturated ketones was designed and synthesized. They were prepared by a combination of Wittig reaction, Sonogashira reaction, and aldol condensation. It was further demonstrated that the double aldol condensation can be performed effectively for highly polarized styrene- and diphenylacetylene-derived aldehydes. The strategic placement of two dialkylamino groups at the periphery of D- $\pi$ -A- $\pi$ -D molecules resulted in dyes with excellent solubility. These ketones absorb light in the region 400-550nm. Many of them display strong solvatochromism so that the emission ranges from 530-580nm in toluene to the near-IR region in benzonitrile. Ketones based on cyclobutanone as central moieties display very high fluorescence quantum yields in nonpolar solvents, which decrease drastically in polar media. Photophysical studies of these new functional dyes revealed that they possess an enhanced two-photon absorption cross section when compared with simpler ketone derivatives. Due to strong polarization of the resulting dyes, values of two-photon absorption cross sections on the level of 200-300GM at 800nm were achieved, and thanks to that as well as the presence of the keto group, these new two-photon initiators display excellent performance so that the operating region is 5-75mW in some cases.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology, Frontier Photonics, Politechnika Warszawska, Foundation for Research and Technology-Hellas, Institute of Electronic Structure and Laser, Institute of Organic Chemistry of the Polish Academy of Sciences

Contributors: Nazir, R., Bourquard, F., Balčiūnas, E., Smoleń, S., Gray, D., Tkachenko, N. V., Farsari, M., Gryko, D. T.  
Number of pages: 9  
Pages: 682–690  
Publication date: 2015  
Peer-reviewed: Yes

#### Publication information

Journal: ChemPhysChem

Volume: 16

Issue number: 3

ISSN (Print): 1439-4235

Ratings:

Scopus rating (2015): CiteScore 3.21 SJR 1.303 SNIP 0.889

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Atomic and Molecular Physics, and Optics

Keywords: Aldol reaction, Ketones, Photosensitizers, Polymerization, Two-photon absorption

DOIs:

10.1002/cphc.201402646

URLs:

<http://www.scopus.com/inward/record.url?scp=84920105777&partnerID=8YFLogxK> (Link to publication in Scopus)

Research output: Contribution to journal › Article › Scientific › peer-review

#### Role of the bridge in photoinduced electron transfer in porphyrin-fullerene dyads

The role of  $\pi$ -conjugated molecular bridges in through-space and through-bond electron transfer is studied by comparing two porphyrin-fullerene donor-acceptor (D-A) dyads. One dyad, ZnP-Ph-C<sub>60</sub> (ZnP=zinc porphyrin), incorporates a phenyl bridge between D and A and behaves very similarly to analogous dyads studied previously. The second dyad, ZnP-EDOTV-C<sub>60</sub>, introduces an additional 3,4-ethylenedioxythienylvinylene (EDOTV) unit into the conjugated bridge, which increases the distance between D and A, but, at the same time, provides increased electronic communication between them. Two essential outcomes that result from the introduction of the EDOTV unit in the bridge are as follows: 1) faster charge recombination, which indicates enhanced electronic coupling between the charge-separated and ground electronic states; and 2) the disappearance of the intramolecular exciplex, which mediates photoinduced charge separation in the ZnP-Ph-C<sub>60</sub> dyad. The latter can be interpreted as a gradual decrease in electronic coupling between locally excited singlet states of D and A when introducing the EDOTV unit into the D-A bridge.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Universitat Politècnica de València, Spain, Universidad de Castilla-La Mancha

Contributors: Pelado, B., Abou-Chahine, F., Calbo, J., Caballero, R., delaCruz, P., Junquera-Hernández, J. M., Ortí, E., Tkachenko, N. V., Langa, F.

Number of pages: 12

Pages: 5814-5825

Publication date: 2015

Peer-reviewed: Yes

#### Publication information

Journal: Chemistry: A European Journal

Volume: 21

Issue number: 15

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2015): CiteScore 4.99 SJR 2.461 SNIP 1.195

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Conjugated bridge, EDOT, Electron transfer, Fullerene, Porphyrin

DOIs:

10.1002/chem.201406514

URLs:

<http://www.scopus.com/inward/record.url?scp=84923917540&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84925396738

Research output: Contribution to journal › Article › Scientific › peer-review

### Ballistic and numerical simulation of impacting goods on conveyor belt rubber

Impact loading is an important process in the transport industry as it causes wear and failure of critical components. Conveyor belts are of particular importance as they are used in practically every industry where large quantities of goods are moved over short (<10 m) or long distances (>1 km). To investigate stress levels inside the material during impact loading, a gas gun was utilized to shoot 9 mm spherical steel balls onto the surface of a rubber conveyor belt. A high speed video recording system was employed in order to determine penetration depth and dissipated energy of the steel ball. Maximal penetration depths of up to 3.9 mm and maximal dissipated energies of up to 86.8 % were measured. Additionally, a numerical simulation using smooth particle applied mechanics was conducted and compared to the experimental results obtained with the gas gun. The calculated von Mises stresses affected the conveyor belts up to a maximum depth of 8.8 mm with at least 20 MPa. Maximum von Mises stresses were calculated to reach 60 MPa.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Materials Characterization, Computational Science X (CompX), Engineering materials science and solutions (EMASS), AC2T Research GmbH

Contributors: Molnar, W., Nugent, S., Lindroos, M., Apostol, M., Varga, M.

Number of pages: 7

Pages: 1-7

Publication date: 2015

Peer-reviewed: Yes

#### Publication information

Journal: Polymer Testing

Volume: 42

ISSN (Print): 0142-9418

Ratings:

Scopus rating (2015): CiteScore 2.58 SJR 0.898 SNIP 1.622

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Polymers and Plastics

Keywords: Ballistic impact, Conveyor belt, Rubber, Simulation, Tribology

DOIs:

10.1016/j.polymertesting.2014.12.001

URLs:

<http://www.scopus.com/inward/record.url?scp=84920749567&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84920749567

Research output: Contribution to journal > Article > Scientific > peer-review

### Synthesis of fluorescent naphthoquinolizines via intramolecular houben-hoesch reaction

The repertoire of synthetic methods leading to aza-analogues of polycyclic aromatic heterocycles has been enlarged by the discovery of the rearrangement of 10-substituted benzo[h]quinolines into compounds bearing an azonia-pyrene moiety. Acid-mediated intramolecular cyclization of derivatives bearing-CH<sub>2</sub>CN and-CH<sub>2</sub>CO<sub>2</sub>Et groups led to compounds bearing a 5-substituted benzo[de]pyrido[3,2,1-ij]quinolinium core. Advanced photophysical studies including time-correlated single photon counting (TCSPC) and transient absorption spectroscopy of 5-aminobenzo[de]pyrido[3,2,1-ij]quinolin-4-ium salt and 5H-benzo[de]pyrido[3,2,1-ij]quinolin-5-one showed their promising optical properties such as high fluorescence quantum yields (37-59%), which was almost independent of the solvent, and high tenability of the absorption band position upon changing the solvent. The benzo[de]pyrido[3,2,1-ij]quinolinium salt selectively stains nucleic acids (in the nucleus and mitochondria) in eukaryotic cells.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Institute of Organic Chemistry of the Polish Academy of Sciences, Politechnika Warszawska, Warsaw Univ Technol, Warsaw University of Technology, Fac Phys, Opt Div, Department of Laboratory Diagnostics and Clinical Immunology of Developmental Age, Medical University of Warsaw, Department of Chemistry and Bioengineering, Tampere University of Technology

Contributors: Stasyuk, A. J., Smoleń, S., Glodkowska-Mrowka, E., Brutkowski, W., Cyrański, M. K., Tkachenko, N., Gryko, D. T.

Number of pages: 6

Pages: 553-558

Publication date: 2015

Peer-reviewed: Yes

### Publication information

Journal: Chemistry - An Asian Journal

Volume: 10

Issue number: 3

ISSN (Print): 1861-4728

Ratings:

Scopus rating (2015): CiteScore 4.41 SJR 1.742 SNIP 0.906

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Cyclization, Fluorescence, Heterocycles, Pyrenes, Quinolines

DOIs:

10.1002/asia.201403339

URLs:

<http://www.scopus.com/inward/record.url?scp=84923364824&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84923364824

Research output: Contribution to journal > Article > Scientific > peer-review

### Synthesis, crystal structure, spectral, dielectric characteristics and conduction mechanism of two novel carboxylates of 1-benzhydrylpiperazine

Two new 1-benzhydrylpiperazinium carboxylates with tartrate and maleate, (C<sub>17</sub>H<sub>21</sub>N<sub>2</sub>)(C<sub>4</sub>H<sub>5</sub>O<sub>6</sub>) and (C<sub>17</sub>H<sub>22</sub>N<sub>2</sub>)(C<sub>4</sub>H<sub>3</sub>O<sub>4</sub>)<sub>2</sub>, have been synthesized and characterized. Crystal structure determinations show that the compounds crystallize in the P21 and the P21/c space groups of the monoclinic system, respectively. Only in the maleate the organic group is protonated on both nitrogen atoms of piperazine ring. The infrared spectra of these compounds reported from 400 to 4000 cm<sup>-1</sup> confirmed the presence of the principal bands assigned to the internal modes of cations and anions of both compounds. The optical band gaps were calculated and found to be 3.46 and 4.14 eV for tartrate and maleate, respectively. Different molecular motions were determined via dielectric relaxation spectroscopy. Measurements of AC conductivity as a function of frequency at different temperatures indicated the hopping conduction mechanism. The number of <sup>13</sup>C CP-MAS NMR lines is in good agreement with the crystallographic data. Graphical abstract: [Figure not available: see fulltext.]

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Laboratory of Chemical Materials, Faculty of Sciences of Bizerte, Carthage University

Contributors: Wacharine, I., Valkonen, A., Rzaigui, M., Smirani, W.

Number of pages: 14

Pages: 2007-2020

Publication date: 2015

Peer-reviewed: Yes

### Publication information

Journal: Monatshefte für Chemie

Volume: 146

Issue number: 12

ISSN (Print): 0026-9247

Ratings:

Scopus rating (2015): CiteScore 1.15 SJR 0.33 SNIP 0.561

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Carboxylic acids, Crystal structure, Hydrogen bonds, NMR spectroscopy, Solid state, X-ray structure determination

DOIs:

10.1007/s00706-015-1553-1

URLs:

<http://www.scopus.com/inward/record.url?scp=84939509914&partnerID=8YFLogxK> (Link to publication in Scopus)

Research output: Contribution to journal > Article > Scientific > peer-review

### Chemolithotrophic denitrification in biofilm reactors

Chemolithotrophic denitrification is an inexpensive and advantageous process for nitrate removal and represents a promising alternative to classical denitrification with organics. Chemolithotrophic denitrifiers are microorganisms able to



reduce nitrate and nitrite using inorganic compounds as source of energy. Ferrous iron, sulfur-reduced compounds (e.g. hydrogen sulfide, elemental sulfur and thiosulfate), hydrogen gas, pyrite and arsenite have been used as inorganic electron donors resulting in diverse outcomes. In the last 40 years, a large number of engineered systems have been used to maintain chemolithotrophic denitrification and improve rate and efficiency of the process. Among them, biofilm reactors proved to be robust and high-performing technologies. Packed bed reactors are particularly suitable for the removal of low nitrate concentrations, since high retention times are required to complete denitrification. Fluidized bed and membrane biofilm reactors result in the highest denitrification rates ( $>20\text{ kg N-NO}_3^-/\text{m}^3\text{d}$ ) when hydrogen gas and sulfur reduced compounds are used as electron donors. Hydrogen gas pressure and current intensity rule the performance of membrane biofilm and biofilm electrode reactors, respectively. Biofouling is the most common and detrimental issue in biofilm reactors. Bed fluidization and hydrogen supply limitation are convenient and effective solutions to mitigate biofouling.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Department of Civil and Mechanical Engineering, University of Cassino and Southern Lazio

Contributors: Di Capua, F., Papirio, S., Lens, P. N. L., Esposito, G.

Number of pages: 15

Pages: 643-657

Publication date: 2015

Peer-reviewed: Yes

Early online date: 15 Jun 2015

#### Publication information

Journal: Chemical Engineering Journal

Volume: 280

ISSN (Print): 1385-8947

Ratings:

Scopus rating (2015): CiteScore 5.68 SJR 1.676 SNIP 1.895

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all), Industrial and Manufacturing Engineering, Environmental Chemistry

Keywords: Biofilm, Biofilm electrode reactor, Chemolithotrophic denitrification, Fluidized bed reactor, Membrane biofilm reactor, Packed bed reactor

DOIs:

10.1016/j.cej.2015.05.131

#### Bibliographical note

AUX=keb,"Di Capua, Francesco"

EXT="Papirio, Stefano"

Source: Scopus

Source ID: 84932636341

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

#### Van der Waals interactions are critical in Car-Parrinello molecular dynamics simulations of porphyrin-fullerene dyads

The interplay between electrostatic and van der Waals (vdW) interactions in porphyrin- $\text{C}_{60}$  dyads is still under debate despite its importance in influencing the structural characteristics of such complexes considered for various applications in molecular photovoltaics. In this article, we sample the conformational space of a porphyrin- $\text{C}_{60}$  dyad using Car-Parrinello molecular dynamics simulations with and without empirical vdW corrections. Long-range vdW interactions, which are poorly described by the commonly used density functional theory functionals, prove to be essential for a proper dynamics of the dyad moieties. Inclusion of vdW corrections brings porphyrin and  $\text{C}_{60}$  close together in an orientation that is in agreement with experimental observations. The structural differences arising from the vdW corrections are shown to be significant for several properties and potentially less important for others. Additionally, our Mulliken population analysis reveals that contrary to the common belief, porphyrin is not the primary electron donating moiety for  $\text{C}_{60}$ . In the considered dyad, fullerene's affinity for electrons is primarily satisfied by charge transfer from the amide group of the linker. However, we show that in the absence of another suitable bound donor,  $\text{C}_{60}$  can withdraw electrons from porphyrin if it is sufficiently close.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Computational Science X (CompX), Frontier Photonics, VTT Technical Research Centre of Finland

Contributors: Karilainen, T., Cramariuc, O., Kuisma, M., Tappura, K., Hukka, T. I.  
Number of pages: 10  
Pages: 612-621  
Publication date: 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Computational Chemistry  
Volume: 36  
Issue number: 9  
ISSN (Print): 0192-8651  
Ratings:

Scopus rating (2015): CiteScore 3.81 SJR 1.382 SNIP 1.368

Original language: English

ASJC Scopus subject areas: Chemistry(all), Computational Mathematics

Keywords: Car-Parrinello molecular dynamics, Fullerene, Porphyrin, Time-dependent-density functional theory

DOIs:

10.1002/jcc.23834

URLs:

<http://www.scopus.com/inward/record.url?scp=84923259668&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

ORG=fys,0.5

ORG=keb,0.5

Source: Scopus

Source ID: 84923259668

Research output: Contribution to journal > Article > Scientific > peer-review

#### Characterisation of novel regenerated cellulosic, viscose, and cotton fibres and the dyeing properties of fabrics

There is a global demand for constant increase in the production of textile fibres. Currently, the market for cellulosic fibres is dominated by cotton and viscose fibres. However, new alternative cellulosic fibres are being sought to meet the growing demand. The dyeing properties of novel fibres aiming at the marketplace are among the properties that determine their applicability to textiles. Recently, a novel process for producing cellulosic fibres, the Biocelsol process, has been scaled up so that the spinning of yarn from Biocelsol fibres is now possible. In this study, the reactive dye Levafix CA Blue was applied to cellulosic fabrics made from viscose, cotton, and Biocelsol yarns. The crystalline structure and morphology of the fibres were studied by Fourier transform infrared spectroscopy and field-emission scanning electron microscopy. The crystalline structure and morphology of the Biocelsol fibres resembled those of viscose fibres, but, owing to higher water absorption, the Biocelsol fabric had a higher dye exhaustion. The colour yield of the Biocelsol fabric was 62% and 41% higher than that of cotton and viscose fabrics respectively, suggesting that less dye is needed to gain a shade in Biocelsol fabric than in viscose and cotton fabrics.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Fibre Materials, Research group: Materials

Characterization, Engineering materials science and solutions (EMASS)

Contributors: Kamppuri, T., Vehviläinen, M., Puolakka, A., Honkanen, M., Vippola, M., Rissanen, M.

Number of pages: 7

Pages: 396-402

Publication date: 2015

Peer-reviewed: Yes

#### Publication information

Journal: Coloration Technology

Volume: 131

Issue number: 5

ISSN (Print): 1472-3581

Ratings:

Scopus rating (2015): CiteScore 1.28 SJR 0.425 SNIP 0.97

Original language: English

ASJC Scopus subject areas: Chemistry (miscellaneous), Chemical Engineering(all), Materials Science (miscellaneous)

DOIs:

10.1111/cote.12163

URLs:

<http://www.scopus.com/inward/record.url?scp=84941702129&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84941940416

Research output: Contribution to journal › Article › Scientific › peer-review

### **Geometry controlled anomalous diffusion in random fractal geometries: Looking beyond the infinite cluster**

We investigate the ergodic properties of a random walker performing (anomalous) diffusion on a random fractal geometry. Extensive Monte Carlo simulations of the motion of tracer particles on an ensemble of realisations of percolation clusters are performed for a wide range of percolation densities. Single trajectories of the tracer motion are analysed to quantify the time averaged mean squared displacement (MSD) and to compare this with the ensemble averaged MSD of the particle motion. Other complementary physical observables associated with ergodicity are studied, as well. It turns out that the time averaged MSD of individual realisations exhibits non-vanishing fluctuations even in the limit of very long observation times as the percolation density approaches the critical value. This apparent non-ergodic behaviour concurs with the ergodic behaviour on the ensemble averaged level. We demonstrate how the non-vanishing fluctuations in single particle trajectories are analytically expressed in terms of the fractal dimension and the cluster size distribution of the random geometry, thus being of purely geometrical origin. Moreover, we reveal that the convergence scaling law to ergodicity, which is known to be inversely proportional to the observation time  $T$  for ergodic diffusion processes, follows a power-law  $\sim T^{-h}$  with  $h < 1$  due to the fractal structure of the accessible space. These results provide useful measures for differentiating the subdiffusion on random fractals from an otherwise closely related process, namely, fractional Brownian motion. Implications of our results on the analysis of single particle tracking experiments are provided.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Institute for Physics and Astronomy, University of Potsdam, School of Physics, Korea Institute for Advanced Study

Contributors: Mardoukhi, Y., Jeon, J., Metzler, R.

Number of pages: 14

Pages: 30134-30147

Publication date: 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Physical Chemistry Chemical Physics

Volume: 17

Issue number: 44

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.188

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1039/c5cp03548a

Source: Scopus

Source ID: 84946811474

Research output: Contribution to journal › Article › Scientific › peer-review

### **Stimuli-Responsive Materials Based on Interpenetrating Polymer Liquid Crystal Hydrogels**

Stimuli-responsive materials based on interpenetrating liquid crystal-hydrogel polymer networks are fabricated. These materials consist of a cholesteric liquid crystalline network that reflects color and an interwoven poly(acrylic acid) network that provides a humidity and pH response. The volume change in the cross-linked hydrogel polymer results in a dimensional alteration in the cholesteric network as well, which, in turn, leads to a color change yielding a dual-responsive photonic material. Furthermore a patterned coating having responsive and static interpenetrating polymer network areas is produced that changes both its surface topography and color.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Eindhoven University of Technology, School of Mathematical Sciences

Contributors: Stumpel, J. E., Gil, E. R., Spoelstra, A. B., Bastiaansen, C. W. M., Broer, D. J., Schenning, A. P. H. J.

Pages: 3314–3320

Publication date: 2015

Peer-reviewed: Yes

### Publication information

Journal: Advanced Functional Materials

Volume: 25

Issue number: 22

ISSN (Print): 1616-301X

Ratings:

Scopus rating (2015): CiteScore 11.93 SJR 4.859 SNIP 2.439

Original language: English

ASJC Scopus subject areas: Biomaterials, Electrochemistry, Condensed Matter Physics, Electronic, Optical and Magnetic Materials

Keywords: Cholesteric liquid crystals, Hydrogels, Interpenetrating polymer networks, Photonic materials, Smart materials

DOIs:

10.1002/adfm.201500745

URLs:

<http://www.scopus.com/inward/record.url?scp=84928138667&partnerID=8YFLogxK> (Link to publication in Scopus)

Research output: Contribution to journal › Article › Scientific › peer-review

### Water-responsive dual-coloured photonic polymer coatings based on cholesteric liquid crystals

This work describes a straightforward method to prepare patterned photonic coatings which alter their colour when exposed to water. Various kinds of dual-coloured patterns were made, which become visible or fade away when placed in water. These effects are reversible and can be repeated many times.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Laboratory of Functional Organic Materials and Devices, Eindhoven University of Technology

Contributors: Stumpel, J. E., Broer, D. J., Schenning, A. P. H. J.

Number of pages: 4

Pages: 94650-94653

Publication date: 2015

Peer-reviewed: Yes

### Publication information

Journal: RSC Advances

Volume: 5

Issue number: 115

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2015): CiteScore 3.42 SJR 0.947 SNIP 0.834

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all)

DOIs:

10.1039/c5ra18017a

URLs:

<http://www.scopus.com/inward/record.url?scp=84946926560&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84946926560

Research output: Contribution to journal › Article › Scientific › peer-review

### Coulomb explosion during the early stages of the reaction of alkali metals with water

Alkali metals can react explosively with water and it is textbook knowledge that this vigorous behaviour results from heat release, steam formation and ignition of the hydrogen gas that is produced. Here we suggest that the initial process enabling the alkali metal explosion in water is, however, of a completely different nature. High-speed camera imaging of liquid drops of a sodium/potassium alloy in water reveals submillisecond formation of metal spikes that protrude from the surface of the drop. Molecular dynamics simulations demonstrate that on immersion in water there is an almost immediate release of electrons from the metal surface. The system thus quickly reaches the Rayleigh instability limit, which leads to a 'coulomb explosion' of the alkali metal drop. Consequently, a new metal surface in contact with water is formed, which explains why the reaction does not become self-quenched by its products, but can rather lead to explosive behaviour.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Technische Universität Braunschweig

Contributors: Mason, P. E., Uhlig, F., Vaněk, V., Buttersack, T., Bauerecker, S., Jungwirth, P.  
Number of pages: 5  
Pages: 250-254  
Publication date: 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Nature Chemistry

Volume: 7

Issue number: 3

ISSN (Print): 1755-4330

Ratings:

Scopus rating (2015): CiteScore 15.17 SJR 11.144 SNIP 4.57

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

DOIs:

10.1038/nchem.2161

URLs:

<http://www.scopus.com/inward/record.url?scp=84923338638&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84923338638

Research output: Contribution to journal > Article > Scientific > peer-review

#### Block co-polymers for nanolithography: Rapid microwave annealing for pattern formation on substrates

The integration of block copolymer (BCP) self-assembled nanopattern formation as an alternative lithographic tool for nanoelectronic device fabrication faces a number of challenges such as defect densities, feature size, pattern transfer, etc. Key barriers are the nanopattern process times and pattern formation on current substrate stack layers such as hard masks (e.g., silicon nitride,  $\text{Si}_3\text{N}_4$ ). We report a rapid microwave assisted solvothermal (in toluene environments) self-assembly and directed self-assembly of a polystyrene-blockpolydimethylsiloxane (PS-b-PDMS) BCP thin films on planar and topographically patterned  $\text{Si}_3\text{N}_4$  substrates. Hexagonally arranged, cylindrical structures were obtained and good pattern ordering was achieved. Factors affecting BCP self-assembly, notably anneal time and temperature, were studied and seen to have significant effects. Graphoepitaxy within the topographical structures provided long range, translational alignment of the patterns. The effect of surface topography feature size and spacing was investigated. The solvothermal microwave based technique used to provide periodic order in the BCP patterns showed significant promise and ordering was achieved in much shorter periods than more conventional thermal and solvent annealing methods. The implications of the work in terms of manufacturing technologies are discussed.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Trinity College Dublin, Materials Chemistry and Analysis Group, University College Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Tyndall National Institute at National University of Ireland, Cork

Contributors: Borah, D., Rasappa, S., Senthamarikannan, R., Holmes, J. D., Morris, M. A.

Number of pages: 18

Pages: 592-609

Publication date: 2015

Peer-reviewed: Yes

#### Publication information

Journal: Polymers

Volume: 7

Issue number: 4

ISSN (Print): 2073-4360

Ratings:

Scopus rating (2015): CiteScore 3.37 SJR 0.888 SNIP 1.325

Original language: English

ASJC Scopus subject areas: Polymers and Plastics, Chemistry(all)

Keywords: Block copolymer, Graphoepitaxy, Microwave anneal, Nanoscale patterns, Plasma etching, Polymer brush, Self-assembly, Silicon nitride substrate, Solvothermal process

DOIs:

10.3390/polym7040592

URLs:

<http://www.scopus.com/inward/record.url?scp=84930638018&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84930638018

Research output: Contribution to journal > Article > Scientific > peer-review

### **Switchavidin: Reversible biotin-avidin-biotin bridges with high affinity and specificity**

Switchavidin is a chicken avidin mutant displaying reversible binding to biotin, an improved binding affinity toward conjugated biotin, and low nonspecific binding due to reduced surface charge. These properties make switchavidin an optimal tool in biosensor applications for the reversible immobilization of biotinylated proteins on biotinylated sensor surfaces. Furthermore, switchavidin opens novel possibilities for patterning, purification, and labeling. (Graph Presented).

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Multi-scaled biodata analysis and modelling (MultiBAM), Fimlab Laboratories Ltd, Johannes Kepler University, Tampere University Hospital

Contributors: Taskinen, B., Zauner, D., Lehtonen, S. I., Koskinen, M., Thomson, C., Kähkönen, N., Kukkurainen, S., Määttä, J. A. E., Ihalainen, T. O., Kulomaa, M. S., Gruber, H. J., Hytönen, V. P.

Number of pages: 11

Pages: 2233-2243

Publication date: 17 Dec 2014

Peer-reviewed: Yes

#### **Publication information**

Journal: Bioconjugate Chemistry

Volume: 25

Issue number: 12

ISSN (Print): 1043-1802

Ratings:

Scopus rating (2014): CiteScore 4.85 SJR 1.711 SNIP 1.164

Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering, Organic Chemistry, Pharmaceutical Science, Biomedical Engineering, Pharmacology, Medicine(all)

DOIs:

10.1021/bc500462w

URLs:

<http://www.scopus.com/inward/record.url?scp=84918539954&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84918539954

Research output: Contribution to journal > Article > Scientific > peer-review

### **DNA lesion can facilitate base ionization: Vertical ionization energies of aqueous 8-oxoguanine and its nucleoside and nucleotide**

8-Oxoguanine is one of the key products of indirect radiation damage to DNA by reactive oxygen species. Here, we describe ionization of this damaged nucleobase and the corresponding nucleoside and nucleotide in aqueous phase, modeled by the nonequilibrium polarizable continuum model, establishing their lowest vertical ionization energies of 6.8-7.0 eV. We thus confirm that 8-oxoguanine has even lower ionization energy than the parental guanine, which is the canonical nucleobase with the lowest ionization energy. Therefore, it can act as a trap for the cationic hole formed by ionizing radiation and thus protect DNA from further radiation damage. We also model using time-dependent density functional theory and measure by liquid jet photoelectron spectroscopy the valence photoelectron spectrum of 8-oxoguanine in water. We show that the calculated higher lying ionization states match well the experiment which, however, is not sensitive enough to capture the electron signal corresponding to the lowest ionization process due to the low solubility of 8-oxoguanine in water.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Helmholtz Center Berlin

Contributors: Palivec, V., Pluharová, E., Unger, I., Winter, B., Jungwirth, P.

Number of pages: 5

Pages: 13833-13837

Publication date: 4 Dec 2014

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 118

Issue number: 48

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2014): CiteScore 3.28 SJR 1.449 SNIP 1.13

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films, Medicine(all)

DOIs:

10.1021/jp5111086

URLs:

<http://www.scopus.com/inward/record.url?scp=84915764488&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84915764488

Research output: Contribution to journal > Article > Scientific > peer-review

### Time-resolved fluorescence methods (IUPAC technical report)

This IUPAC Technical Report describes and compares the currently applied methods for measuring and analyzing time-resolved fluorescence traces using phase-modulation fluorometry as well as pulse fluorometry (direct emission decay measurements, single-photon timing, streak camera measurements, fluorescence upconversion, and optical Kerr gating). The paper starts with a brief description of the basic principles for time and frequency domain fluorescence spectroscopy. The fundamental equations are given, and recommendations for adequate use are emphasized. The up-to-date, commonly employed excitation sources and photodetectors are described in detail. The analysis of time-resolved fluorescence data is discussed. Attention is paid to possible artifacts, and remedies are presented on how to avoid them or to account for them. Finally, fluorescence lifetime standards for the nanosecond and picosecond timescales are collected.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Ecole Normale Supérieure de Cachan, Yamagata University, Hasselt University, Humboldt-Universität zu Berlin, CNRS, IRAMIS, LIDYL, Laboratoire Francis Perrin, KU Leuven

Contributors: Lemmetyinen, H., Tkachenko, N. V., Valeur, B., Hotta, J. I., Ameloot, M., Ernsting, N. P., Gustavsson, T., Boens, N.

Number of pages: 30

Pages: 1969-1998

Publication date: 1 Dec 2014

Peer-reviewed: Yes

### Publication information

Journal: Pure and Applied Chemistry

Volume: 86

Issue number: 12

ISSN (Print): 0033-4545

Ratings:

Scopus rating (2014): CiteScore 2.76 SJR 1.103 SNIP 1.339

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

Keywords: Fluorescence spectroscopy, IUPAC analytical chemistry division, IUPAC organic and biomolecular chemistry division, IUPAC physical and biophysical chemistry division, Phase-modulation fluorometry, Pulse fluorometry, Time-resolved fluorescence

DOIs:

10.1515/pac-2013-0912

URLs:

<http://www.scopus.com/inward/record.url?scp=84928726054&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84928726054

Research output: Contribution to journal > Article > Scientific > peer-review

### Processable aromatic polyesters based on bisphenol derived from cashew nut shell liquid: synthesis and characterization

A new bisphenol viz., 4-(4-hydroxyphenoxy)-3-pentadecylphenol (HPPDP) was synthesized starting from cashew nut shell liquid (CNSL). Aromatic (co)polyesters containing ether linkages in the main chain and pendent pentadecyl chains were

synthesized by the interfacial polycondensation of HPPDP with terephthalic acid chloride (TPC), isophthalic acid chloride (IPC) and a mixture of TPC and IPC (50:50 mol %) and by polycondensation of varying composition of HPPDP and bisphenol-A (BPA) with TPC. The resultant (co)polyesters exhibited inherent viscosities in the range 0.70–1.21 dL g<sup>-1</sup> and number-average molecular weights in the range 16,000–48,200 (GPC, polystyrene standard). Polyesters were soluble in common organic solvents such as chloroform and dichloromethane and could be cast into films from chloroform solution. Polyesters exhibited T<sub>10</sub> values in the range 430–455 °C and T<sub>g</sub> values were in the range 29–202 °C. Dynamic mechanical storage modulus and maximum on transition of tan δ curve decreased with increased content of HPPDP in copolyesters. Importantly, the large difference between T<sub>g</sub> and T<sub>10</sub> values offers the possibility to process these polyesters in the melt.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: CSIR-National Chemical Laboratory, Polymer Science and Engineering Division

Contributors: Tawade, B. V., Salunke, J. K., Sane, P. S., Wadgaonkar, P. P.

Publication date: 18 Nov 2014

Peer-reviewed: Yes

#### Publication information

Journal: JOURNAL OF POLYMER RESEARCH

Volume: 21

Issue number: 12

ISSN (Print): 1022-9760

Ratings:

Scopus rating (2014): CiteScore 1.84 SJR 0.666 SNIP 0.911

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Organic Chemistry

Keywords: Aromatic polyesters, Cashew nut shell liquid, Pentadecyl, Polycondensation, Processability, Thermal properties

DOIs:

10.1007/s10965-014-0617-y

URLs:

<http://www.scopus.com/inward/record.url?scp=84911385848&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

EXT="Salunke, Jagadish"

Source: Scopus

Source ID: 84911385848

Research output: Contribution to journal > Article > Scientific > peer-review

#### Electromagnetic interference shielding effectiveness of MWCNT filled poly(ether sulfone) and poly(ether imide) nanocomposites

Multiwalled carbon nanotube (MWCNT) filled poly(ether sulfone) (PES) and poly(ether imide) (PEI) composites were prepared with different MWCNT weight fractions (0.5–5wt%) by a solution mixing technique. Their electrical conductivities, electromagnetic interference (EMI), shielding effectiveness (SE), return loss (RL), and absorption loss (AL) were investigated. Morphologies of the fracture surfaces of nanocomposites studied by scanning electron and transmission electron microscopy showed relatively good MWCNT dispersion and distribution. The electrical conductivity of compression molded samples measured at room temperature indicated that the electrical percolation network was achieved already at 0.5% loading. The measurements of shielding effectiveness (SE) carried out in the frequency range of 8 to 12 GHz (X-band range) showed that SE increases with measurement frequency and with filler loading, whereby no significant differences could be observed between PES and PEI as matrices. The nanocomposites based on both matrices with 5 wt% loading of MWCNT exhibited shielding levels at 8 GHz between 42 and 45 dB in comparison with the pure polymers which showed value in the range of 1 to 2 dB. RL and AL showed significantly lower values for the composites as compared to unfilled polymers, but no systematic trends were observed on frequency.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Materials Science Centre, Indian Institute of Technology, Department of Applied Science, Symbiosis International University, Leibniz Institute of Polymer Research Dresden (IPF)

Contributors: Mohanty, A. K., Ghosh, A., Sawai, P., Pareek, K., Banerjee, S., Das, A., Pötschke, P., Heinrich, G., Voit, B.

Number of pages: 11

Pages: 2560-2570

Publication date: 1 Nov 2014

Peer-reviewed: Yes



### Publication information

Journal: Polymer Engineering and Science

Volume: 54

Issue number: 11

ISSN (Print): 0032-3888

Ratings:

Scopus rating (2014): CiteScore 1.4 SJR 0.556 SNIP 1.085

Original language: English

ASJC Scopus subject areas: Chemistry(all), Polymers and Plastics, Materials Chemistry

DOIs:

10.1002/pen.23804

URLs:

<http://www.scopus.com/inward/record.url?scp=84907865840&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84907865840

Research output: Contribution to journal > Article > Scientific > peer-review

### A supramolecular approach to photoresponsive thermo/solvoplastic block copolymer elastomers

With the aim of preparing supramolecular photoresponsive block copolymer elastomers, a series of ABA triblock copolymers with a poly(*n*-butyl acrylate) (PnBA) middle block and poly(dimethylaminoethyl methacrylate) (PDMAEMA or PDM) outer blocks were synthesized by atom transfer radical polymerization (ATRP), followed by PDM quaternization (giving PDMQ-PnBA-PDMQ) and then by ionic complexation with methyl orange (MO), an azo-containing and sulfonate-functionalized commercially available compound (giving PDMQ/MO-PnBA-PDMQ/MO). The PnBA block, which has a subambient glass transition, and the quaternized and complexed blocks, which have high glass transitions, form phase-separated soft and hard blocks, respectively. Simple elasticity tests of solvent-cast films show that the PDMQ/MO-PnBA-PDMQ/MO with hard block content between 18 and 29 wt % (as well as PDMQ-PnBA-PDMQ with 18 wt % hard block content) have significant elastomeric character. AFM and TEM (atomic force and transmission electron microscopies) of spin-coated films show a correlation between the elastomeric character and morphologies where the hard block forms a dispersed minority phase (spherical and/or short cylindrical domains). A continuous hard phase is observed for a hard block content of around 37 wt %; these materials show no significant elasticity. Reversible photoisomerization, with relatively high *cis* isomer content in the photostationary state, was also demonstrated.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Computer Systems, Frontier Photonics, Département de Chimie, Succ. Centre-Ville, Université de Sherbrooke

Contributors: Wang, X., Vapaavuori, J., Zhao, Y., Bazuin, C. G.

Number of pages: 10

Pages: 7099-7108

Publication date: 28 Oct 2014

Peer-reviewed: Yes

### Publication information

Journal: Macromolecules

Volume: 47

Issue number: 20

ISSN (Print): 0024-9297

Ratings:

Scopus rating (2014): CiteScore 5.83 SJR 2.524 SNIP 1.685

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry

DOIs:

10.1021/ma501278b

URLs:

<http://www.scopus.com/inward/record.url?scp=84908299127&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84908299127

Research output: Contribution to journal > Article > Scientific > peer-review

### Impact of selective catalytic reduction on exhaust particle formation over excess ammonia events

The introduction of selective catalytic reduction (SCR) aftertreatment to meet stringent diesel NO<sub>x</sub> emission standards around the world increases exhaust ammonia. Further to the direct air quality and health implications of ammonia, this may also lead to particle formation in the exhaust. In this study, an ammonia SCR system was examined with respect to

its impact on both solid and total exhaust particle number and size distribution, downstream of a diesel particulate filter (DPF). Fuel post-injection was conducted in some tests to investigate the effect of ammonia during active DPF regeneration. On average, the post-DPF solid >23 nm and total x control. Ammonia did not have a significant additional effect on the high particle concentrations measured during DPF regeneration. Based on species availability and formation conditions, sulfate, nitrate, and chloride salts with ammonium are possible sources of the new particles formed. Ammonia-induced particle formation corresponds to an environmental problem which is not adequately addressed by current regulations.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), Laboratory of Applied Thermodynamics, Aristotle University of Thessaloniki, European Commission-JRC, AVL List GmbH

Contributors: Amanatidis, S., Ntziachristos, L., Giechaskiel, B., Bergmann, A., Samaras, Z.

Number of pages: 8

Pages: 11527-11534

Publication date: 7 Oct 2014

Peer-reviewed: Yes

#### Publication information

Journal: Environmental Science and Technology

Volume: 48

Issue number: 19

ISSN (Print): 0013-936X

Ratings:

Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 1.992

Original language: English

ASJC Scopus subject areas: Chemistry(all), Environmental Chemistry

DOIs:

10.1021/es502895v

URLs:

<http://www.scopus.com/inward/record.url?scp=84907936083&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84907936083

Research output: Contribution to journal › Article › Scientific › peer-review

#### Global analysis of human nonreceptor tyrosine kinase specificity using high-density peptide microarrays

Protein kinases phosphorylate substrates in the context of specific phosphorylation site sequence motifs. The knowledge of the specific sequences that are recognized by kinases is useful for mapping sites of phosphorylation in protein substrates and facilitates the generation of model substrates to monitor kinase activity. Here, we have adapted a positional scanning peptide library method to a microarray format that is suitable for the rapid determination of phosphorylation site motifs for tyrosine kinases. Peptide mixtures were immobilized on glass slides through a layer of a tyrosine-free Y33F mutant avidin to facilitate the analysis of phosphorylation by radiolabel assay. A microarray analysis provided qualitatively similar results in comparison with the solution phase peptide library "macroarray" method. However, much smaller quantities of kinases were required to phosphorylate peptides on the microarrays, which thus enabled a proteome scale analysis of kinase specificity. We illustrated this capability by microarray profiling more than 80% of the human nonreceptor tyrosine kinases (NRTKs). Microarray results were used to generate a universal NRTK substrate set of 11 consensus peptides for in vitro kinase assays. Several substrates were highly specific for their cognate kinases, which should facilitate their incorporation into kinase-selective biosensors.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Yale School of Medicine, Bio21 Molecular Science and Biotechnology Institute, Fimlab Laboratories Ltd

Contributors: Deng, Y., Alicea-Velázquez, N. L., Bannwarth, L., Lehtonen, S. I., Boggon, T. J., Cheng, H. C., Hytönen, V. P., Turk, B. E.

Number of pages: 8

Pages: 4339-4346

Publication date: 3 Oct 2014

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Proteome Research

Volume: 13

Issue number: 10  
ISSN (Print): 1535-3893  
Ratings:

Scopus rating (2014): CiteScore 4.64 SJR 1.959 SNIP 1.158

Original language: English

ASJC Scopus subject areas: Chemistry(all), Biochemistry

Keywords: drug discovery, enzyme specificity, kinase inhibitors, nonreceptor tyrosine kinases, peptide libraries, peptide microarrays, protein kinases

DOIs:

10.1021/pr500503q

URLs:

<http://www.scopus.com/inward/record.url?scp=84907855794&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84907855794

Research output: Contribution to journal > Article > Scientific > peer-review

### **Rapid, Brushless Self-assembly of a PS-b-PDMS Block Copolymer for Nanolithography**

Block copolymers (BCP) are highly promising self-assembling precursors for scalable nanolithography. Very regular BCP nanopatterns can be used as on-chip etch masks. The first step in the processing of BCP thin films is usually the chemical modification of the substrate surface, typically by grafting of a brush layer that renders the surface energy neutral relative to the constituent blocks. We provide here a first study on rapid, low temperature self-assembly of PS- b-PDMS (polystyrene- block-polydimethylsiloxane) on silicon substrates without a brush layer. We show that it forms line and antidot patterns after short solvo-thermal annealing. Unlike previous reports on this system, low temperature and short annealing time provide self-assembly in homogeneous thin films covering large substrate areas. This on-chip mask was then used for pattern transfer to the underlying silicon substrate. SEM (scanning electron microscope) images reveal silicon nanowires relative to the PDMS patterns of the BCP mask.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Micro and Nanotechnology, Danmarks Tekniske Universitet, DTU Informatik, Center for Nanostructured Graphene, Trinity College Dublin

Contributors: Rasappa, S., Schulte, L., Borah, D., Morris, M. A., Ndoni, S.

Number of pages: 5

Pages: 1-5

Publication date: 1 Oct 2014

Peer-reviewed: Yes

#### **Publication information**

Journal: Colloids and Interface Science Communications

Volume: 2

ISSN (Print): 2215-0382

Original language: English

ASJC Scopus subject areas: Biotechnology, Colloid and Surface Chemistry, Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

Keywords: Aspect ratio, Brushless, Dry etching, Lines and antidots, Pattern transfer, PS-b-PDMS, Self-assembly, Silicon nanostructures, Soft mask template, Solvo-thermal annealing

DOIs:

10.1016/j.colcom.2014.07.001

URLs:

<http://www.scopus.com/inward/record.url?scp=84919650698&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84919650698

Research output: Contribution to journal > Article > Scientific > peer-review

### **Effect of head group size on the photoswitching applications of azobenzene Disperse Red 1 analogues**

We investigate the effect of the increased molecular bulk in the 'head' group for a class of newly synthesized azobenzene chromophores with a clickable ethynyl group para and a nitro group ortho to the azo bond on the distal benzene ring. This 'variable-head' functionalization provides a family of dyes with photophysical characteristics very similar to those of Disperse Red 1, one of the most commonly used azo dyes in materials science. Phenyl, naphthyl, and anthracyl derivatives were synthesized as small molecules, monomers, homopolymers, and copolymers in a rapid and facile manner using click chemistry, confirming the versatility of this parent chromophore. Photochemical and spectral studies indicate that this strategy is suitable to build a 'bulkiness series' of stimuli-responsive materials, as the various material derivatives retain the absorption and kinetic characteristics of the parent chromophore necessary for all optical patterning applications that DR1 dyes have been optimized for. In thin films, larger head group size was found to increase the stability of light-

induced birefringence in copolymers. The homopolymers formed stable surface-relief gratings upon interference irradiation, whose grating depths correlate with head group size, demonstrating that this new class of polymers can also undergo tailored macroscopic photoinduced motions, which could have applications in all optical nano-patterning.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Humboldt-Universität zu Berlin, McGill University, Aalto University

Contributors: Goulet-Hanssens, A., Corkery, T. C., Priimagi, A., Barrett, C. J.

Number of pages: 8

Pages: 7505-7512

Publication date: 28 Sep 2014

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Materials Chemistry C

Volume: 2

Issue number: 36

ISSN (Print): 2050-7534

Ratings:

Scopus rating (2014): CiteScore 4.64 SJR 1.517 SNIP 1.351

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Chemistry

DOIs:

10.1039/c4tc00996g

URLs:

<http://www.scopus.com/inward/record.url?scp=84906539664&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84906539664

Research output: Contribution to journal > Article > Scientific > peer-review

#### Pyrene based conjugated materials: Synthesis, characterization and electroluminescent properties

In this work, three novel pyrene cored small conjugated molecules, namely 1,3,6,8-tetrakis(6-(octyloxy)naphthalene-2-yl)pyrene (PY-1), 1,3,6,8-tetrakis((E)-2-(6-(n-octyloxy)naphthalene-2-yl)vinyl)pyrene (PY-2) and 1,3,6,8-tetrakis((6-(n-octyloxy)naphthalene-2-yl)ethynyl)pyrene (PY-3) have been synthesized by Suzuki, Heck and Sonogashira organometallic coupling reactions, respectively. The effects of single, double and triple bonds on their optical, electrochemical, and thermal properties are studied in detail. These are all materials fluorescent and they have been used in organic light-emitting diodes (OLEDs) and their electroluminescent properties have been studied. This journal is

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Polymer Science and Engineering Division, CSIR-National Chemical Laboratory, Queensland University of Technology QUT, University of Hong Kong

Contributors: Salunke, J. K., Sonar, P., Wong, F. L., Roy, V. A. L., Lee, C. S., Wadgaonkar, P. P.

Number of pages: 9

Pages: 23320-23328

Publication date: 26 Sep 2014

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 16

Issue number: 42

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.231

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1039/c4cp03693j

URLs:

<http://www.scopus.com/inward/record.url?scp=84908081510&partnerID=8YFLogxK> (Link to publication in Scopus)

### Bibliographical note

EXT="Salunke, Jagadish"

Source: Scopus

Source ID: 84908081510

Research output: Contribution to journal › Article › Scientific › peer-review

### Density functional theory study of transition metals doped B<sub>80</sub> fullerene

Density functional theory calculations have been carried out to investigate 3d, Pd and Pt transition metal (TM) atoms exohedrally and endohedrally doped B<sub>80</sub> fullerene. We find that the most preferred doping site of the TM atom gradually moves from the outer surface (TM = Sc), to the inner surface (TM = Ti and V) and the center (TM = Cr, Mn, Fe and Zn), then to the outer surface (TM = Co, Ni, Cu, Pd, and Pt) again with the TM atom varying from Sc to Pt. From the formation energy calculations, we find that doping TM atom can further improve the stability of B<sub>80</sub> fullerene. The magnetic moments of doped V, Cr, Mn, Fe, Co and Ni atoms are reduced from their free-atom values and other TM atoms are completely quenched. Charge transfer and hybridization between 4s and 3d states of TM and 2s and 2p states of B were observed. The energy gaps of TM@B<sub>80</sub> are usually smaller than that of the pure B<sub>80</sub>. Endohedrally doped B<sub>80</sub> fullerene with two Mn and two Fe atoms were also considered, respectively. It is found that the antiferromagnetic (AFM) state is more energetically favorable than the ferromagnetic (FM) state for Mn<sub>2</sub>- and Fe<sub>2</sub>@B<sub>80</sub>. The Mn and Fe atoms carry the residual magnetic moments of  $\sim 3 \mu_B$  and  $2 \mu_B$  in the AFM states.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), National Key Laboratory of Photoelectric Technology and Functional Materials in Shaanxi Province, Northwest University China, Nanjing University

Contributors: Wang, J., Ma, L., Liang, Y., Gao, M., Wang, G.

Publication date: 22 Sep 2014

Peer-reviewed: Yes

### Publication information

Journal: Journal of Theoretical and Computational Chemistry

Volume: 13

Issue number: 6

Article number: 1450050

ISSN (Print): 0219-6336

Ratings:

Scopus rating (2014): CiteScore 0.48 SJR 0.22 SNIP 0.243

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Computational Theory and Mathematics, Computer Science Applications

Keywords: B<sub>80</sub> fullerene, density functional theory, doped, Transition metal

DOIs:

10.1142/S0219633614500503

URLs:

<http://www.scopus.com/inward/record.url?scp=84929575039&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84929575039

Research output: Contribution to journal › Article › Scientific › peer-review

### Recent twists in photoactuation and photoalignment control

The design of functional and stimuli-responsive materials is among the key goals of modern materials science. The structure and properties of such materials can be controlled via various stimuli, among which light is often times the most attractive choice. Light is ubiquitous and a gentle energy source and its properties can be optimized for a specific target remotely, with high spatial and temporal resolution. Light-control over molecular alignment has in recent years attracted particular interest, for potential applications such as reconfigurable photonic elements and optical-to-mechanical energy conversion. Herein, we bring forward some recent examples and emerging trends in this exciting field of research, focusing on liquid crystals, liquid-crystalline polymers and photochromic organic crystals, which we believe serve to highlight the immense potential of light-responsive materials to a wide variety of current and future high-tech applications in photonics, energy harvesting and conversion. This journal is

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Politecnico di Milano, McGill University, Tokyo Institute of Technology

Contributors: Primagi, A., Barrett, C. J., Shishido, A.

Number of pages: 8  
Pages: 7155-7162  
Publication date: 21 Sep 2014  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Materials Chemistry C  
Volume: 2

Issue number: 35  
ISSN (Print): 2050-7534

Ratings:

Scopus rating (2014): CiteScore 4.64 SJR 1.517 SNIP 1.351

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Chemistry

DOIs:

10.1039/c4tc01236d

URLs:

<http://www.scopus.com/inward/record.url?scp=84906079173&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84906079173

Research output: Contribution to journal > Article > Scientific > peer-review

#### Optical spectroscopy of the bulk and interfacial hydrated electron from ab initio calculations

The optical spectrum of the hydrated (aqueous) electron,  $e_{aq}^-$ , is the primary observable by means of which this species is detected, monitored, and studied. In theoretical calculations, this spectrum has most often been simulated using one-electron models. Here, we present ab initio simulations of that spectrum in both bulk water and, for the first time, at the water/vapor interface, using density functional theory and its time-dependent variant. Our results indicate that this approach provides a reliable description, and quantitative agreement with the experimental spectrum for the bulk species is obtained using a "tuned" long-range corrected functional. The spectrum of the interfacial electron is found to be very similar to the bulk spectrum. (Figure Presented).

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Ohio State University

Contributors: Uhlig, F., Herbert, J. M., Coons, M. P., Jungwirth, P.

Number of pages: 9

Pages: 7507-7515

Publication date: 4 Sep 2014

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry A

Volume: 118

Issue number: 35

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2014): CiteScore 2.65 SJR 1.159 SNIP 1.061

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1021/jp5004243

URLs:

<http://www.scopus.com/inward/record.url?scp=84920104276&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84920104276

Research output: Contribution to journal > Article > Scientific > peer-review

#### The role of linked phospholipids in the rubber-filler interaction in carbon nanotube (CNT) filled natural rubber (NR) composites

The aim of the present work is to evidence the role of the linked phospholipids of natural rubber (NR) in the rubber-carbon nanotube (CNT) interactions in rubber composites. Three rubbers namely NR, deproteinized NR (DPNR) and a synthetic rubber isoprene (IR) were used as matrix for CNTs. The selective wetting of CNTs in miscible NR/IR and DPNR/IR blends

was investigated by means of the modified wetting concept based on Fourier transformed infrared (FTIR) analysis of the rubber-filler gel of blends. It revealed that the surface of CNTs is entirely wetted by NR or DPNR molecules, respectively, but not by IR. This result emphasizes that proteins do not influence the affinity between NR and CNTs, while the linked phospholipids interact with CNT surface through cation- $\pi$  linkage. This linkage acts as anchor point supporting NR molecules to wet CNT surface effectively. The modified wetting concept can be used for characterization of selective wetting of different fillers in blends consisting of miscible rubber components.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Polymer Service GmbH Merseburg, Martin-Luther-University Halle-Wittenberg, Styron Deutschland GmbH, Fraunhofer IWM, Malaysian Rubber Board, Elastomer Technology and Engineering, University of Twente, Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems, Tribhuvan University, Borealis Polyolefine GmbH

Contributors: Le, H. H., Abhijeet, S., Ilisch, S., Klehm, J., Henning, S., Beiner, M., Sarkawi, S. S., Dierkes, W., Das, A., Fischer, D., Stöckelhuber, K. W., Wiessner, S., Khatiwada, S. P., Adhikari, R., Pham, T., Heinrich, G., Radosch, H. J.

Number of pages: 10

Pages: 4738-4747

Publication date: 2 Sep 2014

Peer-reviewed: Yes

#### Publication information

Journal: Polymer

Volume: 55

Issue number: 18

ISSN (Print): 0032-3861

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Scopus rating (2014): CiteScore 3.85 SJR 1.326 SNIP 1.602

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Polymers and Plastics

Keywords: Carbon nanotubes, Filler wetting, Non-rubber components

DOIs:

10.1016/j.polymer.2014.07.043

URLs:

<http://www.scopus.com/inward/record.url?scp=84906787813&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84906787813

Research output: Contribution to journal > Article > Scientific > peer-review

#### Effect of silane integrated sol-gel derived in situ silica on the properties of nitrile rubber

Nitrile rubber/silica composites are prepared by a sol-gel process using tetraethoxysilane as precursor in the presence of  $\gamma$ - mercaptopropyltrimethoxysilane as a silane coupling agent. Here, we follow a novel processing route where the silica particles are generated inside the rubber matrix before compounding with vulcanizing ingredients. The effect of in situ generated silanized silica on the properties of the rubber composite has been evaluated by studying curing characteristics, morphology, mechanical and dynamic mechanical properties. Enhanced rubber-filler interaction of these composites is revealed from stress-strain studies and dynamic mechanical analysis. Excessive use of silane shows an adverse effect on mechanical properties of the composites. Due to finer dispersed state of the in situ silica and enhanced rubber-filler interaction, the mechanical properties and thermal stability of the composites are improved compared to corresponding ex situ processed composite.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Visvesvaraya National Institute of Technology, Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V.

Contributors: Kapgate, B. P., Das, C., Basu, D., Das, A., Heinrich, G., Reuter, U.

Publication date: 5 Aug 2014

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Applied Polymer Science

Volume: 131

Issue number: 15

Article number: 40531

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2014): CiteScore 1.76 SJR 0.664 SNIP 0.98

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)

Keywords: elastomers, mechanical properties, morphology, rheology, structure-property relations

DOIs:

10.1002/app.40531

URLs:

<http://www.scopus.com/inward/record.url?scp=84900485659&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84900485659

Research output: Contribution to journal › Article › Scientific › peer-review

### **Molecular engineering of avidin and hydrophobin for functional self-assembling interfaces**

Control over the functionality of interfaces through biomolecular engineering is a central tool for nanoscale technology as well as many current applications of biology. In this work we designed fusion proteins that combined the surface adhesion and interfacial activity of a hydrophobin-protein together with the high affinity biotin-binding capability of an avidin-protein. We found that an overall architecture that was based on a circularly permuted version of avidin, dual-chain avidin, and hydrophobin gave a highly functional combination. The protein was produced in the filamentous fungus *Trichoderma reesei* and was efficiently purified using an aqueous two-phase partitioning procedure. The surface adhesive properties were widely different compared to wild-type avidin. Functional characterization showed that the protein assembled on hydrophobic surfaces as a thin layer even at very low concentrations and efficiently bound a biotinylated compound. The work shows how the challenge of creating a fusion protein with proteins that form multimers can be solved by structural design and how protein self-assembly can be used to efficiently functionalize interfaces.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), VTT Technical Research Centre of Finland, Fimlab Laboratories Ltd, Tampere University Hospital, Aalto University

Contributors: Kurppa, K., Hytönen, V. P., Nakari-Setälä, T., Kulomaa, M. S., Linder, M. B.

Number of pages: 8

Pages: 102-109

Publication date: 1 Aug 2014

Peer-reviewed: Yes

### **Publication information**

Journal: Colloids and Surfaces B: Biointerfaces

Volume: 120

ISSN (Print): 0927-7765

Ratings:

Scopus rating (2014): CiteScore 4.53 SJR 1.21 SNIP 1.56

Original language: English

ASJC Scopus subject areas: Surfaces and Interfaces, Biotechnology, Colloid and Surface Chemistry, Physical and Theoretical Chemistry, Medicine(all)

Keywords: Avidin, Biofunctional surface, Hydrophobin, Nanomaterial, Protein engineering

DOIs:

10.1016/j.colsurfb.2014.05.010

URLs:

<http://www.scopus.com/inward/record.url?scp=84901790623&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84901790623

Research output: Contribution to journal › Article › Scientific › peer-review

### **Performance testing of iron based thermally sprayed HVOF coatings in a biomass-fired fluidised bed boiler**

Managing high temperature corrosion problems in biomass firing boilers has been challenging especially due to high amounts of chemically active compounds, in particular alkali chlorides. Thermally sprayed coatings with high chromium content can offer a solution for protecting low alloyed substrate materials in locations prone to high temperature corrosion. Two thermally sprayed (HVOF - high velocity oxy-fuel) iron based coatings (Fe-27Cr-11Ni-4Mo and Fe-19Cr-9W-7Nb-4Mo) were exposed to biomass boiler conditions for two years. The fluidised bed boiler for district heating used mainly wood-based fuels mixed with small amounts of peat. The coated tubes were located at the hot economiser of the boiler, where the estimated material temperature was about 200. °C maximum. After the exposure the coatings and the carbon steel St35.8 substrate material were analysed with SEM-EDX. It was detected that corrosion due to elements such as chlorine, potassium, zinc, lead and copper had caused severe material wastage in the biomass boiler with relatively low



heat exchanger surface temperatures. The low alloyed boiler tubes had suffered severely with a corrosion rate as high as 2. mm/year, whereas dense thermal spray coatings offered excellent protection during the exposure.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland

Contributors: Oksa, M., Varis, T., Ruusuvoori, K.

Number of pages: 10

Pages: 191-200

Publication date: 25 Jul 2014

Peer-reviewed: Yes

#### Publication information

Journal: Surface and Coatings Technology

Volume: 251

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2014): CiteScore 2.44 SJR 0.983 SNIP 1.652

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces

Keywords: Biomass, Chlorine corrosion, Corrosion protection, High temperature corrosion, HVOF, Thermal spray coating

DOIs:

10.1016/j.surfcoat.2014.04.025

URLs:

<http://www.scopus.com/inward/record.url?scp=84901601150&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84901601150

Research output: Contribution to journal > Article > Scientific > peer-review

#### Accurate description of calcium solvation in concentrated aqueous solutions

Calcium is one of the biologically most important ions; however, its accurate description by classical molecular dynamics simulations is complicated by strong electrostatic and polarization interactions with surroundings due to its divalent nature. Here, we explore the recently suggested approach for effectively accounting for polarization effects via ionic charge rescaling and develop a new and accurate parametrization of the calcium dication. Comparison to neutron scattering and viscosity measurements demonstrates that our model allows for an accurate description of concentrated aqueous calcium chloride solutions. The present model should find broad use in efficient and accurate modeling of calcium in aqueous environments, such as those encountered in biological and technological applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Kohagen, M., Mason, P. E., Jungwirth, P.

Number of pages: 8

Pages: 7902-7909

Publication date: 17 Jul 2014

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 118

Issue number: 28

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2014): CiteScore 3.28 SJR 1.449 SNIP 1.13

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films, Medicine(all)

DOIs:

10.1021/jp5005693

URLs:

<http://www.scopus.com/inward/record.url?scp=84904581115&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84904581115

Research output: Contribution to journal > Article > Scientific > peer-review

### **Surface behavior of hydrated guanidinium and ammonium ions: A comparative study by photoelectron spectroscopy and molecular dynamics**

Through the combination of surface sensitive photoelectron spectroscopy and molecular dynamics simulation, the relative surface propensities of guanidinium and ammonium ions in aqueous solution are characterized. The fact that the N 1s binding energies differ between these two species was exploited to monitor their relative surface concentration through their respective photoemission intensities. Aqueous solutions of ammonium and guanidinium chloride, and mixtures of these salts, have been studied in a wide concentration range, and it is found that the guanidinium ion has a greater propensity to reside at the aqueous surface than the ammonium ion. A large portion of the relative excess of guanidinium ions in the surface region of the mixed solutions can be explained by replacement of ammonium ions by guanidinium ions in the surface region in combination with a strong salting-out effect of guanidinium by ammonium ions at increased concentrations. This interpretation is supported by molecular dynamics simulations, which reproduce the experimental trends very well. The simulations suggest that the relatively higher surface propensity of guanidinium compared with ammonium ions is due to the ease of dehydration of the faces of the almost planar guanidinium ion, which allows it to approach the water-vapor interface oriented parallel to it.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Swedish University of Agricultural Sciences, Lund University, Uppsala University, FOM-Institute AMOLF, Science Park 102, Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Werner, J., Wernersson, E., Ekholm, V., Ottosson, N., Öhrwall, G., Heyda, J., Persson, I., Söderström, J., Jungwirth, P., Björneholm, O.

Number of pages: 9

Pages: 7119-7127

Publication date: 26 Jun 2014

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry Part B

Volume: 118

Issue number: 25

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2014): CiteScore 3.28 SJR 1.449 SNIP 1.13

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry

DOIs:

10.1021/jp500867w

URLs:

<http://www.scopus.com/inward/record.url?scp=84903466740&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84903466740

Research output: Contribution to journal > Article > Scientific > peer-review

### **Carbon nanotubes-filled thermoplastic polyurethane-urea and carboxylated acrylonitrile butadiene rubber blend nanocomposites**

This article reports the preparation and characterization of multiwalled carbon nanotubes (MWCNTs)-filled thermoplastic polyurethane-urea (TPUU) and carboxylated acrylonitrile butadiene rubber (XNBR) blend nanocomposites. The dispersion of the MWCNTs was carried out using a laboratory two roll mill. Three different loadings, that is, 1, 3, and 5 wt % of the MWCNTs were used. The electron microscopy image analysis proves that the MWCNTs are evenly dispersed along the shear flow direction. Through incorporation of the nanotubes in the blend, the tensile modulus was increased from  $9.90 \pm 0.5$  to  $45.30 \pm 0.3$  MPa, and the tensile strength at break was increased from  $25.4 \pm 2.5$  to  $33.0 \pm 1.5$  MPa. The wide angle X-ray scattering result showed that the TPUU:XNBR blends were arranged in layered structures. These structures are formed through chemical reactions of -NH group from urethane and urea with the carboxylic group on XNBR. Furthermore, even at a very low loading, the high degree of nanotubes dispersion results in a significant increase in the electrical percolation threshold. © 2014 Wiley Periodicals, Inc. J. Appl. Polym. Sci. 2014, 131, 40341.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), COMSATS Institute of Information Technology Lahore, Leibniz-Institut für Polymerforschung Dresden E.V., Institut für Polymerwerkstoffe, Vodafone Department of Mobile Communications Systems

Contributors: Mahmood, N., Khan, A. U., Stöckelhuber, K. W., Das, A., Jehnichen, D., Heinrich, G.

Publication date: 5 Jun 2014

Peer-reviewed: Yes

### Publication information

Journal: Journal of Applied Polymer Science

Volume: 131

Issue number: 11

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2014): CiteScore 1.76 SJR 0.664 SNIP 0.98

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)

Keywords: blends, elastomers, graphene and fullerenes, nanotubes, polyurethanes, rubber

DOIs:

10.1002/app.40341

URLs:

<http://www.scopus.com/inward/record.url?scp=84897664169&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84897664169

Research output: Contribution to journal > Article > Scientific > peer-review

### Hydration of the chloride ion in concentrated aqueous solutions using neutron scattering and molecular dynamics

Neutron scattering experiments were performed on 6 m LiCl solutions in order to obtain the solvation structure around the chloride ion. Molecular dynamics simulations on systems mirroring the concentrated electrolyte conditions of the experiment were carried out with a variety of chloride force-fields. In each case the simulations were run with both full ionic charges and employing the electronic continuum correction (implemented through charge scaling) to account effectively for electronic polarisation. The experimental data were then used to assess the successes and shortcomings of the investigated force-fields. We found that due to the very good signal-to-noise ratio in the experimental data, they provide a very narrow window for the position of the first hydration shell of the chloride ion. This allowed us to establish the importance of effectively accounting for electronic polarisation, as well as adjusting the ionic size, for obtaining a force-field which compares quantitatively to the experimental data. The present results emphasise the utility of performing neutron diffraction with isotopic substitution as a powerful tool in gaining insight and examining the validity of force-fields in concentrated electrolyte solutions.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Institut Laue-Langevin

Contributors: Pluhařová, E., Fischer, H. E., Mason, P. E., Jungwirth, P.

Number of pages: 11

Pages: 1230-1240

Publication date: 19 May 2014

Peer-reviewed: Yes

### Publication information

Journal: Molecular Physics

Volume: 112

Issue number: 9-10

ISSN (Print): 0026-8976

Ratings:

Scopus rating (2014): CiteScore 1.48 SJR 0.693 SNIP 0.642

Original language: English

ASJC Scopus subject areas: Biophysics, Molecular Biology, Condensed Matter Physics, Physical and Theoretical Chemistry

Keywords: Chloride, Lithium, Molecular dynamics, Neutron scattering, Solution

DOIs:

10.1080/00268976.2013.875231

URLs:

<http://www.scopus.com/inward/record.url?scp=84901191483&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84901191483

Research output: Contribution to journal › Article › Scientific › peer-review

### **Bioprocessing of enhanced cellulase production from a mutant of *Trichoderma asperellum* RCK2011 and its application in hydrolysis of cellulose**

A mutant strain of *Trichoderma asperellum* RCK2011 was developed through UV-irradiation for enhanced cellulase production and lower catabolite repression. The production of FPase, CMCase and  $\beta$ -glucosidase was optimized under solid state fermentation; up to 20 mM of glucose did not inhibit cellulase production. The mutant strain *T. asperellum* SR1-7 produced FPase (2.2 IU/gds), CMCase (13.2 IU/gds), and  $\beta$ -glucosidase (9.2 IU/gds) under optimized conditions, which is, 1.4, 1.3, 1.5-fold higher than the wild type. The wild as well as mutant strain produced the cellulases at pH range, 4.0-10.0. Saccharification of pretreated corn cob, wheat straw, and sugarcane bagasse by cellulase from mutant strain SR1-7 resulted in release of reducing sugar at the rate of 530.0 mg/g, 290.0 mg/g, and 335.0 mg/g of substrate, respectively; this is 1.6-fold higher than the wild type strain. © 2014 Published by Elsevier Ltd.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Tampere University of Technology, Urban circular bioeconomy (UrCirBio), Department of Microbiology, University of Delhi South Campus, Lignocellulose Biotechnology Laboratory

Contributors: Raghuwanshi, S., Deswal, D., Karp, M., Kuhad, R. C.

Number of pages: 7

Pages: 183-189

Publication date: 15 May 2014

Peer-reviewed: Yes

#### **Publication information**

Journal: Fuel

Volume: 124

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2014): CiteScore 4.14 SJR 1.634 SNIP 2.281

Original language: English

ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

Keywords: Alkaline cellulase, Catabolite repression, Saccharification, Solid state fermentation

DOIs:

10.1016/j.fuel.2014.01.107

URLs:

<http://www.scopus.com/inward/record.url?scp=84894571819&partnerID=8YFLogxK> (Link to publication in Scopus)

#### **Bibliographical note**

Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-03-15

Source: researchoutputwizard

Source ID: 1327

Research output: Contribution to journal › Article › Scientific › peer-review

### **Light-fuelled transport of large dendrimers and proteins**

This work presents a facile water-based supramolecular approach for light-induced surface patterning. The method is based upon azobenzene- functionalized high-molecular weight triazine dendrimers up to generation 9, demonstrating that even very large globular supramolecular complexes can be made to move in response to light. We also demonstrate light-fuelled macroscopic movements in native biomolecules, showing that complexes of apoferritin protein and azobenzene can effectively form light-induced surface patterns. Fundamentally, the results establish that thin films comprising both flexible and rigid globular particles of large diameter can be moved with light, whereas the presented material concepts offer new possibilities for the yet marginally explored biological applications of azobenzene surface patterning.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Aalto University, Texas Christian University

Contributors: Koskela, J. E., Liljeström, V., Lim, J., Simanek, E. E., Ras, R. H. A., Priimagi, A., Kostianen, M. A.  
Number of pages: 4  
Pages: 6850-6853  
Publication date: 14 May 2014  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of the American Chemical Society

Volume: 136

Issue number: 19

ISSN (Print): 0002-7863

Ratings:

Scopus rating (2014): CiteScore 11.92 SJR 6.294 SNIP 2.573

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis, Biochemistry, Colloid and Surface Chemistry, Medicine(all)

DOIs:

10.1021/ja502623m

URLs:

<http://www.scopus.com/inward/record.url?scp=84900818359&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84900818359

Research output: Contribution to journal > Article > Scientific > peer-review

#### Microphase mechanism of "superquenching" of luminescent probes in aqueous solutions of DNA and some other polyelectrolytes

A new approach in terms of microphase model of aqueous solutions of polyelectrolytes is proposed for explanation of a very strong quenching of luminescent probes ("superquenching") in these solutions. This phenomenon is used in literature for creation of extremely sensitive chemical and biosensors and was attributed predominantly to efficient energy or electron transfer. Microphase approach considers this phenomenon in terms of local concentrations of both the luminescent compound and of the quencher in microphase, formed by DNA and other polyelectrolytes, which can be several (4-10) orders of magnitude greater than their apparent concentrations in solution. Large local concentrations of the light absorbing centers in the microphase also provide conditions for aggregation of these centers and efficient energy transfer, which provides a significant increase in quenching constants ( $\sim 10^2$ - $10^3$ ). Microphase approach provides good quantitative description of all the features of the superquenching, new possibilities for analysis and control of kinetics of DNA reactions, and for improvement of the sensitivity of luminescent sensors. It reveals nonspecific localization of the luminescent centers and of Au<sub>n</sub> nanoparticles in different positions of DNA molecules that hinders from the simultaneous use of optical methods and electron or tunneling microscopy for the combined study of the structure of DNA.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Moscow State University, Emanuel' Institute of Biochemical Physics, Russian Academy of Sciences

Contributors: Kuzmin, M. G., Soboleva, I. V., Durandin, N. A., Lisitsyna, E. S., Kuzmin, V. A.

Number of pages: 8

Pages: 4245-4252

Publication date: 17 Apr 2014

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 118

Issue number: 15

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2014): CiteScore 3.28 SJR 1.449 SNIP 1.13

Original language: English

ASJC Scopus subject areas: Surfaces, Coatings and Films, Physical and Theoretical Chemistry, Materials Chemistry

DOIs:

10.1021/jp500713q

URLs:

<http://www.scopus.com/inward/record.url?scp=84899003075&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84899003075

### Protein conformation as a regulator of cell-matrix adhesion

The dynamic regulation of cell-matrix adhesion is essential for tissue homeostasis and architecture, and thus numerous pathologies are linked to altered cell-extracellular matrix (ECM) interaction and ECM scaffold. The molecular machinery involved in cell-matrix adhesion is complex and involves both sensory and matrix-remodelling functions. In this review, we focus on how protein conformation controls the organization and dynamics of cell-matrix adhesion. The conformational changes in various adhesion machinery components are described, including examples from ECM as well as cytoplasmic proteins. The discussed mechanisms involved in the regulation of protein conformation include mechanical stress, post-translational modifications and allosteric ligand-binding. We emphasize the potential role of intrinsically disordered protein regions in these processes and discuss the role of protein networks and co-operative protein interactions in the formation and consolidation of cell-matrix adhesion and extracellular scaffolds.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Fimlab Laboratories Ltd, University of Geneva

Contributors: Hytönen, V. P., Wehrle-Haller, B.

Number of pages: 16

Pages: 6342-6357

Publication date: 14 Apr 2014

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 16

Issue number: 14

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.231

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

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10.1039/c3cp54884h

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<http://www.scopus.com/inward/record.url?scp=84896364401&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84896364401

Research output: Contribution to journal › Article › Scientific › peer-review

### Deciphering the infrared spectrum of the protonated water pentamer and the hybrid Eigen-Zundel cation

Traditionally, infrared band assignment for the protonated water clusters, such as  $\text{H}^+(\text{H}_2\text{O})_5$ , is based on their lowest energy isomer. Recent experiments extend the observation spectral window to lower frequencies, for which such assignment appears to be inadequate. Because this hydrogen-bonded system is highly anharmonic, harmonic spectral calculations are insufficient for reliable interpretation. Consequently, we have calculated the IR spectrum of several isomers of the protonated water pentamer using an inherently anharmonic methodology, utilizing dipole and velocity autocorrelation functions computed from ab initio molecular dynamic trajectories. While the spectrum of  $\text{H}^+(\text{H}_2\text{O})_5$  is universally assumed to represent the branched Eigen isomer, we find a better agreement for a mixture of a ring and linear isomers. The first has an Eigen core and contributes at high frequencies, whereas the latter accounts for all prominent low-frequency bands. Interestingly, its core is neither a classical Eigen nor a Zundel cation, but rather has hybrid geometry. Such an isomer may play a role in proton conductance along short proton wires.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Hebrew University of Jerusalem

Contributors: Kulig, W., Agmon, N.

Number of pages: 9

Pages: 4933-4941

Publication date: 14 Mar 2014

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 16  
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Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.231

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1039/c3cp54029d

URLs:

<http://www.scopus.com/inward/record.url?scp=84894129482&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84894129482

Research output: Contribution to journal > Article > Scientific > peer-review

### **Fabrication of ssDNA/oligo(ethylene glycol) monolayers by promoted exchange reaction with thiol and disulfide substituents**

Biorepulsive oligo(ethylene glycol)-substituted alkanethiolate (OEG-AT) monolayers on gold can serve as primary templates for promoted (by electron irradiation) exchange reaction with thiolated ssDNA species, resulting in the formation of mixed OEG-AT/ssDNA monolayers of desired composition. Here we test the ability of alternative, disulfide precursors to serve as substituents in such a reaction. Two representative molecules, based on adenine-based homo-oligonucleotide (25-mer), were used, viz., asymmetric disulfide with a short second chain (A25SSOH) and symmetric disulfide (A25SSA25). The results were compared to the reference system of thiolated ssDNA (A25SH). Both disulfide precursors were found to be suitable for the reaction, further extending the types of commercially available compounds which can be used for this approach. A25SSOH exhibited quite high efficiency, similar to A25SH, while the efficiency of A25SSA25 was noticeably lower, especially at low irradiation doses (2). Also, the single component, A25SSA25-based ssDNA monolayer, was of lower quality as compared to the films prepared from the A25SH and A25SSOH precursors. The above observations were explained by the bulky character and conformational flexibility of A25SSA25, which hinder the proper assembly and efficient exchange reaction.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Universitat Heidelberg

Contributors: Khan, M. N., Zharnikov, M.

Number of pages: 9

Pages: 3093-3101

Publication date: 13 Feb 2014

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry C

Volume: 118

Issue number: 6

ISSN (Print): 1932-7447

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ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

10.1021/jp411353f

URLs:

<http://www.scopus.com/inward/record.url?scp=84894037828&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84894037828

Research output: Contribution to journal > Article > Scientific > peer-review

### **Azopolymer-based micro- and nanopatterning for photonic applications**

Azopolymers comprise a unique materials platform, in which the photoisomerization reaction of azobenzene molecules can induce substantial material motions at molecular, mesoscopic, and even macroscopic length scales. In particular, amorphous azopolymer films can form stable surface relief patterns upon exposure to interfering light. This allows obtaining large-area periodic micro- and nanostructures in a remarkably simple way. Herein, recent progress in the development of azopolymer-based surface-patterning techniques for photonic applications is reviewed. Starting with a thin

azopolymer layer, one can create a variety of photonic elements, such as diffraction gratings, microlens arrays, plasmonic sensors, antireflection coatings, and nanostructured light-polarization converters, either by using the azopolymer surface patterns themselves as optical elements or by utilizing them to microstructure or nanostructure other materials. Both of these domains are covered, with the aim of triggering further research in this fascinating field of science and technology that is far from being harnessed. © 2013 Wiley Periodicals, Inc. *J. Polym. Sci., Part B: Polym. Phys.* 2014, 52, 163-182

The aim of this review is to cover the existing research and trigger future research on the development of azopolymer-based micro- and nanopatterning techniques for applications in photonics. These techniques exploit a remarkably simple inscription of large-area surface relief gratings on azopolymer films. Starting with such an azopolymer pattern, one can create a variety of photonic elements, including diffraction gratings, distributed Bragg reflectors, microlens arrays, plasmonic sensors, antireflection coatings, and nanostructured converters of light polarization.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Frontier Photonics, Aalto University  
Contributors: Priimagi, A., Shevchenko, A.  
Number of pages: 20  
Pages: 163-182  
Publication date: 1 Feb 2014  
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#### Publication information

Journal: *Journal of Polymer Science. Part B, Polymer Physics*  
Volume: 52  
Issue number: 3  
ISSN (Print): 0887-6266  
Ratings:  
Scopus rating (2014): CiteScore 3.91 SJR 1.503 SNIP 1.412  
Original language: English  
ASJC Scopus subject areas: Condensed Matter Physics, Physical and Theoretical Chemistry, Polymers and Plastics, Materials Chemistry  
Keywords: azo polymers, isomer/isomerization, lithography, nanotechnology, periodic arrays, photonics; surface-relief grating  
DOIs:  
10.1002/polb.23390  
URLs:  
<http://www.scopus.com/inward/record.url?scp=84890653328&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 84890653328  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Both zundel and eigen isomers contribute to the IR spectrum of the gas-phase H<sub>9</sub>O<sup>+</sup> cluster

The "Eigen cation", H<sub>3</sub>O<sup>+</sup>(H<sub>2</sub>O)<sub>3</sub>, is the most prevalent protonated water structure in the liquid phase and the most stable gas-phase isomer of the H<sup>+</sup>(H<sub>2</sub>O)<sub>4</sub> cluster. Nevertheless, its 50 K argon predissociation vibrational spectrum contains unexplainable low frequency peak(s). We have simulated the IR spectra of 10 gas-phase H<sup>+</sup>(H<sub>2</sub>O)<sub>4</sub> isomers, that include zero to three argon ligands, using dipole autocorrelation functions from ab initio molecular dynamics with the CP2K software. We have also tested the effect of elevated temperature and dispersion correction. The Eigen isomers describe well the high frequency portion of the spectrum but do not agree with experiment below 2000 cm<sup>-1</sup>. Most notably, they completely lack the "proton transfer bands" observed at 1050 and 1750 cm<sup>-1</sup>, which characterize Zundel-type (H<sub>5</sub>O<sub>2</sub><sup>+</sup>) isomers. In contrast, linear isomers with a Zundel core, although not the lowest in energy, show very good agreement with experiment, particularly at low frequencies. Peak assignments made with partial velocity autocorrelation functions verify that the 1750 cm<sup>-1</sup> band does not originate with the Eigen isomer but is rather due to coupled proton transfer/water bend in the Zundel isomer.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Computational Science X (CompX), Tallinn Technical University, Institute of Chemistry, Hebrew University of Jerusalem  
Contributors: Kulig, W., Agmon, N.  
Number of pages: 9  
Pages: 278-286  
Publication date: 9 Jan 2014  
Peer-reviewed: Yes



### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 118

Issue number: 1

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2014): CiteScore 3.28 SJR 1.449 SNIP 1.13

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/jp410446d

URLs:

<http://www.scopus.com/inward/record.url?scp=84892594412&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84892594412

Research output: Contribution to journal > Article > Scientific > peer-review

### Natural thermal adaptation increases heat shock protein levels and decreases oxidative stress

Heat shock proteins (HSPs), originally identified as heat-inducible gene products, are a family of highly conserved proteins that respond to a wide variety of stress including oxidative stress. Although both acute and chronic oxidative stress have been well demonstrated to induce HSP responses, little evidence is available whether increased HSP levels provide enhanced protection against oxidative stress under elevated yet sublethal temperatures. We studied relationships between oxidative stress and HSPs in a physiological model by using *Garra rufa* (doctor fish), a fish species naturally acclimatized to different thermal conditions. We compared fish naturally living in a hot spring with relatively high water temperature ( $34.4 \pm 0.6$  °C) to those living in normal river water temperature ( $25.4 \pm 4.7$  °C), and found that levels of all the studied HSPs (HSP70, HSP60, HSP90, HSC70 and GRP75) were higher in fish living in elevated water temperature compared with normal river water temperature. In contrast, indicators of oxidative stress, including protein carbonyls and lipid hydroperoxides, were decreased in fish living in the elevated temperature, indicating that HSP levels are inversely associated with oxidative stress. The present results provide evidence that physiologically increased HSP levels provide protection against oxidative stress and enhance cytoprotection.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), University of Tampere, Medical School, University of Hacettepe, University of Düzce, Ita-Suomen yliopisto, University Central Hospital Kuopio

Contributors: Oksala, N. K. J., Ekmeççi, F. G., Özsoy, E., Kirankaya, Ş., Kokkola, T., Emecen, G., Lappalainen, J., Kaarniranta, K., Atalay, M.

Number of pages: 4

Pages: 25-28

Publication date: 1 Jan 2014

Peer-reviewed: Yes

### Publication information

Journal: REDOX BIOLOGY

Volume: 3

ISSN (Print): 2213-2317

Ratings:

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Original language: English

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Keywords: *Garra rufa*, Oxidation, Regulation, Stress, Thermal

DOIs:

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URLs:

<http://www.scopus.com/inward/record.url?scp=84912102339&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84912102339

Research output: Contribution to journal > Article > Scientific > peer-review

### A microscopic view of the mechanisms of active transport across the cellular membrane

Membrane transporters are molecular machines that couple active transport of their specific substrates to various sources of cellular energy through a set of highly coordinated protein conformational changes. The alternating-access mechanism of transport in these proteins, which ensures that the substrate is only accessible from one side of the membrane at any

given time, relies on complex and global protein conformational changes that are also closely coupled to molecular events such as substrate binding and translocation. In this review, we describe the application of advanced molecular modeling and simulation technologies to a number of membrane transport proteins studied in our laboratory. The goal is to demonstrate the power of the methods in describing functionally relevant molecular events ranging from more localized events such as substrate binding and gating motions to large, global protein conformational changes governing the transition of the protein between major functional states.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Department of Biochemistry, Univ Illinois, University of Illinois System, University of Illinois Urbana-Champaign, Frederick Seitz Mat Res Lab, Dept Mat Sci & Engr

Contributors: Enkavi, G., Li, J., Wen, P., Thangapandian, S., Moradi, M., Jiang, T., Han, W., Tajkhorshid, E.

Number of pages: 49

Pages: 77-125

Publication date: 2014

Peer-reviewed: Yes

#### Publication information

Journal: Annual Reports in Computational Chemistry

Volume: 10

ISSN (Print): 1574-1400

Ratings:

Scopus rating (2014): CiteScore 1.25 SJR 0.74 SNIP 0.985

Original language: English

ASJC Scopus subject areas: Chemistry(all), Computational Mathematics

Keywords: Conformational changes, Membrane transporters, Molecular dynamics, Nonequilibrium simulation, Primary transporters, Secondary transporters, Substrate binding

DOIs:

10.1016/B978-0-444-63378-1.00004-5

URLs:

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Source: Scopus

Source ID: 84919386963

Research output: Contribution to journal › Article › Scientific › peer-review

#### Direct observation of the collapse of the delocalized excess electron in water

It is generally assumed that the hydrated electron occupies a quasi-spherical cavity surrounded by only a few water molecules in its equilibrated state. However, in the very moment of its generation, before water has had time to respond to the extra charge, it is expected to be significantly larger in size. According to a particle-in-a-box picture, the frequency of its absorption spectrum is a sensitive measure of the initial size of the electronic wavefunction. Here, using transient terahertz spectroscopy, we show that the excess electron initially absorbs in the far-infrared at a frequency for which accompanying ab initio molecular dynamics simulations estimate an initial delocalization length of  $\approx 40$  Å. The electron subsequently shrinks due to solvation and thereby leaves the terahertz observation window very quickly, within  $\approx 200$  fs.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Zurich, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Savolainen, J., Uhlig, F., Ahmed, S., Hamm, P., Jungwirth, P.

Number of pages: 5

Pages: 697-701

Publication date: 2014

Peer-reviewed: Yes

#### Publication information

Journal: Nature Chemistry

Volume: 6

Issue number: 8

ISSN (Print): 1755-4330

Ratings:

Scopus rating (2014): CiteScore 13.67 SJR 10.562 SNIP 4.441

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

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10.1038/nchem.1995

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<http://www.scopus.com/inward/record.url?scp=84904805160&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84904805160

Research output: Contribution to journal > Article > Scientific > peer-review

### **A full-potential linearized augmented plane wave study of the interaction of CO<sub>2</sub> with $\alpha$ -Pu (020) surface nanolayers**

Adsorption of CO<sub>2</sub> on  $\alpha$ -Pu (020) surface nanolayers is investigated using GGA-DFT and the suite of software DMOL<sup>3</sup> and WIEN2k. Completely dissociated configurations (C+O+O) exhibit the strongest binding with the surface (7.94 eV), followed by partially dissociated (CO+O) and molecular CO<sub>2</sub> configurations (5.18 and 1.90 eV, respectively). For initial vertically upright orientations, final configuration of the CO<sub>2</sub> molecule does not change after optimization. For initial flat lying orientations, the final states correspond to bent geometry with a bond angle of ~130°. For CO+O coadsorptions, the stable configurations correspond to CO dipole moment orientations of 105°-167° with respect to the normal surface.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Texas at Arlington

Contributors: Wang, J., Ray, A. K.

Number of pages: 8

Pages: 1710-1717

Publication date: 2014

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Computational and Theoretical Nanoscience

Volume: 11

Issue number: 7

ISSN (Print): 1546-1955

Ratings:

Scopus rating (2014): CiteScore 1.17 SJR 0.326 SNIP 0.778

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Electrical and Electronic Engineering, Materials Science(all), Computational Mathematics, Chemistry(all)

Keywords: Adsorption, Alpha-Plutonium, Carbon Dioxide, Density Functional Theory, Nanolayers

DOIs:

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<http://www.scopus.com/inward/record.url?scp=84898458971&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84898458971

Research output: Contribution to journal > Article > Scientific > peer-review

### **Molekuly a ionty v pohybu: Počítačové simulace biochemických a biofyzikálních procesů**

The review presents research activities aimed at better understanding of the effects of salt ions on biological processes (protein salting out/in, protein denaturation, enzymatic activity, processes in biological membranes, and radiation damage to DNA) using molecular simulations in close contact with the experiment.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Jungwirth, P.

Number of pages: 7

Pages: 278-284

Publication date: 2014

Peer-reviewed: Yes

#### **Publication information**

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Volume: 108

Issue number: 4  
ISSN (Print): 0009-2770  
Ratings:

Scopus rating (2014): CiteScore 0.33 SJR 0.198 SNIP 0.504

Original language: Undefined/Unknown

ASJC Scopus subject areas: Chemistry(all)

URLs:

<http://www.scopus.com/inward/record.url?scp=84899732053&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84899732053

Research output: Contribution to journal > Article > Scientific > peer-review

### **Magnetic origin of the chemical balance in alloyed Fe-Cr stainless steels: First-principles and Ising model study**

Iron-chromium is the base material for most of the stainless steel grades. Recently, new insights into the origins of fundamental physical and chemical characteristics of Fe-Cr based alloys have been achieved. Some of the new results are quite unexpected and call for further investigations. The present study focuses on the magnetic contribution in the atomic driving forces related to the chemical composition in Fe-Cr when alloyed with Al, Ti, V, Mn, Co, Ni, and Mo. Using the ab initio exact muffin-tin orbitals method combined with an Ising-type spin model, we demonstrate that the magnetic moment of the solute atoms with the induced changes in the magnetic moments of the host atoms form the main factor in determining the mixing energy and chemical potentials of low-Cr Fe-Cr based alloys. The results obtained in the present work are related to the designing and tuning of the microstructure and corrosion protection of low-Cr steels.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Turun Yliopisto/Turun Biomateriaalikeskus, Department of Physics and Astronomy, University of Turku, Abo Akad Univ, Abo Akademi University, Dept Phys, Uppsala University, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences

Contributors: Airiskallio, E., Nurmi, E., Väyrynen, I. J., Kokko, K., Ropo, M., Punkkinen, M. P. J., Johansson, B., Vitos, L.

Number of pages: 6

Pages: 135-140

Publication date: 2014

Peer-reviewed: Yes

#### **Publication information**

Journal: Computational Materials Science

Volume: 92

ISSN (Print): 0927-0256

Ratings:

Scopus rating (2014): CiteScore 2.47 SJR 1.098 SNIP 1.612

Original language: English

ASJC Scopus subject areas: Computer Science(all), Chemistry(all), Materials Science(all), Mechanics of Materials, Physics and Astronomy(all), Computational Mathematics

Keywords: Al, Chemical potential, Co, Corrosion protection, Cr, Fe, First principles calculation, Ising model, Magnetic moment, Mixing energy, Mn, Mo, Ni, Stainless steel, Ti, V

DOIs:

[10.1016/j.commatsci.2014.05.036](https://doi.org/10.1016/j.commatsci.2014.05.036)

URLs:

<http://www.scopus.com/inward/record.url?scp=84902660256&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84902660256

Research output: Contribution to journal > Article > Scientific > peer-review

### **Effect of non-rubber components of NR on the carbon nanotube (CNT) localization in SBR/NR blends**

Carbon nanotubes (CNTs) are mixed into SBR/NR and SBR/IR blends using a wet mixing process. The phase specific localization of CNTs in rubber blends is predicted theoretically using surface energy data of blend components and determined experimentally by means of the wetting concept. Almost all CNTs are found to be localized in the SBR matrix of SBR/IR blends due to the better affinity of CNTs to SBR than to IR. In contrast, a high CNT loading localized in the NR phase of SBR/NR blends results from the presence of phospholipids in NR. Electrical and mechanical properties of the rubber blends depend strongly on CNT localization. A lower CNT loading in SBR matrix of SBR/NR blends imparts a better wet grip and lower rolling resistance to tire tread compounds.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Martin-Luther-University Halle-Wittenberg, Styron Deutschland GmbH, Fraunhofer IWM, Leibniz-Institut für Polymerforschung Dresden E.V., Dau Mot University, Tribhuvan University, Vodafone Department of Mobile Communications Systems

Contributors: Le, H. H., Parsekar, M., Ilisch, S., Henning, S., Das, A., Stöckelhuber, K. W., Beiner, M., Ho, C. A., Adhikari, R., Wießner, S., Heinrich, G., Radusch, H. J.

Number of pages: 14

Pages: 569-582

Publication date: 2014

Peer-reviewed: Yes

### Publication information

Journal: Macromolecular Materials and Engineering

Volume: 299

Issue number: 5

ISSN (Print): 1438-7492

Ratings:

Scopus rating (2014): CiteScore 2.81 SJR 1.009 SNIP 1.294

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Chemical Engineering(all)

Keywords: carbon nanotubes, filler localization, nanocomposites, rubber blends

DOIs:

10.1002/mame.201300254

URLs:

<http://www.scopus.com/inward/record.url?scp=84899990693&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84899990693

Research output: Contribution to journal > Article > Scientific > peer-review

## Novel derivatives of bacteriochlorophyll a: Complex formation with albumin and the mechanism of tumor cell photodamage

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Emanuel' Institute of Biochemical Physics, Russian Academy of Sciences, M.V.

Lomonosov Moscow State University of Fine Chemical Technologies, Georgian Technical University, St. Petersburg State Polytechnical University, N.N. Blokhin Russian Cancer Research Center, Russian Academy of Medical Sciences

Contributors: Akimova, A. V., Grin, M. A., Golovina, G. V., Kokrashvili, T. A., Vinogradov, A. M., Mironov, A. F., Rychkov, G. N., Shtil, A. A., Kuzmin, V. A., Durandin, N. A.

Number of pages: 4

Pages: 17-20

Publication date: 2014

Peer-reviewed: Yes

### Publication information

Journal: DOKLADY BIOCHEMISTRY AND BIOPHYSICS

Volume: 454

Issue number: 1

ISSN (Print): 1607-6729

Ratings:

Scopus rating (2014): CiteScore 0.38 SJR 0.208 SNIP 0.312

Original language: English

ASJC Scopus subject areas: Biophysics, Chemistry(all), Medicine(all), Biochemistry

DOIs:

10.1134/S1607672914010062

URLs:

<http://www.scopus.com/inward/record.url?scp=84896349301&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84896349301

Research output: Contribution to journal > Article > Scientific > peer-review

## Fabrication of 3-D nanodimensioned electric double layer capacitor structures using block copolymer templates

The need for materials for high energy storage has led to very significant research in supercapacitor systems. These can exhibit electrical double layer phenomena and capacitances up to hundreds of F/g. Here, we demonstrate a new

supercapacitor fabrication methodology based around the microphase separation of PS-b-PMMA which has been used to prepare copper nanoelectrodes of dimension ~13 nm. These structures provide excellent capacitive performance with a maximum specific capacitance of ~836 F/g for a current density of 8.06 A/g at a discharge current as high as 75 mA. The excellent performance is due to a high surface area: volume ratio. We suggest that this highly novel, easily fabricated structure might have a number of important applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Materials Chemistry and Analysis Group, University College Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Tyndall National Institute at National University of Ireland, Cork

Contributors: Rasappa, S., Borah, D., Senthamaraiannan, R., Faulkner, C. C., Holmes, J. D., Morris, M. A.

Number of pages: 7

Pages: 5221-5227

Publication date: 2014

Peer-reviewed: Yes

#### Publication information

Journal: Journal Nanoscience and Nanotechnology

Volume: 14

Issue number: 7

ISSN (Print): 1533-4880

Ratings:

Scopus rating (2014): CiteScore 1.36 SJR 0.327 SNIP 0.515

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Biomedical Engineering, Materials Science(all), Condensed Matter Physics

Keywords: 3-D Nanostructure, Block Copolymer, Capacitance, Copper Nanowires, PS-b-PMMA, Supercapacitor

DOIs:

10.1166/jnn.2014.8668

URLs:

<http://www.scopus.com/inward/record.url?scp=84903822885&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84903822885

Research output: Contribution to journal > Article > Scientific > peer-review

#### Study of the kinetics and mechanism of rapid self-assembly in block copolymer thin films during solvo-microwave annealing

Microwave annealing is an emerging technique for achieving ordered patterns of block copolymer films on substrates. Little is understood about the mechanisms of microphase separation during the microwave annealing process and how it promotes the microphase separation of the blocks. Here, we use controlled power microwave irradiation in the presence of tetrahydrofuran (THF) solvent, to achieve lateral microphase separation in high- $\chi$  lamellar-forming poly(styrene-b-lactic acid) PS-b-PLA. A highly ordered line pattern was formed within seconds on silicon, germanium and silicon on insulator (SOI) substrates. In-situ temperature measurement of the silicon substrate coupled to condition changes during "solvomicrowave" annealing allowed understanding of the processes to be attained. Our results suggest that the substrate has little effect on the ordering process and is essentially microwave transparent but rather, it is direct heating of the polar THF molecules that causes microphase separation. It is postulated that the rapid interaction of THF with microwaves and the resultant temperature increase to 55 °C within seconds causes an increase of the vapor pressure of the solvent from 19.8 to 70 kPa. This enriched vapor environment increases the plasticity of both PS and PLA chains and leads to the fast self-assembly kinetics. Comparing the patterns formed on silicon, germanium and silicon on insulator (SOI) and also an in situ temperature measurement of silicon in the oven confirms the significance of the solvent over the role of substrate heating during "solvo-microwave" annealing. Besides the short annealing time which has technological importance, the coherence length is on a micron scale and dewetting is not observed after annealing. The etched pattern (PLA was removed by an Ar/O<sub>2</sub> reactive ion etch) was transferred to the underlying silicon substrate fabricating sub-20 nm silicon nanowires over large areas demonstrating that the morphology is consistent both across and through the film.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Trinity College Dublin, Tyndall National Institute at National University of Ireland, Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Department of Micro and Nanotechnology, Danmarks Tekniske Universitet, DTU Informatik, Universitat Autònoma de Barcelona, Catalan Institute for Research and Advanced Studies (ICREA)

Contributors: Mokarian-Tabari, P., Cummins, C., Rasappa, S., Simao, C., Torres, C. M. S., Holmes, J. D., Morris, M. A.

Number of pages: 12  
Pages: 10728-10739  
Publication date: 2014  
Peer-reviewed: Yes

#### Publication information

Journal: Langmuir  
Volume: 30  
Issue number: 35  
ISSN (Print): 0743-7463  
Ratings:

Scopus rating (2014): CiteScore 4.59 SJR 1.81 SNIP 1.363

Original language: English

ASJC Scopus subject areas: Medicine(all), Materials Science(all), Condensed Matter Physics, Surfaces and Interfaces, Spectroscopy, Electrochemistry

DOIs:

10.1021/la503137q

URLs:

<http://www.scopus.com/inward/record.url?scp=84925424888&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84925424888

Research output: Contribution to journal > Article > Scientific > peer-review

#### Kinetics of bioconjugate nanoparticle label binding in a sandwich-type immunoassay

Nanoparticle labels have enhanced the performance of diagnostic, screening, and other measurement applications and hold further promise for more sensitive, precise, and cost-effective assay technologies. Nevertheless, a clear view of the biomolecular interactions on the molecular level is missing. Controlling the ratio of molecular recognition over undesired nonspecific adhesion is the key to improve biosensing with nanoparticles. To improve this ratio with an aim to disallow nonspecific binding, a more detailed perspective into the kinetic differences between the cases is needed. We present the application of two novel methods to determine complex binding kinetics of bioconjugate nanoparticles, interferometry, and force spectroscopy. Force spectroscopy is an atomic force microscopy technique and optical interferometry is a direct method to monitor reaction kinetics in second-hour timescale, both having steadily increasing importance in nanomedicine. The combination is perfectly suited for this purpose, due to the high sensitivity to detect binding events and the ability to investigate biological samples under physiological conditions. We have attached a single biofunctionalized nanoparticle to the outer tip apex and studied the binding behavior of the nanoparticle in a sandwich-type immunoassay using dynamic force spectroscopy in millisecond timescale. Utilization of the two novel methods allowed characterization of binding kinetics in a time range spanning from 50 ms to 4 h. These experiments allowed detection and demonstration of differences between specific and nonspecific binding. Most importantly, nonspecific binding of a nanoparticle was reduced at contact times below 100 ms with the solid-phase surface.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Turun Yliopisto/Turun Biomateriaalikeskus, Johannes Kepler University, Agilent Technologies Österreich GmbH, Fimlab Laboratories Ltd, Center for Advanced Bioanalysis

Contributors: Näreoja, T., Ebner, A., Gruber, H. J., Taskinen, B., Kienberger, F., Hänninen, P. E., Hytönen, V. P., Hinterdorfer, P., Härmä, H.

Number of pages: 11

Pages: 493-503

Publication date: 2014

Peer-reviewed: Yes

#### Publication information

Journal: Analytical and Bioanalytical Chemistry

Volume: 406

Issue number: 2

ISSN (Print): 1618-2642

Ratings:

Scopus rating (2014): CiteScore 3.26 SJR 1.126 SNIP 1.212

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Biochemistry

Keywords: Biofunctionalized nanoparticle labels, Biolayer interferometry, Force spectroscopy, Nonspecific binding, Sandwich-type immunoassay

DOIs:

10.1007/s00216-013-7474-0

URLs:

<http://www.scopus.com/inward/record.url?scp=84899084023&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84899084023

Research output: Contribution to journal > Article > Scientific > peer-review

### **Self-assembly of polystyrene-block-poly(4-vinylpyridine) block copolymer on molecularly functionalized silicon substrates: Fabrication of inorganic nanostructured etchmask for lithographic use**

Block copolymers (BCPs) are seen as a possible cost effective complementary technique to traditional lithography currently used in the semiconductor industry. This unconventional approach has received increased attention in recent years as a process capable of facilitating the ever decreasing device size demanded. Control over microdomain orientation and enhancing long range order are key aspects for the utility of BCPs for future lithographic purposes. This paper provides an efficient route for the fabrication of highly ordered nanostructures suitable for such application. We investigate the significant effect of surface treatment regarding the self-assembly process of polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) by employing an ethylene glycol layer, producing well defined perpendicular P4VP cylinders with long range order over large surface areas. Nanopores are generated through surface reconstruction using a preferential solvent, which allows for the incorporation of an inorganic moiety. Treatment of this pattern with UV/Ozone leads to formation of well-ordered iron oxide nanodots with a pitch of ~26 nm. Furthermore, high aspect ratio silicon nanopillars result following pattern transfer (using Ar/O<sub>2</sub>).

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Tyndall National Institute at National University of Ireland, Cork, Trinity College Dublin, University College Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN)

Contributors: Cummins, C., Borah, D., Rasappa, S., Chaudhari, A., Ghoshal, T., O'Driscoll, B. M. D., Carolan, P., Petkov, N., Holmes, J. D., Morris, M. A.

Number of pages: 11

Pages: 7941-7951

Publication date: 21 Dec 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Materials Chemistry C

Volume: 1

Issue number: 47

ISSN (Print): 2050-7534

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Chemistry

DOIs:

10.1039/c3tc31498g

URLs:

<http://www.scopus.com/inward/record.url?scp=84887902210&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84887902210

Research output: Contribution to journal > Article > Scientific > peer-review

### **Analysis of free, mono- and diacetylated polyamines from human urine by LC-MS/MS**

Polyamines are promising biochemical markers of cancer and many other pathophysiological conditions, and thus their concentrations in biological fluids are a matter of interest. However, since the concentrations of these compounds are low, their quantitation is typically based on methods requiring laborious sample preparation. Here we developed and validated an LC-MS/MS method to analyze simultaneously free (DAP, PUT, CAD, SPD, SPM) monoacetylated (AcPUT, AcCAD, N<sup>1</sup>AcSPD, N<sup>8</sup>AcSPD, N<sup>1</sup>AcSPM) and diacetylated (DiAcPUT, DiAcCAD, DiAcSPD, DiAcSPM) polyamines from human urine without the need for derivatization. Deuterium labeled polyamines were the internal standards for each analyte. Diluted urine samples spiked with internal standards were filtered through a strong anion exchange resin prior to LC-MS/MS analysis. The chromatographic separation of 14 polyamines was achieved in 12min on C18 column with 0.1% HFBA (v/v) as the ion-pairing agent and a water-acetonitrile gradient. Ionization was performed with positive electrospray ionization (ESI) and detection was with a triple quadrupole mass spectrometer with selected reaction monitoring. Calibration curves ranged from up to 5 to 10,000nM. The accuracy and precision of the method were determined using urine based quality control samples, and matrix effects were examined by using standard addition methods. This novel method is suitable for elucidating differences in urinary polyamine excretion in cancer patients and healthy humans.

#### **General information**



Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Ita-Suomen yliopisto, Tampere University Hospital, Karolinska University Hospital, School of Management (JKK)

Contributors: Häkkinen, M. R., Roine, A., Auriola, S., Tuokko, A., Veskimäe, E., Keinänen, T. A., Lehtimäki, T., Oksala, N., Vepsäläinen, J.

Number of pages: 9

Pages: 81-89

Publication date: 15 Dec 2013

Peer-reviewed: Yes

#### Publication information

Journal: JOURNAL OF CHROMATOGRAPHY B: ANALYTICAL TECHNOLOGIES IN THE BIOMEDICAL AND LIFE SCIENCES

Volume: 941

ISSN (Print): 1570-0232

Ratings:

Scopus rating (2013): CiteScore 2.78 SJR 1.061 SNIP 1.278

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Biochemistry, Clinical Biochemistry, Cell Biology

Keywords: Cancer diagnostic markers, Liquid chromatography-tandem mass spectrometry, N-acetylated, Polyamines, Prostate cancer, Urine

DOIs:

10.1016/j.jchromb.2013.10.009

URLs:

<http://www.scopus.com/inward/record.url?scp=84887097655&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84887097655

Research output: Contribution to journal › Article › Scientific › peer-review

#### Location of dispersing agent in rubber nanocomposites during mixing process

In the present work, the development of morphology and selective wetting of nanoclay and carbon nanotubes (CNTs) in rubber nanocomposites were characterized qualitatively by means of the optical microscopy, TEM and AFM and quantitatively by means of the wetting concept. Carboxylated hydrogenated nitrile butadiene rubber (XHNBR), ionic liquid and ethanol were used as dispersing agent and they show very good effect on the macro- and microdispersion of nanofillers in different rubbers. It was found that the selective wetting of filler surface by the dispersing agent and rubber matrix is controlled by thermodynamic and kinetic factors. A model basing on surface energy data of polymer components (rubber and dispersing agent) and filler was introduced in order to determine the thermodynamic equilibrium state of filler wetting, which is found to be simultaneously determined by the filler-polymer affinity and the rubber/dispersing agent mass ratio. During the mixing process a replacement process of bound polymer components takes place on the filler surface until the predicted state is reached.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V., University of Applied Sciences Merseburg, Martin-Luther-University Halle-Wittenberg, Vodafone Department of Mobile Communications Systems, Polymer Service Merseburg

Contributors: Le, H. H., Oßwald, K., Wießner, S., Das, A., Stöckelhuber, K. W., Boldt, R., Gupta, G., Heinrich, G., Radosch, H. J.

Number of pages: 13

Pages: 7009-7021

Publication date: 13 Dec 2013

Peer-reviewed: Yes

#### Publication information

Journal: Polymer

Volume: 54

Issue number: 26

ISSN (Print): 0032-3861

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Original language: English

ASJC Scopus subject areas: Polymers and Plastics, Organic Chemistry

Keywords: Carbon nanotubes, Dispersing agent, Localization

DOIs:

10.1016/j.polymer.2013.10.038

URLs:

<http://www.scopus.com/inward/record.url?scp=84889099442&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84889099442

Research output: Contribution to journal > Article > Scientific > peer-review

### **Proliferation and differentiation of adipose stem cells towards smooth muscle cells on poly(trimethylene carbonate) membranes**

**Summary** Multipotent human adipose stem cells (hASCs) are an abundant and potential source of cells for vascular tissue engineering when combined with a suitable biomaterial scaffold. Poly(trimethylene carbonate) (PTMC) has been shown to be a useful biodegradable material for tissue engineered vascular grafts due to its flexibility, excellent biocompatibility and enzymatic degradation by surface erosion in vivo. The purpose of the current study was to evaluate the proliferation and differentiation of hASCs towards smooth muscle cells (SMCs) on gamma-crosslinked and photo-crosslinked PTMC membranes. PTMC macromers were functionalized with methacrylate end groups and crosslinked by UV initiated radical polymerization. High molecular weight linear PTMC was crosslinked by gamma irradiation. Cell viability, cell numbers and SMC differentiation of hASCs were evaluated on the differently crosslinked PTMC films at 7 and 14 days (d). On the photo-crosslinked membranes, homogenous monolayers of hASC were detected by live/dead assay. Consistently, cells on the photo-crosslinked membranes had significantly higher cell numbers compared to cells on the gamma-crosslinked membranes after 14 d of culture. SMC specific genes were expressed on both membranes at 14 d. Photo-crosslinked membranes showed higher expression of SMC specific proteins at 14 d compared to gamma-crosslinked membranes. These results suggest that especially the photo-crosslinked PTMC membranes are suitable for vascular tissue engineering applications when combined with hASCs.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Aachen University of Applied Sciences, University of Groningen

Contributors: German, S. J., Behbahani, M., Miettinen, S., Grijpma, D. W., Haimi, S. P.

Number of pages: 10

Pages: 133-142

Publication date: Dec 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Macromolecular symposia

Volume: 334

Issue number: 1

ISSN (Print): 1022-1360

Ratings:

Scopus rating (2013): CiteScore 0.71 SJR 0.326 SNIP 0.388

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Polymers and Plastics, Organic Chemistry, Materials Chemistry

Keywords: adipose stem cell differentiation, poly (trimethylene carbonate), smooth muscle cells, tissue engineering

DOIs:

10.1002/masy.201300100

URLs:

<http://www.scopus.com/inward/record.url?scp=84890729494&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84890729494

Research output: Contribution to journal > Article > Scientific > peer-review

### **Effect of surface morphology of poly( $\epsilon$ -caprolactone) scaffolds on adipose stem cell adhesion and proliferation**

**Summary** The effect of the surface morphology of flat poly( $\epsilon$ -caprolactone) (PCL) scaffolds on human adipose stem cell (hASC) adherence and proliferation was studied. During fabrication of the scaffolds by phase inversion, the employment of different non-solvents (water (W), ethanol (EtOH) or isopropanol (IPA)) led to distinct surface morphologies. It was found that PCL scaffolds fabricated using IPA as a non-solvent had a higher roughness and porosity compared to the other groups. Moreover, during culturing of hASCs under static conditions, best cell attachment, spreading and growth were observed on the PCL scaffold. Our results show the potential of PCL scaffolds prepared using IPA as a non-solvent for especially soft tissue engineering applications.

#### **General information**

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), University of Twente, University of Groningen  
Contributors: Diban, N., Haimi, S. P., Bolhuis-Versteeg, L., Teixeira, S., Miettinen, S., Poot, A. A., Grijpma, D. W., Stamatialis, D.  
Number of pages: 7  
Pages: 126-132  
Publication date: Dec 2013  
Peer-reviewed: Yes

#### Publication information

Journal: Macromolecular symposia  
Volume: 334  
Issue number: 1  
ISSN (Print): 1022-1360  
Ratings:  
Scopus rating (2013): CiteScore 0.71 SJR 0.326 SNIP 0.388  
Original language: English  
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Condensed Matter Physics  
Keywords: morphology, phase inversion, poly( $\mu$ -caprolactone), roughness, scaffold porosity  
DOIs:  
10.1002/masy.201300106  
URLs:  
<http://www.scopus.com/inward/record.url?scp=84890745371&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 84890745371  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Human adipose stem cells in chondrogenic differentiation medium without growth factors differentiate towards annulus fibrosus phenotype in vitro

Summary Intervertebral disc degeneration is the main cause of chronic back pain. Disc degeneration mainly leads to tearing of annulus fibrosus (AF), which is with current methods difficult to restore and impossible to regenerate. Stem cell technology offers a potential technique to repair the ruptured AF by enabling new matrix synthesis at the defect site. Previous studies have shown that human adipose stem cells (hASCs) are able to differentiate towards AF phenotype when treated with suitable growth factors. There are concerns about the use of growth factors in clinical applications because of their short half-lives, high costs and low effectiveness. The main aim of this research project was to regenerate AF tissue in vitro using hASCs and serum free chondrogenic medium without supplementation of growth factors. Differentiation of hASCs was induced by using the micromass culture technique. Human annulus fibrosus cell (hAFCs) cultured in commercial AF growth medium were used as positive control. Assessment of AF phenotype of hASCs and hAFCs was done at 14 and 21 days of culture. Quantification of sulphated glycosaminoglycan (GAG) content showed that hASCs cultured in chondrogenic medium expressed similar levels of sulphated GAGs as hAFCs. qRT-PCR confirmed the similarity of the differentiated hASCs with AF phenotype. Several markers for AF phenotype (aggrecan, collagen type I and glypican-3) were expressed in both hAFCs and differentiated hASCs. This is the first study that demonstrated that hASCs can be differentiated towards AF phenotype using serum free chondrogenic medium without growth factors. In a next step, scaffolds manufactured from biodegradable polymers will be used in combination with ASCs to find an optimal construct to repair AF defects.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), University of Twente, University of Groningen  
Contributors: Gebraad, A. W. H., Miettinen, S., Grijpma, D. W., Haimi, S. P.  
Number of pages: 8  
Pages: 49-56  
Publication date: Dec 2013  
Peer-reviewed: Yes

#### Publication information

Journal: Macromolecular symposia  
Volume: 334  
Issue number: 1  
ISSN (Print): 1022-1360  
Ratings:

Scopus rating (2013): CiteScore 0.71 SJR 0.326 SNIP 0.388

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Condensed Matter Physics

Keywords: adipose stem cells, annulus fibrosus, intervertebral disc, tissue engineering

DOIs:

10.1002/masy.201300104

URLs:

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Source: Scopus

Source ID: 84890722713

Research output: Contribution to journal > Article > Scientific > peer-review

### **Fabrication of ssDNA/Oligo(ethylene glycol) monolayers and patterns by exchange reaction promoted by ultraviolet light irradiation**

Using a representative test system, we present here a versatile approach to prepare mixed monolayers of thiolated single-stranded DNA (ssDNA) and oligo(ethylene glycol) substituted alkanethiols (OEG-AT) in a broad range of compositions as well as ssDNA/OEG-AT patterns of desired shape imbedded into a biorepulsive background. The procedure involves two steps. First, a primary, well-defined OEG-AT monolayer on a solid support is exposed to UV light in either homogeneous or lithographic fashion. Second, the exchange reaction between the damaged OEG-AT species in the film and ssDNA substituents in solution occurs, resulting in formation of ssDNA/OEG-AT monolayer or pattern. The above procedure relies on commercially available compounds and does not require vacuum, which simplifies its application in research and industrial laboratories. The composition of the mixed films or ssDNA/OEG-AT spots (lithography) can be precisely adjusted by UV dose in an almost entire composition range. It was demonstrated that the procedure can be performed with UV light of different wavelengths (254 or 365 nm), which opens new possibilities for lithography. Using advanced spectroscopic tools, it was shown that ssDNA molecules imbedded into the OEG-AT matrix maintain their identity and intact character as well as exhibit predominant upright orientation typical of one-component films of thiolated ssDNA. The OEG-AT constituents of the mixed monolayers were found to be intact as well, with all UV damaged OEG-AT species being exchanged for ssDNA. Finally, a representative ssDNA/OEG-AT pattern was fabricated.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Universitat Heidelberg

Contributors: Khan, M. N., Zhamnikov, M.

Number of pages: 11

Pages: 24883-24893

Publication date: 27 Nov 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry C

Volume: 117

Issue number: 47

ISSN (Print): 1932-7447

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Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.432

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

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URLs:

<http://www.scopus.com/inward/record.url?scp=84889582340&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84889582340

Research output: Contribution to journal > Article > Scientific > peer-review

### **Release of halide ions from the buried active site of the haloalkane dehalogenase LinB revealed by stopped-flow fluorescence analysis and free energy calculations**

Release of halide ions is an essential step of the catalytic cycle of haloalkane dehalogenases. Here we describe experimentally and computationally the process of release of a halide anion from the buried active site of the haloalkane dehalogenase LinB. Using stopped-flow fluorescence analysis and umbrella sampling free energy calculations, we show that the anion binding is ion-specific and follows the ordering  $I^- > Br^- > Cl^-$ . We also address the issue of the protonation state of the catalytic His272 residue and its effect on the process of halide release. While deprotonation of His272

increases binding of anions in the access tunnel, we show that the anionic ordering does not change with the switch of the protonation state. We also demonstrate that a sodium cation could relatively easily enter the active site, provided the His272 residue is singly protonated, and replace thus the missing proton. In contrast,  $\text{Na}^+$  is strongly repelled from the active site containing the doubly protonated His272 residue. Our study contributes toward understanding of the reaction mechanism of haloalkane dehalogenase enzyme family. Determination of the protonation state of the catalytic histidine throughout the catalytic cycle remains a challenge for future studies.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Masaryk University

Contributors: Hladilkova, J., Prokop, Z., Chaloupkova, R., Damborsky, J., Jungwirth, P.

Number of pages: 7

Pages: 14329-14335

Publication date: 21 Nov 2013

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 117

Issue number: 46

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2013): CiteScore 3.53 SJR 1.504 SNIP 1.194

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

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Source: Scopus

Source ID: 84888618153

Research output: Contribution to journal > Article > Scientific > peer-review

#### Ion pairing in aqueous lithium salt solutions with monovalent and divalent counter-anions

Molecular dynamics simulations of concentrated aqueous solutions of LiCl and  $\text{Li}_2\text{SO}_4$  were conducted in order to provide molecular insight into recent neutron scattering data. The structures predicted from the molecular dynamics simulations using standard nonpolarizable force fields provided a very poor fit to the experiment; therefore, refinement was needed. The electronic polarizability of the medium was effectively accounted for by implementing the electronic continuum correction, which practically means rescaling the ionic charges. Consistent with previous studies, we found that this approach in each case provided a significantly improved fit to the experimental data, which was further enhanced by slightly adjusting the radius of the lithium ion. The polarization effect was particularly pronounced in the  $\text{Li}_2\text{SO}_4$  solution where the ions in the nonpolarizable simulations tended to cluster unphysically. With the above alterations, the employed force field displayed an excellent fit to the neutron scattering data and provided a useful interpretative framework for the experimental measurements. At the same time, the present study underlines the importance of solvent polarization effects in hydration of ions with high charge density.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Pluhařová, E., Mason, P. E., Jungwirth, P.

Number of pages: 8

Pages: 11766-11773

Publication date: 21 Nov 2013

Peer-reviewed: Yes

#### Publication information

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ISSN (Print): 1089-5639

Ratings:

Scopus rating (2013): CiteScore 2.84 SJR 1.205 SNIP 1.1  
Original language: English  
ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1021/jp402532e

URLs:

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Source: Scopus

Source ID: 84879340380

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **The Halogen Bond in the Design of Functional Supramolecular Materials: Recent Advances**

Halogen bonding is an emerging noncovalent interaction for constructing supramolecular assemblies. Though similar to the more familiar hydrogen bonding, four primary differences between these two interactions make halogen bonding a unique tool for molecular recognition and the design of functional materials. First, halogen bonds tend to be much more directional than (single) hydrogen bonds. Second, the interaction strength scales with the polarizability of the bond-donor atom, a feature that researchers can tune through single-atom mutation. In addition, halogen bonds are hydrophobic whereas hydrogen bonds are hydrophilic. Lastly, the size of the bond-donor atom (halogen) is significantly larger than hydrogen. As a result, halogen bonding provides supramolecular chemists with design tools that cannot be easily met with other types of noncovalent interactions and opens up unprecedented possibilities in the design of smart functional materials. This Account highlights the recent advances in the design of halogen-bond-based functional materials. Each of the unique features of halogen bonding, directionality, tunable interaction strength, hydrophobicity, and large donor atom size, makes a difference. Taking advantage of the hydrophobicity, researchers have designed small-size ion transporters. The large halogen atom size provided a platform for constructing all-organic light-emitting crystals that efficiently generate triplet electrons and have a high phosphorescence quantum yield. The tunable interaction strengths provide tools for understanding light-induced macroscopic motions in photoresponsive azobenzene-containing polymers, and the directionality renders halogen bonding useful in the design of functional supramolecular liquid crystals and gel-phase materials. Although halogen bond based functional materials design is still in its infancy, we foresee a bright future for this field. We expect that materials designed based on halogen bonding could lead to applications in biomimetics, optics/photonics, functional surfaces, and photoswitchable supramolecules.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Aalto University, Politecnico di Milano, VTT Technical Research Centre of Finland

Contributors: Priimagi, A., Cavallo, G., Metrangolo, P., Resnati, G.

Number of pages: 10

Pages: 2686-2695

Publication date: 19 Nov 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Accounts of Chemical Research

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Issue number: 11

ISSN (Print): 0001-4842

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Original language: English

ASJC Scopus subject areas: Chemistry(all)

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Source: Scopus

Source ID: 84888619396

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **How conformational flexibility stabilizes the hyperthermophilic elongation factor G-domain**

Proteins from thermophilic organisms are stable and functional well above ambient temperature. Understanding the molecular mechanism underlying such a resistance is of crucial interest for many technological applications. For some time, thermal stability has been assumed to correlate with high mechanical rigidity of the protein matrix. In this work we address this common belief by carefully studying a pair of homologous G-domain proteins, with their melting temperatures differing by 40 K. To probe the thermal-stability content of the two proteins we use extensive simulations covering the

microsecond time range and employ several different indicators to assess the salient features of the conformational landscape and the role of internal fluctuations at ambient condition. At the atomistic level, while the magnitude of fluctuations is comparable, the distribution of flexible and rigid stretches of amino-acids is more regular in the thermophilic protein causing a cage-like correlation of amplitudes along the sequence. This caging effect is suggested to favor stability at high T by confining the mechanical excitations. Moreover, it is found that the thermophilic protein, when folded, visits a higher number of conformational substates than the mesophilic homologue. The entropy associated with the occupation of the different substates and the thermal resilience of the protein intrinsic compressibility provide a qualitative insight on the thermal stability of the thermophilic protein as compared to its mesophilic homologue. Our findings potentially open the route to new strategies in the design of thermostable proteins.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Laboratoire de Biochimie Théorique, Université Paris Diderot, Centro S3

Contributors: Kalimeri, M., Rahaman, O., Melchionna, S., Sterpone, F.

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Publication date: 7 Nov 2013

Peer-reviewed: Yes

#### Publication information

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Ratings:

Scopus rating (2013): CiteScore 3.53 SJR 1.504 SNIP 1.194

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

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#### Bibliographical note

EXT="Kalimeri, Maria"

Source: Scopus

Source ID: 84887752230

Research output: Contribution to journal > Article > Scientific > peer-review

#### Embedded cluster models for reactivity of the hydrated electron

Our computational study presents embedded cluster models of the hydrated electron focusing on its reactivity with the hydrated proton and the nitrous oxide molecule leading to formation of a hydrogen atom in the former case and a nitrogen molecule plus hydroxyl radical and hydroxide anion in the latter case. We show using ab initio calculations combined with the nudged elastic band method for determining minimum energy paths that carefully chosen cluster models with no more than six water molecules embedded in a polarizable continuum are able to capture the essential features of the reactive processes of the hydrated electron.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Uhlig, F., Jungwirth, P.

Number of pages: 11

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Publication date: Nov 2013

Peer-reviewed: Yes

#### Publication information

Journal: ZEITSCHRIFT FUR PHYSIKALISCHE CHEMIE-INTERNATIONAL JOURNAL OF RESEARCH IN PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

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ISSN (Print): 0942-9352

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Scopus rating (2013): CiteScore 1.13 SJR 0.463 SNIP 0.603

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

Keywords: Clusters, Hydrated Electron, Hydronium, Nitrous Oxide, Reactivity

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Source: Scopus

Source ID: 84888629620

Research output: Contribution to journal > Article > Scientific > peer-review

### **Soft-graphoepitaxy using nanoimprinted polyhedral oligomeric silsesquioxane substrates for the directed self-Assembly of PS-b-PDMS**

We report here the fabrication of periodic sub-25 nm diameter size cylinder structures using block copolymer (BCP) directed self-Assembly on nanoimprinted topographically patterned substrates. Tailored polyhedral oligomeric silsesquioxanes (POSSs) films were spin coated onto silicon substrates and were patterned by nanoimprint lithography to produce topographies commensurable with the BCP domain spacing. The chemistry of the POSS was tuned to control the alignment and orientation of the BCP films. The substrates were used to direct the microphase separation (following toluene solvent annealing) of a hexagonal structure forming polystyrene-block-polydimethylsiloxane (PS-b-PDMS) having a domain spacing of 42.6 nm and PDMS cylinder widths of 23.7 nm. On more hydrophilic POSS substrates the cylinders were obtained parallel to the substrate plane and aligned with the topography. In contrast, in more hydrophobic POSS patterns, the cylinders align perpendicular to the substrate plane. The use of these methods for the nanofabrication of vias, nanofluidic devices or interconnect structures of sub-25 nm feature size is discussed.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Nanophotonics, Frontier Photonics, Trinity College Dublin, Edifici CM3, University College Cork, Tyndall National Institute at National University of Ireland, Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Profactor GmbH, CNRS/UJF-Grenoble1/CEA LTM, Catalan Institute for Research and Advanced Studies (ICREA)

Contributors: Borah, D., Simao, C. D., Senthamaraiannan, R., Rasappa, S., Francone, A., Lorret, O., Salaun, M., Kosmala, B., Kehagias, N., Zelsmann, M., Sotomayor-Torres, C. M., Morris, M. A.

Number of pages: 10

Pages: 3512-3521

Publication date: Nov 2013

Peer-reviewed: Yes

#### **Publication information**

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ISSN (Print): 0014-3057

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Original language: English

ASJC Scopus subject areas: Polymers and Plastics, Physics and Astronomy(all), Organic Chemistry

Keywords: Block copolymer-Polyhedral oligomeric silsesquioxanes, Directed self-Assembly, Graphoepitaxy, Nanoimprint lithography, Surface chemistry

DOIs:

10.1016/j.eurpolymj.2013.08.011

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Source: Scopus

Source ID: 84885020807

Research output: Contribution to journal > Article > Scientific > peer-review

### **Porphyrim adsorbed on the (1010) surface of the wurtzite structure of ZnO-conformation induced effects on the electron transfer characteristics**

Electron transfer at the adsorbate-surface interface is crucial in many applications but the steps taking place prior to and during the electron transfer are not always thoroughly understood. In this work a model system of 4-(porphyrim-5-



yl)benzoic acid adsorbed as a corresponding benzoate on the ZnO wurtzite (1010) surface is studied using density functional theory (DFT) and time-dependent DFT. Emphasis is on the initial photoexcitation of porphyrin and on the strength of coupling between the porphyrin LUMO or LUMO + 1 and the ZnO conduction band that plays a role in the electron transfer. Firstly, ZnO wurtzite bulk is optimized to minimum energy geometry and the properties of the isolated ZnO (1010) surface model and the porphyrin model are discussed to gain insight into the combined system. Secondly, various orientations of the model porphyrin on the ZnO surface are studied: the porphyrin model standing perpendicularly to the surface and gradually brought close to the surface by tilting the linker in a few steps. The porphyrin model approaches the surface either sideways with hydrogen atoms of the porphyrin ring coming down first or twisted in a ca. 45° angle, giving rise to  $\pi$ -interactions of the porphyrin ring with ZnO. Because porphyrins are closely packed and near the surface, emerging van der Waals (vdW) interactions are examined using Grimme's D2 method. While the orientation affects the initial excitation of porphyrin only slightly, the coupling between the LUMO and LUMO + 1 of porphyrin and the conduction band of ZnO increases considerably if porphyrin is close to the surface, especially if the  $\pi$ -electrons are interacting with the surface. Based on the results of coupling studies, not only the distance between porphyrin and the ZnO surface but also the orientation of porphyrin can greatly affect the electron transfer. © 2013 the Owner Societies.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Supramolecular photochemistry, Department of Chemistry and Bioengineering, Tampere University of Technology, Department of Physics, Department of Physics, Research area: Computational Physics, Research group: Electronic Structure Theory, Computational Science X (CompX), Frontier Photonics

Contributors: Niskanen, M., Kuisma, M., Cramariuc, O., Golovanov, V., Hukka, T. I., Tkachenko, N., Rantala, T. T.

Number of pages: 11

Pages: 17408-17418

Publication date: 28 Oct 2013

Peer-reviewed: Yes

### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 15

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ISSN (Print): 1463-9076

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

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URLs:

<http://www.scopus.com/inward/record.url?scp=84886933383&partnerID=8YFLogxK> (Link to publication in Scopus)

### Bibliographical note

poistettu tuplat r=2454 ja r=3218<br/>Contribution: organisation=keb,FACT1=0.5<br/>Contribution: organisation=fys,FACT2=0.5<br/>Portfolio EDEND: 2013-10-29<br/>Publisher name: R S C Publications

Source: researchoutputwizard

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Research output: Contribution to journal › Article › Scientific › peer-review

### Reversible biofunctionalization of surfaces with a switchable mutant of avidin

Label-free biosensors detect binding of prey molecules ("analytes") to immobile bait molecules on the sensing surface. Numerous methods are available for immobilization of bait molecules. A convenient option is binding of biotinylated bait molecules to streptavidin-functionalized surfaces, or to biotinylated surfaces via biotin-avidin-biotin bridges. The goal of this study was to find a rapid method for reversible immobilization of biotinylated bait molecules on biotinylated sensor chips. The task was to establish a biotin-avidin-biotin bridge which was easily cleaved when desired, yet perfectly stable under a wide range of measurement conditions. The problem was solved with the avidin mutant M96H which contains extra histidine residues at the subunit-subunit interfaces. This mutant was bound to a mixed self-assembled monolayer (SAM) containing biotin residues on 20% of the oligo(ethylene glycol)-terminated SAM components. Various biotinylated bait molecules were bound on top of the immobilized avidin mutant. The biotin-avidin-biotin bridge was stable at pH  $\geq 3$ , and it was insensitive to sodium dodecyl sulfate (SDS) at neutral pH. Only the combination of citric acid (2.5%, pH 2) and SDS (0.25%) caused instantaneous cleavage of the biotin-avidin-biotin bridge. As a consequence, the biotinylated bait molecules could be immobilized and removed as often as desired, the only limit being the time span for reproducible chip function when kept in buffer (2-3 weeks at 25 C). As expected, the high isoelectric pH (pI) of the avidin mutant caused nonspecific adsorption of proteins. This problem was solved by acetylation of avidin (to pI <5), or by optimization of SAM formation and passivation with biotin-BSA and BSA.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Johannes Kepler University, Fimlab Laboratories Ltd, University of Salzburg, University of Basel, University of South Bohemia, Goethe-University Frankfurt

Contributors: Pollheimer, P., Taskinen, B., Scherfler, A., Gusenkov, S., Creus, M., Wiesauer, P., Zauner, D., Schöfberger, W., Schwarzinger, C., Ebner, A., Tampé, R., Stutz, H., Hytönen, V. P., Gruber, H. J.

Number of pages: 13

Pages: 1656-1668

Publication date: 16 Oct 2013

Peer-reviewed: Yes

### Publication information

Journal: Bioconjugate Chemistry

Volume: 24

Issue number: 10

ISSN (Print): 1043-1802

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Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering, Organic Chemistry, Pharmaceutical Science, Biomedical Engineering, Pharmacology

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10.1021/bc400087e

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Source: Scopus

Source ID: 84886070072

Research output: Contribution to journal › Article › Scientific › peer-review

### Importance of the ion-pair interactions in the OPEP coarse-grained force field: Parametrization and validation

We have derived new effective interactions that improve the description of ion pairs in the Optimized Potential for Efficient protein structure Prediction (OPEP) coarse-grained force field without introducing explicit electrostatic terms. The iterative Boltzmann inversion method was used to extract these potentials from all-atom simulations by targeting the radial distribution function of the distance between the center of mass of the side chains. The new potentials have stabilities, and number of ion pairs. Our modeling, by refining the packing of the charged amino acids, impacts the stability of secondary structure motifs and the population of intermediate states during temperature folding/unfolding; it also improves the aggregation propensity of peptides. The new version of the OPEP force field has the potentiality to describe more realistically a large spectrum of situations where salt-bridges are key interactions. (Figure Presented)

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Université Paris Diderot, Laboratoire de Biochimie Théorique, Institut Universitaire de France

Contributors: Sterpone, F., Nguyen, P. H., Kalimeri, M., Derreumaux, P.

Number of pages: 11

Pages: 4574-4584

Publication date: 8 Oct 2013

Peer-reviewed: Yes

### Publication information

Journal: Journal of Chemical Theory and Computation

Volume: 9

Issue number: 10

ISSN (Print): 1549-9618

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Computer Science Applications

DOIs:

10.1021/ct4003493

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<http://www.scopus.com/inward/record.url?scp=84891948959&partnerID=8YFLogxK> (Link to publication in Scopus)

## Bibliographical note

EXT="Kalimeri, Maria"

Source: Scopus

Source ID: 84891948959

Research output: Contribution to journal › Article › Scientific › peer-review

## Zinc coordination spheres in protein structures

Zinc metalloproteins are one of the most abundant and structurally diverse proteins in nature. In these proteins, the Zn(II) ion possesses a multifunctional role as it stabilizes the fold of small zinc fingers, catalyzes essential reactions in enzymes of all six classes, or assists in the formation of biological oligomers. Previously, a number of database surveys have been conducted on zinc proteins to gain broader insights into their rich coordination chemistry. However, many of these surveys suffer from severe flaws and misinterpretations or are otherwise limited. To provide a more comprehensive, up-to-date picture on zinc coordination environments in proteins, zinc containing protein structures deposited in the Protein Data Bank (PDB) were analyzed in detail. A statistical analysis in terms of zinc coordinating amino acids, metal-to-ligand bond lengths, coordination number, and structural classification was performed, revealing coordination spheres from classical tetrahedral cysteine/histidine binding sites to more complex binuclear sites with carboxylated lysine residues. According to the results, coordination spheres of hundreds of crystal structures in the PDB could be misinterpreted due to symmetry-related molecules or missing electron densities for ligands. The analysis also revealed increasing average metal-to-ligand bond length as a function of crystallographic resolution, which should be taken into account when interrogating metal ion binding sites. Moreover, one-third of the zinc ions present in crystal structures are artifacts, merely aiding crystal formation and packing with no biological significance. Our analysis provides solid evidence that a minimal stable zinc coordination sphere is made up by four ligands and adopts a tetrahedral coordination geometry.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Ita-Suomen yliopisto, School of Management (JKK)

Contributors: Laitaoja, M., Valjakka, J., Jänis, J.

Number of pages: 9

Pages: 10983-10991

Publication date: 7 Oct 2013

Peer-reviewed: Yes

## Publication information

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Volume: 52

Issue number: 19

ISSN (Print): 0020-1669

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Original language: English

ASJC Scopus subject areas: Inorganic Chemistry, Physical and Theoretical Chemistry

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<http://www.scopus.com/inward/record.url?scp=84885131955&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84885131955

Research output: Contribution to journal › Article › Scientific › peer-review

## Spectroscopic study of a DNA brush synthesized in situ by surface initiated enzymatic polymerization

We used a combination of synchrotron-based X-ray photoelectron spectroscopy (XPS) and angle-resolved near-edge X-ray absorption fine structure (NEXAFS) spectroscopy to study the chemical integrity, purity, and possible internal alignment of single-strand (ss) adenine deoxynucleotide (poly(A)) DNA brushes. The brushes were synthesized by surface-initiated enzymatic polymerization (SIEP) on a 25-mer of adenine self-assembled monolayer (SAM) on gold (A25-SH), wherein the terminal 3'-OH of the A25-SH serve as the initiation sites for SIEP of poly(A). XPS and NEXAFS spectra of poly(A) brushes were found to be almost identical to those of A25-SH initiator, with no unambiguous traces of contamination. Apart from the well-defined chemical integrity and contamination-free character, the brushes were found to have a high degree of orientational order, with an upright orientation of individual strands, despite their large thickness up to ~55 nm, that corresponds to a chain length of at least several hundred nucleotides for individual ssDNA molecules. The orientational order exhibited by these poly(A) DNA brushes, mediated presumably by base stacking, was found to be independent of the brush thickness as long as the packing density was high enough. The well-defined character and orientational ordering of the ssDNA brushes make them a potentially promising system for different applications.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Universitat Heidelberg, Duke University

Contributors: Khan, M. N., Tjong, V., Chilkoti, A., Zharnikov, M.

Number of pages: 10

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Peer-reviewed: Yes

### Publication information

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ISSN (Print): 1520-6106

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

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Source: Scopus

Source ID: 84883395998

Research output: Contribution to journal > Article > Scientific > peer-review

### Mechanisms of acceleration and retardation of water dynamics by ions

There are fundamental and not yet fully resolved questions concerning the impact of solutes, ions in particular, on the structure and dynamics of water, which can be formulated as follows: Are the effects of ions local or long-ranged? Is the action of cations and anions on water cooperative or not? Here, we investigate how the reorientation and hydrogen-bond dynamics of water are affected by ions in dilute and concentrated aqueous salt solutions. By combining simulations and analytic modeling, we first show that ions have a short-ranged influence on the reorientation of individual water molecules and that depending on their interaction strength with water, they may accelerate or slow down water dynamics. A simple additive picture combining the effects of the cations and anions is found to provide a good description in dilute solutions. In concentrated solutions, we show that the average water reorientation time ceases to scale linearly with salt concentration due to overlapping hydration shells and structural rearrangements which reduce the translational displacements induced by hydrogen-bond switches and increase the solution viscosity. This effect is not ion-specific and explains why all concentrated salt solutions slow down water dynamics. Our picture, which is demonstrated to be robust vis-a-vis a change in the force-field, reconciles the seemingly contradictory experimental results obtained by ultrafast infrared and NMR spectroscopies, and suggests that there are no long-ranged cooperative ion effects on the dynamics of individual water molecules in dilute solutions.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Columbia University in the City of New York, Lund University, Institute

of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, UMR ENS-CNRS-UPMC 8640

Contributors: Stirnemann, G., Wernersson, E., Jungwirth, P., Laage, D.

Number of pages: 8

Pages: 11824-11831

Publication date: 14 Aug 2013

Peer-reviewed: Yes

### Publication information

Journal: Journal of the American Chemical Society

Volume: 135

Issue number: 32

ISSN (Print): 0002-7863

Ratings:

Scopus rating (2013): CiteScore 11.38 SJR 5.993 SNIP 2.446

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis, Biochemistry, Colloid and Surface Chemistry

DOIs:

10.1021/ja405201s

URLs:

<http://www.scopus.com/inward/record.url?scp=84882270662&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84882270662

Research output: Contribution to journal › Article › Scientific › peer-review

### **Irradiation promoted exchange reaction with disulfide substituents**

Exchange reaction between the primary self-assembled monolayer (SAM) on gold and potential molecular substituents capable of forming a SAM on the same substrate can be promoted by electron irradiation. Here we demonstrate that such a promoted reaction can be performed not only with thiols but with disulfides as substituents as well. This extends significantly the assortments of the suitable compounds, resulting in a broader variety of mixed SAMs and chemical patterns which can be fabricated by this technique. The kinetics of the promoted exchange reaction was studied in detail. The feasibility and practical usefulness of the approach were demonstrated by the experiments with a disulfide substituent bearing a tail group which can serve as an initiator for surface-initiated polymerization. A variety of complex polymer brush patterns was prepared using several representative polymers, relevant for biomedical research and applications, as test systems.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Universitat Heidelberg

Contributors: Khan, M. N., Zharnikov, M.

Number of pages: 10

Pages: 14534-14543

Publication date: 18 Jul 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry C

Volume: 117

Issue number: 28

ISSN (Print): 1932-7447

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Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.432

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

10.1021/jp4006026

URLs:

<http://www.scopus.com/inward/record.url?scp=84880559790&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84880559790

Research output: Contribution to journal › Article › Scientific › peer-review

### **Tuning PDMS brush chemistry by UV-O<sub>3</sub> exposure for PS-b-PDMS microphase separation and directed self-assembly**

The directed self-assembly (DSA) of block copolymer (BCP) thin films could enable a scalable, bottom-up alternative to photolithography for the generation of substrate features. The PS-b-PDMS (polystyrene-b-polydimethylsiloxane) system is attractive as it can be extended toward very small feature sizes as well as having two blocks that can be readily differentiated during pattern transfer. However, PS-b-PDMS offers a considerable challenge because of the chemical differences in the blocks which lead to poor surface-wetting, poor pattern orientation control, and structural instabilities. These challenges can be mitigated by careful definition of the interface chemistry between the substrate and the BCP. Here, we report controlled pattern formation in cylinder forming PS-b-PDMS system by use of a carefully controlled PDMS brush. Control of the brush was achieved using exposure to UV-O<sub>3</sub> for varying time. It is demonstrated that this treatment enhances surface wetting and coverage of the BCP. The modified brushes also enable DSA of the BCP on topographically patterned substrates. UV-O<sub>3</sub> exposure was also used to reveal the BCP structure and provide an in situ "hard mask" for pattern transfer to the substrate.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Tyndall National Institute at National University of Ireland, Cork, Materials Chemistry and Analysis Group, University College Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin

Contributors: Borah, D., Rasappa, S., Senthamaraiannan, R., Holmes, J. D., Morris, M. A.  
Number of pages: 10  
Pages: 8959-8968  
Publication date: 16 Jul 2013  
Peer-reviewed: Yes

#### Publication information

Journal: Langmuir  
Volume: 29  
Issue number: 28  
ISSN (Print): 0743-7463  
Ratings:

Scopus rating (2013): CiteScore 4.55 SJR 1.896 SNIP 1.333

Original language: English

ASJC Scopus subject areas: Electrochemistry, Condensed Matter Physics, Surfaces and Interfaces, Materials Science(all), Spectroscopy

DOIs:

10.1021/la401561k

URLs:

<http://www.scopus.com/inward/record.url?scp=84880308592&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84880308592

Research output: Contribution to journal > Article > Scientific > peer-review

#### Reversal of the Hofmeister series: Specific ion effects on peptides

Ion-specific effects on salting-in and salting-out of proteins, protein denaturation, as well as enzymatic activity are typically rationalized in terms of the Hofmeister series. Here, we demonstrate by means of NMR spectroscopy and molecular dynamics simulations that the traditional explanation of the Hofmeister ordering of ions in terms of their bulk hydration properties is inadequate. Using triglycine as a model system, we show that the Hofmeister series for anions changes from a direct to a reversed series upon uncapping the N-terminus. Weakly hydrated anions, such as iodide and thiocyanate, interact with the peptide bond, while strongly hydrated anions like sulfate are repelled from it. In contrast, reversed order in interactions of anions is observed at the positively charged, uncapped N-terminus, and by analogy, this should also be the case at side chains of positively charged amino acids. These results demonstrate that the specific chemical and physical properties of peptides and proteins play a fundamental role in ion-specific effects. The present study thus provides a molecular rationalization of Hofmeister ordering for the anions. It also provides a route for tuning these interactions by titration or mutation of basic amino acid residues on the protein surface.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Pennsylvania State University, Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Texas A and M University

Contributors: Paterová, J., Rembert, K. B., Heyda, J., Kurra, Y., Okur, H. I., Liu, W. R., Hilty, C., Cremer, P. S., Jungwirth, P.

Number of pages: 9

Pages: 8150-8158

Publication date: 11 Jul 2013

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 117

Issue number: 27

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2013): CiteScore 3.53 SJR 1.504 SNIP 1.194

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/jp405683s

URLs:

<http://www.scopus.com/inward/record.url?scp=84880155215&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84880155215

Research output: Contribution to journal › Article › Scientific › peer-review

### Photoswitchable hydrogel surface topographies by polymerisation-induced diffusion

Herein, we describe the preparation of patterned photoresponsive hydrogels by using a facile method. This polymer-network hydrogel coating consists of N-isopropylacrylamide (NIPAAM), cross-linking agent tripropylene glycol diacrylate (TPGDA), and a new photochromic spiropyran monoacrylate. In a pre-study, a linear NIPAAM copolymer (without TPGDA) that contained the spiropyran dye was synthesised, which showed relatively fast photoswitching behaviour. Subsequently, the photopolymerisation of a similar monomer mixture that included TPGDA afforded freestanding hydrogel polymer networks. The light-induced isomerisation of protonated merocyanine into neutral spiropyran under slightly acidic conditions resulted in macroscopic changes in the hydrophilicity of the entire polymer film, that is, shrinkage of the hydrogel. The degree of shrinkage could be controlled by changing the chemical composition of the acrylate mixture. After these pre-studies, a hydrogel film with spatially modulated cross-link density was fabricated through polymerisation-induced diffusion, by using a patterned photomask. The resulting smooth patterned hydrogel coating swelled in slightly acidic media and the swelling was higher in the regions with lower cross-linking densities, thus yielding a corrugated surface. Upon exposure to visible light, the surface topography flattened again, thus showing that a hydrogel coating could be created, the topography of which could be controlled by light irradiation.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Laboratory of Functional Organic Materials and Devices, Eindhoven University of Technology

Contributors: Stumpel, J. E., Liu, D., Broer, D. J., Schenning, A. P. H. J.

Number of pages: 6

Pages: 10922-10927

Publication date: 2 Jul 2013

Peer-reviewed: Yes

#### Publication information

Journal: Chemistry: A European Journal

Volume: 19

Issue number: 33

ISSN (Print): 0947-6539

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Scopus rating (2013): CiteScore 5.68 SJR 2.643 SNIP 1.239

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: hydrogels, photoresponsive materials, polymerization, spiropyran compounds, surface chemistry

DOIs:

10.1002/chem.201300852

URLs:

<http://www.scopus.com/inward/record.url?scp=84881229562&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

EXT="Stumpel, Jelle"

Source: Scopus

Source ID: 84881229562

Research output: Contribution to journal › Article › Scientific › peer-review

### Development and characterization of poly( $\epsilon$ -caprolactone) hollow fiber membranes for vascular tissue engineering

The fabrication of tissue-engineered scaffolds for small-caliber blood vessels still remains a challenge. In the present work, we prepared poly( $\epsilon$ -caprolactone) (PCL) hollow fiber (HF) membranes, suitable for small-diameter blood vessel regeneration, by a phase separation spinning technique. The difficulty of processing PCL, a highly elastic material prone to suffer die swelling by extrusion, was overcome by tailoring the dope solution temperature and extrusion flow rate during the spinning procedure. The influence of the composition of the coagulation bath (water, ethanol, isopropanol) on the HF membrane physico-chemical properties (morphology, transport and mechanical properties) and cell attachment and proliferation was studied. The HF membranes fabricated using ethanol as coagulation bath had the most uniform morphology, good mechanical and transport properties and showed human adipose stem cell attachment and proliferation. Therefore, these fibers are promising scaffolds for small-caliber blood vessel regeneration.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), University of Cantabria, University of Twente

Contributors: Diban, N., Haimi, S., Bolhuis-Versteeg, L., Teixeira, S., Miettinen, S., Poot, A., Grijpma, D., Stamatialis, D.  
Number of pages: 9  
Pages: 29-37  
Publication date: 1 Jul 2013  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Membrane Science

Volume: 438

ISSN (Print): 0376-7388

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Science(all), Biochemistry, Filtration and Separation

Keywords: Adipose stem cell, Hollow fiber, Phase-inversion, Poly( $\epsilon$ -caprolactone), Vascular regeneration

DOIs:

10.1016/j.memsci.2013.03.024

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<http://www.scopus.com/inward/record.url?scp=84876440642&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84876440642

Research output: Contribution to journal > Article > Scientific > peer-review

#### Shape-dependent plasmonic response and directed self-assembly in a new semiconductor building block, indium-doped cadmium oxide (ICO)

The influence of particle shape on plasmonic response and local electric field strength is well-documented in metallic nanoparticles. Morphologies such as rods, plates, and octahedra are readily synthesized and exhibit drastically different extinction spectra than spherical particles. Despite this fact, the influence of composition and shape on the optical properties of plasmonic semiconductor nanocrystals, in which free electrons result from heavy doping, has not been well-studied. Here, we report the first observation of plasmonic resonance in indium-doped cadmium oxide (ICO) nanocrystals, which exhibit the highest quality factors reported for semiconductor nanocrystals. Furthermore, we are able to independently control the shape and free electron concentration in ICO nanocrystals, allowing for the influence of shape on the optical response of a plasmonic semiconductor to be conclusively demonstrated. The highly uniform particles may be self-assembled into ordered single component and binary nanocrystal superlattices, and in thin films, exhibit negative permittivity in the near infrared (NIR) region, validating their use as a new class of tunable low-loss plasmonic building blocks for 3-D optical metamaterials.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Pennsylvania, Purdue University, Department of Electrical and Systems Engineering

Contributors: Gordon, T. R., Paik, T., Klein, D. R., Naik, G. V., Caglayan, H., Boltasseva, A., Murray, C. B.

Number of pages: 7

Pages: 2857-2863

Publication date: 12 Jun 2013

Peer-reviewed: Yes

#### Publication information

Journal: Nano Letters

Volume: 13

Issue number: 6

ISSN (Print): 1530-6984

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Scopus rating (2013): CiteScore 14.23 SJR 9.081 SNIP 3.355

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Materials Science(all), Condensed Matter Physics, Mechanical Engineering

Keywords: indium-doped cadmium oxide, metamaterials, nanocrystal superlattices, Plasmonics, shape effects, transparent conducting oxide

DOIs:

10.1021/nl4012003

URLs:

<http://www.scopus.com/inward/record.url?scp=84879097164&partnerID=8YFLogxK> (Link to publication in Scopus)



## Bibliographical note

EXT="Caglayan, Humeyra"

Source: Scopus

Source ID: 84879097164

Research output: Contribution to journal › Article › Scientific › peer-review

## Cell toxicity and oxidative potential of engine exhaust particles: Impact of using particulate filter or biodiesel fuel blend

The link between emissions of vehicular particulate matter (PM) and adverse health effects is well established. However, the influence of new emission control technologies and fuel types on both PM emissions and health effects has been less well investigated. We examined the health impact of PM emissions from two vehicles equipped with or without a diesel particulate filter (DPF). Both vehicles were powered either with diesel (B0) or a 50% v/v biodiesel blend (B50). The DPF effectively decreased PM mass emissions (~85%), whereas the fuel B50 without DPF led to less reduction (~50%). The hazard of PM per unit distance driven was decreased for the DPF-equipped vehicle as indicated by a reduced cytotoxicity, oxidative, and pro-inflammatory potential. This was not evident and even led to an increase when the hazard was expressed on a per unit of mass basis. In general, the PM oxidative potential was similar or reduced for the B50 compared to the B0 powered vehicle. However, the use of B50 resulted in increased cytotoxicity and IL-6 release in BEAS-2B cells irrespective of the expression metric. This study shows that PM mass reduction achieved by the use of B50 will not necessarily decrease the hazard of engine emissions, while the application of a DPF has a beneficial effect on both PM mass emission and PM hazard.

## General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), National Institute for Public Health and the Environment, Norwegian Institute of Public Health, Aristotle University of Thessaloniki, Laboratory of Applied Thermodynamics, Utrecht University

Contributors: Gerlofs-Nijland, M. E., Totlandsdal, A. I., Tzamkiozis, T., Leseman, D. L. A. C., Samaras, Z., Låg, M., Schwarze, P., Ntziachristos, L., Cassee, F. R.

Number of pages: 8

Pages: 5931-5938

Publication date: 4 Jun 2013

Peer-reviewed: Yes

## Publication information

Journal: Environmental Science and Technology

Volume: 47

Issue number: 11

ISSN (Print): 0013-936X

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Original language: English

ASJC Scopus subject areas: Chemistry(all), Environmental Chemistry

DOIs:

10.1021/es305330y

URLs:

<http://www.scopus.com/inward/record.url?scp=84878655379&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84878655379

Research output: Contribution to journal › Article › Scientific › peer-review

## Cation-specific effects on enzymatic catalysis driven by interactions at the tunnel mouth

Cationic specificity which follows the Hofmeister series has been established for the catalytic efficiency of haloalkane dehalogenase LinB by a combination of molecular dynamics simulations and enzyme kinetic experiments. Simulations provided a detailed molecular picture of cation interactions with negatively charged residues on the protein surface, particularly at the tunnel mouth leading to the enzyme active site. On the basis of the binding affinities, cations were ordered as  $\text{Na}^+ > \text{K}^+ > \text{Rb}^+ > \text{Cs}^+$ . In agreement with this result, a steady-state kinetic analysis disclosed that the smaller alkali cations influence formation and productivity of enzyme-substrate complexes more efficiently than the larger ones. A subsequent systematic investigation of two LinB mutants with engineered charge in the cation-binding site revealed that the observed cation affinities are enhanced by increasing the number of negatively charged residues at the tunnel mouth, and vice versa, reduced by decreasing this number. However, the cation-specific effects are overwhelmed by strong electrostatic interactions in the former case. Interestingly, the substrate inhibition of the mutant LinB L177D in the presence of chloride salts was 7 times lower than that of LinB wild type in glycine buffer. Our work provides new insight into the mechanisms of specific cation effects on enzyme activity and suggests a potential strategy for suppression of substrate inhibition by the combination of protein and medium engineering.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), International Clinical Research Center, St. Anne's University Hospital Brno, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Department of Experimental Biology, Research Centre for Toxic Compounds in the Environment, Masaryk University

Contributors: Štěpánková, V., Paterová, J., Damborský, J., Jungwirth, P., Chaloupková, R., Heyda, J.

Number of pages: 9

Pages: 6394-6402

Publication date: 30 May 2013

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 117

Issue number: 21

ISSN (Print): 1520-6106

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/jp401506v

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<http://www.scopus.com/inward/record.url?scp=84878363659&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84878363659

Research output: Contribution to journal > Article > Scientific > peer-review

### Surface properties and interaction forces of biopolymer-doped conductive polypyrrole surfaces by atomic force microscopy

Surface properties and electrical charges are critical factors elucidating cell interactions on biomaterial surfaces. The surface potential distribution and the nanoscopic and microscopic surface elasticity of organic polypyrrole-hyaluronic acid (PPy-HA) were studied by atomic force microscopy (AFM) in a fluid environment in order to explain the observed enhancement in the attachment of human adipose stem cells on positively charged PPy-HA films. The electrostatic force between the AFM tip and a charged PPy-HA surface, the tip-sample adhesion force, and elastic moduli were estimated from the AFM force curves, and the data were fitted to electrostatic double-layer and elastic contact models. The surface potential of the charged and dried PPy-HA films was assessed with Kelvin probe force microscopy (KPFM), and the KPFM data were correlated to the fluid AFM data. The surface charge distribution and elasticity were both found to correlate well with the nodular morphology of PPy-HA and to be sensitive to the electrochemical charging conditions. Furthermore, a significant change in the adhesion was detected when the surface was electrochemically charged positive. The results highlight the potential of positively charged PPy-HA as a coating material to enhance the stem cell response in tissue-engineering scaffolds.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), VTT Technical Research Centre of Finland, University of Wollongong

Contributors: Pelto, J. M., Haimi, S. P., Siljander, A. S., Miettinen, S. S., Tappura, K. M., Higgins, M. J., Wallace, G. G.

Number of pages: 10

Pages: 6099-6108

Publication date: 21 May 2013

Peer-reviewed: Yes

### Publication information

Journal: Langmuir

Volume: 29

Issue number: 20

ISSN (Print): 0743-7463

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Scopus rating (2013): CiteScore 4.55 SJR 1.896 SNIP 1.333

Original language: English

ASJC Scopus subject areas: Materials Science(all), Condensed Matter Physics, Surfaces and Interfaces, Spectroscopy, Electrochemistry

DOIs:

10.1021/la4009366

URLs:

<http://www.scopus.com/inward/record.url?scp=84878234949&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84878234949

Research output: Contribution to journal > Article > Scientific > peer-review

### **Depth profiling of PLGA copolymer in a novel biomedical bilayer using confocal raman spectroscopy**

Confocal Raman spectroscopy was undertaken to identify separate layers of PLGA and gentamicin sulfate (GS) coatings on a titanium alloy substrate for a novel drug-delivery system. Additionally, it was found that it was possible to measure the layer thickness and uniformity of the PLGA accurately by detecting intensity and wavelength changes in the vibrational bands of the copolymer bonds. Further analysis of the materials was done using FIB, SEM/EDX, and profilometry; these techniques were used to confirm the findings of the Raman data. It was determined that the substrate was extremely rough and therefore the coating was not uniform in thickness but the materials were uniformly dispersed. Most importantly, two distinct GS and PLGA layers were present.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, University College Cork, DePuy Ireland, Trinity College Dublin, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN)

Contributors: McManamon, C., Delaney, P., Kavanagh, C., Wang, J. J., Rasappa, S., Morris, M. A.

Number of pages: 6

Pages: 5905-5910

Publication date: 14 May 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Langmuir

Volume: 29

Issue number: 19

ISSN (Print): 0743-7463

Ratings:

Scopus rating (2013): CiteScore 4.55 SJR 1.896 SNIP 1.333

Original language: English

ASJC Scopus subject areas: Electrochemistry, Condensed Matter Physics, Surfaces and Interfaces, Materials Science(all), Spectroscopy

DOIs:

10.1021/la400402a

URLs:

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Source: Scopus

Source ID: 84877784340

Research output: Contribution to journal > Article > Scientific > peer-review

### **Screening pretreatment methods to enhance thermophilic anaerobic digestion of pulp and paper mill wastewater treatment secondary sludge**

The effect of hydrothermal (150°C for 10min and 70°C for 40min), enzymatic (Accelerase 1500, 0.07g/g volatile solids (VS)), ultrasound (45kHz for 30min) and chemical pretreatments (HNO<sub>3</sub> at pH3 and NaOH at pH12) alone or in combination on the chemical composition and methane yield of the pulp and paper mill secondary sludge was studied in batch assays at 55°C. In total, 12 different pretreatment combinations were compared. Chemical analyses showed that all pretreatments except for HNO<sub>3</sub> and ultrasound pretreatments improved the organic matter solubilization. Among the studied pretreatments, hydrothermal (150°C, 10min) pretreatment alone or in combination with enzymatic and/or ultrasound pretreatment had the highest impact on sludge solubilization and methane yield. The increase in methane yield was 31% (from 108ml/g VS<sub>original</sub> to 141ml/gVS<sub>original</sub>). In addition, enzymatic pretreatment also improved the methane yields but only when combined with hydrothermal pretreatment at 150°C or ultrasound+hydrothermal pretreatment at 150°C. On the other hand, ultrasound pretreatment did not improve the methane yields while acid and alkaline pretreatments resulted in lower methane yields than control. Improved hydrolysis and higher methane production rates noticed in assays subjected to hydrothermal pretreatment alone or in combination with enzymes and/or ultrasound could make these treatments more attractive in reducing the retention times required during full-scale anaerobic digestion of pulp and paper mill wastewater sludges. © 2013 Elsevier B.V.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Tampere University of Technology, Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), Jyväskylän yliopisto, University of Jyväskylä

Contributors: Bayr, S., Kaparaju, P., Rintala, J.

Number of pages: 8

Pages: 479-486

Publication date: 1 May 2013

Peer-reviewed: Yes

### Publication information

Journal: Chemical Engineering Journal

Volume: 223

ISSN (Print): 1385-8947

Ratings:

Scopus rating (2013): CiteScore 4.59 SJR 1.597 SNIP 1.902

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all), Industrial and Manufacturing Engineering, Environmental Chemistry

Keywords: Anaerobic digestion, Methane yield, Pretreatment, Pulp and paper mill, Secondary sludge

DOIs:

10.1016/j.cej.2013.02.119

URLs:

<http://www.scopus.com/inward/record.url?scp=84876300888&partnerID=8YFLogxK> (Link to publication in Scopus)

### Bibliographical note

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Source: researchoutputwizard

Source ID: 1974

Research output: Contribution to journal > Article > Scientific > peer-review

### Immobilized bioactive agents onto polyurethane surface with heparin and phosphorylcholine group

Heparin (HEP) and phosphorylcholine groups (PC) were grafted onto the polyurethane (PU) surface in order to improve biocompatibility and anticoagulant activity. After the surface grafting sites of PU were amplified with the primary amine groups of polyethylenimine (PEI), heparin was covalently linked onto the surface by the reaction between the amino group and the carboxyl group. PC groups were covalently immobilized on the PU-PEI surface through the reaction between the amino group and the aldehyde group of phosphorylcholine glyceraldehyde (PCGA). The surface density of primary amine groups was determined by a ninhydrin assay. The amino group density reached a maximum of 0.88  $\mu\text{mol}/\text{cm}^2$  upon incorporation of 10 wt% PEI. The amount of heparin covalently immobilized on the PU-PEI surface was determined by the toluidine blue method. The grafting chemistry resulted in the comparatively dense immobilization of HEP (2.6  $\mu\text{g}/\text{cm}^2$ ) and PC to the PU-PEI surfaces. The HEP and PC modified surfaces were characterized by water uptake (PU 0.15  $\text{mg}/\text{cm}^2$ , PU-PEI 3.54  $\text{mg}/\text{cm}^2$ , PU-HEP 2.04  $\text{mg}/\text{cm}^2$ , PU-PC 2.38  $\text{mg}/\text{cm}^2$ ), water contact angle (PU 95.3, PU-PEI 34.0, PU-HEP 39.5, PU-PC 37.2), attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and scanning electron microscope (SEM). The results demonstrated that the PUPEI surface was successfully grafted with HEP and PC. The hydrophilicity and hemocompatibility of these grafted surfaces were significantly improved. These results suggested that the PU-HEP and PU-PC composite films are promising candidates for blood contacting tissue engineering.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Tianjin University, Shihezi University, School of Chemical Engineering and Technology, Tianjin Chest Hospital

Contributors: Tan, M., Feng, Y., Wang, H., Zhang, L., Khan, M., Guo, J., Chen, Q., Liu, J.

Number of pages: 9

Pages: 541-549

Publication date: May 2013

Peer-reviewed: Yes

### Publication information

Journal: Macromolecular Research

Volume: 21

Issue number: 5

ISSN (Print): 1598-5032

Ratings:

Scopus rating (2013): CiteScore 1.66 SJR 0.553 SNIP 0.769

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Chemical Engineering(all)  
Keywords: hemocompatibility, heparin, phosphorylcholine group, polyethylenimine, polyurethane

DOIs:

10.1007/s13233-013-1028-3

URLs:

<http://www.scopus.com/inward/record.url?scp=84877763417&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84877763417

Research output: Contribution to journal > Article > Scientific > peer-review

### Nanoindentation study of light-induced softening of supramolecular and covalently functionalized azo polymers

Nanoindentation studies on thin films of the widely used azo polymer pDR1A and a supramolecular polymer-azobenzene complex p4VP(DY7)<sub>0.5</sub> demonstrate significant light-induced softening upon visible-light irradiation due to trans-cis-trans photoisomerization of the azobenzene units. More specifically, the strain-rate sensitivities of pDR1A and p4VP(DY7)<sub>0.5</sub> upon 532 nm irradiation increase by 80% and 120%, respectively. These results imply a photosoftering contribution to the mechanisms of light-induced surface patterning of azo polymers and the photomechanical effect. The finding that under the experimental conditions used photosoftering is more significant in the supramolecular complex than in the covalently functionalized polymer highlights the potential of noncovalent functionalization strategies in designing materials with efficient photomechanical response, and nanoindentation provides a powerful technique to quantify the connection between the photoinduced changes in mechanical properties and photoinduced macroscopic movement of azo polymer films.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Applied Physics, Aalto University, McGill University

Contributors: Vapaavuori, J., Mahimwalla, Z., Chromik, R. R., Kaivola, M., Priimagi, A., Barrett, C. J.

Number of pages: 5

Pages: 2806-2810

Publication date: 28 Apr 2013

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Materials Chemistry C

Volume: 1

Issue number: 16

ISSN (Print): 2050-7534

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Chemistry

DOIs:

10.1039/c3tc30246f

URLs:

<http://www.scopus.com/inward/record.url?scp=84879524974&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84879524974

Research output: Contribution to journal > Article > Scientific > peer-review

### Understanding the reinforcing behavior of expanded clay particles in natural rubber compounds

We report the unusual mechanical percolation behavior of expanded clay nanoparticles in a natural rubber (NR) matrix. This phenomenon is discussed in terms of fractal dimensions of the nanoparticle cluster. Highly exfoliated structures of nanoparticles in NR are obtained by a process we call the 'propping-open approach'. The impact of filler dispersion and rubber-filler interactions on the viscoelastic behavior of NR-clay nanocomposites is systematically investigated. We observe non-linear viscoelastic behavior (Payne effect) at very low nanoparticle concentrations which we attribute to the formation of a network-like structure of the exfoliated clay particles. We rely on the Kraus and Maier-Göritz models to interpret such nonlinear viscoelastic behavior. We find that the chain mobility of the NR is greatly reduced based on the viscoelastic master curves. The value of the mechanical percolation threshold ( $\phi_p$ ) and the fractal nature of nanoparticle clusters are determined through an analysis of the experimental data based on a theory put forward by Huber and Vilgis. The nature of rubber-filler interactions is further understood from swelling experiments utilizing the Kraus and Cunneen-Russell equations.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V.  
Contributors: Rooj, S., Das, A., Stöckelhuber, K. W., Wang, D. Y., Galiatsatos, V., Heinrich, G.  
Number of pages: 11  
Pages: 3798-3808  
Publication date: 14 Apr 2013  
Peer-reviewed: Yes

#### Publication information

Journal: Soft Matter  
Volume: 9  
Issue number: 14  
ISSN (Print): 1744-683X  
Ratings:  
Scopus rating (2013): CiteScore 4.2 SJR 1.748 SNIP 1.193  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics  
DOIs:  
10.1039/c3sm27519a  
URLs:  
<http://www.scopus.com/inward/record.url?scp=84875027182&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 84875027182  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Biomimetic zinc chlorin-poly(4-vinylpyridine) assemblies: Doping level dependent emission-absorption regimes

To develop biomimetic dye-polymers for photonics, two different types of Zn chlorin-poly(4-vinylpyridine) (P4VP) assemblies were prepared by varying Zn pyro-pheophorbide a methylester (ZnPPME) and Zn 3<sup>1</sup>-OH-pyro- pheophorbide a methylester (Zn-3<sup>1</sup>-OH-PPME) doping levels. <sup>1</sup>H NMR spectroscopy and diffusion ordered NMR spectroscopy (DOSY) studies revealed that a coordinative interaction between Zn chlorin and P4VP was predominant in solution (d<sub>5</sub>-nitrobenzene). Small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM) characterization of bulk samples of polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) doped with variable amounts of Zn chlorin showed that the pigment doping transformed the native cylindrical block copolymer nanostructures to lamellar morphologies. The result indicates that the pyridine moiety-Zn chlorin coordination is stronger than the aggregation tendency between the pigment molecules even in the solid state. UV-Vis absorption spectroscopy studies of a Zn chlorin-P4VP thin film showed characteristic monomeric chlorin spectra, while steady-state fluorescence spectroscopy displayed quenching of fluorescence and time-resolved studies indicated shortening of fluorescence lifetimes with an increasing chlorin doping level. Notably, time-resolved fluorescence spectroscopy revealed that the lifetime decay changed from monoexponential to biexponential above 0.5 wt% (ca. 0.001 equiv.) loadings. The Förster analysis implies that excitonic chlorin-chlorin interactions are observed in the thin films when the distance between the pigment molecules is approximately 50 Å. The Zn chlorin-P4VP solid films emit strongly up to 1 wt% (ca. 0.002 equiv.) doping level above which the chlorin-chlorin interactions start to linearly dominate with an increase of doping level, while with 10 wt% (ca. 0.02 equiv.) loading less than 10% of fluorescence remains. Doping levels up to 300 wt% (0.5 equiv.) can be used in absorbing materials without the formation of chlorin aggregates. These defined optical response regions pave the way for photonic materials based on biopigment assemblies.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Frontier Photonics, Aalto University, University of Helsinki, Department of Applied Physics  
Contributors: Pale, V., Nikkonen, T., Vapaavuori, J., Kostianen, M., Kavakka, J., Selin, J., Tittonen, I., Helaja, J.  
Number of pages: 8  
Pages: 2166-2173  
Publication date: 21 Mar 2013  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Materials Chemistry C  
Volume: 1  
Issue number: 11  
ISSN (Print): 2050-7534  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Materials Chemistry  
DOIs:  
10.1039/c3tc00499f

URLs:

<http://www.scopus.com/inward/record.url?scp=84875847322&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84875847322

Research output: Contribution to journal > Article > Scientific > peer-review

### Site-specific analysis of dipole polarizabilities of heterogeneous systems: Iron-doped $\text{Si}_n$ ( $n = 1-14$ ) clusters

Following the recent work of decomposing the total dipole moment and polarizability of a homogeneous system into site-specific contributions, we extend the study to the heterogeneous systems of iron-doped  $\text{Si}_n$  ( $n = 1-14$ ) clusters by introducing a weighting function. The structure-/shape- and size-specific aspects of the dipole moments and polarizabilities of  $\text{Si}_n\text{Fe}$  ( $n = 1-14$ ) clusters are analyzed and compared with pure silicon clusters. It is shown that the polarizabilities associated with the individual constituent atoms vary considerably with the structure/shape of the cluster and the location of the atom or site within a given structure. For atoms at peripheral sites, the polarizabilities are substantially larger than atoms at the interior sites, and the more peripheral an atom is, the larger is its polarizability. The polarizability of the Fe atom in  $\text{Si}_n\text{Fe}$  clusters decreases as the cluster size increases. This is related to the position of Fe atom in  $\text{Si}_n\text{Fe}$  clusters and indicates significant screening of the interior of the cluster by its surface. The correlation between the anisotropy of the total polarizability and the anisotropy of the cluster shape is also analyzed. Comparing with pure  $\text{Si}_n$  clusters, the polarizabilities of Si atoms are increased after Fe atom doping. The structures are more compact for  $\text{Si}_n\text{Fe}$  than the same sizes of  $\text{Si}_{n+1}$  clusters and the polarizabilities of  $\text{Si}_n\text{Fe}$  are smaller than  $\text{Si}_{n+1}$  for the sizes of  $n = 7-14$ .

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Northwest University China, National Laboratory of Solid State Microstructures, Nanjing University, Institute of Photonics and Photo-technology

Contributors: Ma, L., Wang, J., Wang, G.

Publication date: 7 Mar 2013

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chemical Physics

Volume: 138

Issue number: 9

Article number: 094304

ISSN (Print): 0021-9606

Ratings:

Scopus rating (2013): CiteScore 2.95 SJR 1.559 SNIP 1.182

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1063/1.4793276

URLs:

<http://www.scopus.com/inward/record.url?scp=84874852980&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84874852980

Research output: Contribution to journal > Article > Scientific > peer-review

### Molecularly functionalized silicon substrates for orientation control of the microphase separation of PS-b-PMMA and PS-b-PDMS block copolymer systems

The use of block copolymer (BCP) thin films to generate nanostructured surfaces for device and other applications requires precise control of interfacial energies to achieve the desired domain orientation. Usually, the surface chemistry is engineered through the use of homo- or random copolymer brushes grown or attached to the surface. Herein, we demonstrate a facile, rapid, and tunable approach to surface functionalization using a molecular approach based on ethylene glycol attachment to the surface. The effectiveness of the molecular approach is demonstrated for the microphase separation of PS-b-PMMA and PS-b-PDMS BCPs in thin films and the development of nanoscale features at the substrate.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Tyndall National Institute at National University of Ireland, Cork, Selcuk University, Materials Chemistry and Analysis Group, University College Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Collinstown Industrial Estate

Contributors: Borah, D., Ozmen, M., Rasappa, S., Shaw, M. T., Holmes, J. D., Morris, M. A.

Number of pages: 12  
Pages: 2809-2820  
Publication date: 5 Mar 2013  
Peer-reviewed: Yes

#### Publication information

Journal: Langmuir  
Volume: 29  
Issue number: 9  
ISSN (Print): 0743-7463  
Ratings:

Scopus rating (2013): CiteScore 4.55 SJR 1.896 SNIP 1.333

Original language: English

ASJC Scopus subject areas: Electrochemistry, Condensed Matter Physics, Surfaces and Interfaces, Materials Science(all), Spectroscopy

DOIs:

10.1021/la304140q

URLs:

<http://www.scopus.com/inward/record.url?scp=84874584704&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84874584704

Research output: Contribution to journal > Article > Scientific > peer-review

#### Optical vortex generation in nematic liquid crystal light valves

A nematic liquid crystal light valve (LCLV) is made by using a photosensitive material as one of the cell-confining walls. The liquid crystals (LCs) are homeotropically aligned and with a negative anisotropy; therefore, they naturally produce topological defects when they reorient under the application of an electric field. In our work, we show that by sending circularly polarized light beams onto the photosensitive wall of the light valve, it is possible to locally induce the reorientation and to generate vortex-like defects that remain, each stable and trapped at the chosen location. We demonstrate the ability of the system to create optical vortices with opposite topological charge that, consistently with angular momentum conservation, both derive from the same defect created in the LC texture. The efficiency of the spin-to-orbital angular momentum conversion is measured as a function of the system control parameters, namely the low-frequency electric field applied to the light valve and the intensity of the optical beam inducing the matter defect.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, CNRS, NooEL (Nonlinear Optics and OptoElectronics Laboratory), University "Roma Tre"

Contributors: Barboza, R., Bortolozzo, U., Assanto, G., Residori, S.

Number of pages: 7

Pages: 24-30

Publication date: 1 Mar 2013

Peer-reviewed: Yes

#### Publication information

Journal: Molecular Crystals and Liquid Crystals

Volume: 572

Issue number: 1

ISSN (Print): 1542-1406

Ratings:

Scopus rating (2013): CiteScore 0.52 SJR 0.279 SNIP 0.38

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Science(all)

Keywords: Liquid crystal light valves, optical vortices, spin-to-orbital angular momentum conversion, topological defects

DOIs:

10.1080/15421406.2012.763206

URLs:

<http://www.scopus.com/inward/record.url?scp=84876183883&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84876183883

Research output: Contribution to journal > Article > Scientific > peer-review



### **Fabrication of a sub-10 nm silicon nanowire based ethanol sensor using block copolymer lithography**

This paper details the fabrication of ultrathin silicon nanowires (SiNWs) on a silicon-on-insulator (SOI) substrate as an electrode for the electro-oxidation and sensing of ethanol. The nanowire surfaces were prepared by a block copolymer (BCP) nanolithographic technique using low molecular weight symmetric poly(styrene)-block-poly(methyl methacrylate) (PS-*b*-PMMA) to create a nanopattern which was transferred to the substrate using plasma etching. The BCP orientation was controlled using a hydroxyl-terminated random polymer brush of poly(styrene)-random-poly(methyl methacrylate) (HO-PS-*r*-PMMA). TEM cross-sections of the resultant SiNWs indicate an anisotropic etch process with nanowires of sub-10 nm feature size. The SiNWs obtained by etching show high crystallinity and there is no evidence of defect inclusion or amorphous region production as a result of the pattern transfer process. The high density of SiNWs at the substrate surface allowed the fabrication of a sensor for cyclic voltammetric detection of ethanol. The sensor shows better sensitivity to ethanol and a faster response time compared to widely used polymer nanocomposite based sensors.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Materials Chemistry and Analysis Group, University College Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Tyndall National Institute at National University of Ireland, Cork, Collinstown Industrial Estate

Contributors: Rasappa, S., Borah, D., Faulkner, C. C., Lutz, T., Shaw, M. T., Holmes, J. D., Morris, M. A.

Publication date: 15 Feb 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Nanotechnology

Volume: 24

Issue number: 6

Article number: 065503

ISSN (Print): 0957-4484

Ratings:

Scopus rating (2013): CiteScore 2.74 SJR 1.602 SNIP 1.27

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Electrical and Electronic Engineering, Mechanical Engineering, Mechanics of Materials, Materials Science(all)

DOIs:

10.1088/0957-4484/24/6/065503

URLs:

<http://www.scopus.com/inward/record.url?scp=84872971946&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84872971946

Research output: Contribution to journal > Article > Scientific > peer-review

### **Aqueous guanidinium-carbonate interactions by molecular dynamics and neutron scattering: Relevance to ion-protein interactions**

Guanidinium carbonate was used in this study as a simple proxy for the biologically relevant arginine-carbonate interactions in water. Molecular dynamics (MD) simulations of guanidinium carbonate were performed with nonpolarizable water using two implementations of the ion force fields. In the first, the ions had full charges, while in the second, the ions had reduced charges in order to effectively account for electronic polarization effects of water. The results from the simulations were then compared to data from previous neutron scattering experiments. It was found that there were significant discrepancies between the full charge force field MD simulations and the experimental results due to excessive ion pairing and clustering in the former. In contrast, reducing the ionic charges yields a more regular solution with a simulated structure, which fits well the experimental data.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Division of Organic Chemistry and Biochemistry, Bijenička Cesta 54

Contributors: Vazdar, M., Jungwirth, P., Mason, P. E.

Number of pages: 5

Pages: 1844-1848

Publication date: 14 Feb 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry Part B

Volume: 117  
Issue number: 6  
ISSN (Print): 1520-6106  
Ratings:

Scopus rating (2013): CiteScore 3.53 SJR 1.504 SNIP 1.194

Original language: English

ASJC Scopus subject areas: Surfaces, Coatings and Films, Physical and Theoretical Chemistry, Materials Chemistry  
DOIs:

10.1021/jp310719g

URLs:

<http://www.scopus.com/inward/record.url?scp=84873899176&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84873899176

Research output: Contribution to journal > Article > Scientific > peer-review

### **Chemically tailored dielectric-to-metal transition for the design of metamaterials from nanoimprinted colloidal nanocrystals**

We demonstrate optical metamaterial design using colloidal gold nanocrystal building blocks. In the solid state, chemically exchanging the nanocrystals' surface-capping molecules provides a tailorable dielectric-to-metal transition exhibiting a  $10^{10}$  range in DC conductivity and dielectric permittivity ranging from everywhere positive to everywhere negative throughout the visible-to-near-IR. Direct, wide-area nanoimprinting of subwavelength superstructures at room temperature, on plastic and glass substrates, affords plasmonic resonances ranging from 660 to 1070 nm, in agreement with numerical simulations.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Pennsylvania, Department of Electrical and Systems Engineering

Contributors: Fafarman, A. T., Hong, S. H., Caglayan, H., Ye, X., Diroll, B. T., Paik, T., Engheta, N., Murray, C. B., Kagan, C. R.

Number of pages: 8

Pages: 350-357

Publication date: 13 Feb 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Nano Letters

Volume: 13

Issue number: 2

ISSN (Print): 1530-6984

Ratings:

Scopus rating (2013): CiteScore 14.23 SJR 9.081 SNIP 3.355

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Materials Science(all), Condensed Matter Physics, Mechanical Engineering

Keywords: ammonium thiocyanate, dielectric function, gold nanoparticles, ligand exchange, Plasmonics, soft lithography

DOIs:

10.1021/nl303161d

URLs:

<http://www.scopus.com/inward/record.url?scp=84873680258&partnerID=8YFLogxK> (Link to publication in Scopus)

#### **Bibliographical note**

EXT="Caglayan, Humeyra"

Source: Scopus

Source ID: 84873680258

Research output: Contribution to journal > Article > Scientific > peer-review

### **Growth behavior and magnetic properties of spherical uranium oxide nanoclusters**

The growth behavior and magnetic properties of spherical uranium oxide nanoclusters have been investigated using the generalized gradient approximation (GGA) to density functional theory (DFT). The geometries of  $U_nO_m$  clusters remain the  $O_h$  symmetry after DFT relaxation. The largest binding energy corresponds to the cluster with the smallest deviation from the bulk ( $UO_2$ ) ratio. The electronic structures and magnetic properties of these nanoclusters are presented. We find the chemical bonding between the U and O atoms has a significant ionic character. The reduction of magnetism in the inner positions can be understood by the charge transfer and the hybridization between U atoms and the neighboring O atoms.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Computational Science X (CompX), University of Texas at Arlington  
Contributors: Ma, L., Ray, A. K.  
Number of pages: 7  
Pages: 334-340  
Publication date: Feb 2013  
Peer-reviewed: Yes

### Publication information

Journal: Journal of Computational and Theoretical Nanoscience  
Volume: 10  
Issue number: 2  
ISSN (Print): 1546-1955  
Ratings:  
Scopus rating (2013): CiteScore 0.96 SJR 0.384 SNIP 0.593  
Original language: English  
ASJC Scopus subject areas: Condensed Matter Physics, Electrical and Electronic Engineering, Materials Science(all), Computational Mathematics, Chemistry(all)  
Keywords: Growth behavior, Magnetism, Nanoclusters, Uranium oxide  
DOIs:  
10.1166/jctn.2013.2701  
URLs:  
<http://www.scopus.com/inward/record.url?scp=84876525693&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 84876525693  
Research output: Contribution to journal > Article > Scientific > peer-review

### Density functional theory study of FePd<sub>n</sub> (n = 2-14) clusters and interactions with small molecules

First-principles calculations have been conducted to investigate the properties of FePd<sub>n</sub> (n = 2-14) clusters. In the lowest energy structures of FePd<sub>n</sub> clusters, the Fe atom gradually moves from the convex to the surface, and then to the interior site with the number of Pd atoms increasing from 2 to 14. The magnetic moments of Pd<sub>n</sub> clusters have been enhanced by the doping of Fe impurity. Furthermore, the adsorption of small molecules, including NH<sub>3</sub>, H<sub>2</sub>O, CO, H<sub>2</sub>, and O<sub>2</sub>, on the higher stability of FePd<sub>n</sub> (n = 5, 7, 10, and 12) clusters were studied. The lowest energy adsorption structures are obtained for each molecule. On the whole, the adsorption energies vary as the order of E<sub>a</sub>(H<sub>2</sub>O) < E<sub>a</sub>(H<sub>2</sub>) < E<sub>a</sub>(NH<sub>3</sub>) < E<sub>a</sub>(O<sub>2</sub>) < E<sub>a</sub>(CO). NH<sub>3</sub>, CO and H<sub>2</sub> molecules prefer to adsorb on the FePd<sub>10</sub> cluster with the highest adsorption energy, while H<sub>2</sub>O and O<sub>2</sub> are more like to adsorb on the FePd<sub>5</sub>. The magnetic moments of FePd<sub>n</sub> clusters are reduced with the adsorption of molecules.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Computational Science X (CompX), Northwest University China, National Laboratory of Solid State Microstructures, Nanjing University, Institute of Photonics and Photo-technology  
Contributors: Ma, L., Wang, J., Hao, Y., Wang, G.  
Number of pages: 8  
Pages: 166-173  
Publication date: Feb 2013  
Peer-reviewed: Yes

### Publication information

Journal: Computational Materials Science  
Volume: 68  
ISSN (Print): 0927-0256  
Ratings:  
Scopus rating (2013): CiteScore 2.15 SJR 0.951 SNIP 1.306  
Original language: English  
ASJC Scopus subject areas: Computer Science(all), Chemistry(all), Materials Science(all), Mechanics of Materials, Physics and Astronomy(all), Computational Mathematics  
Keywords: Cluster, Density functional theory, Small molecule adsorption  
DOIs:  
10.1016/j.commatsci.2012.10.014  
URLs:

<http://www.scopus.com/inward/record.url?scp=84869874680&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84869874680

Research output: Contribution to journal > Article > Scientific > peer-review

### Networking of ionic liquid modified CNTs in SSBR

Carbon nanotubes (CNTs) were modified using an ionic liquid (IL) and were admixed with a non-polar solution styrene butadiene rubber (SSBR). A local re-agglomeration of ionic liquid modified CNTs (m-CNTs) was found to occur in the SSBR composites, which was confirmed from transmission electron micrographs, as IL cannot couple CNTs and elastomer in order to maintain the disentangled state of the tubes. The conducting networks were established as a consequence of agglomerate-tube percolation and the maximum electrical conductivity of the investigated samples was found to be ~0.01 S/cm. The reinforcing effect of m-CNTs was not profound in the composites due to the plasticizing nature of IL in non-polar SSBR.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V.

Contributors: Subramaniam, K., Das, A., Simon, F., Heinrich, G.

Number of pages: 8

Pages: 345-352

Publication date: Feb 2013

Peer-reviewed: Yes

#### Publication information

Journal: European Polymer Journal

Volume: 49

Issue number: 2

ISSN (Print): 0014-3057

Ratings:

Scopus rating (2013): CiteScore 3.43 SJR 1.087 SNIP 1.66

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Organic Chemistry, Polymers and Plastics

Keywords: Carbon nanotubes, Electrical properties, Ionic liquids, Mechanical properties, Nanocomposites

DOIs:

10.1016/j.eurpolymj.2012.10.023

URLs:

<http://www.scopus.com/inward/record.url?scp=84873192692&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84873192692

Research output: Contribution to journal > Article > Scientific > peer-review

### A potential nonthrombogenic small-diameter vascular scaffold with polyurethane/poly(ethylene glycol) hybrid materials by electrospinning technique

A small-diameter vascular graft (inner diameter 4 mm) was fabricated from polyurethane (PU) and poly(ethylene glycol) (PEG) solutions by electrospinning technology. The fiber diameter decreased from 1023±185 nm to 394±106 nm with increasing weight ratio of PEG in electrospinning solutions. The PU/PEG scaffolds showed randomly nanofibrous morphology and well-interconnected porous structure. The hydrophilicity of these scaffolds was improved significantly with increasing weight ratio of PEG. The mechanical properties of electrospun PU/PEG scaffolds were obviously different from that of pure PU scaffold, which was caused by plasticizing or hardening effect imparted by PEG composition. Under hydrated state, the PU/PEG scaffolds demonstrated low mechanical performance due to the hydrophilic property of materials. Compared with dry PU/PEG scaffolds with the same weight ratio of PEG, the tensile strength and elastic modulus of hydrated PU/PEG scaffolds decreased significantly, while the elongation at break increased. The results demonstrated that the electrospun PU/PEG hybrid tubular scaffolds are potential candidates for artificial blood vessels.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Tianjin University, School of Chemical Engineering and Technology

Contributors: Wang, H., Feng, Y., Zhao, H., Fang, Z., Khan, M., Guo, J.

Number of pages: 5

Pages: 1578-1582

Publication date: Feb 2013

Peer-reviewed: Yes

### Publication information

Journal: Journal Nanoscience and Nanotechnology

Volume: 13

Issue number: 2

ISSN (Print): 1533-4880

Ratings:

Scopus rating (2013): CiteScore 1.26 SJR 0.339 SNIP 0.545

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Chemistry(all), Materials Science(all), Bioengineering, Biomedical Engineering

Keywords: Electrospinning, Nanofiber, Poly(ethylene glycol), Polyurethane, Vascular scaffold

DOIs:

10.1166/jnn.2013.6051

URLs:

<http://www.scopus.com/inward/record.url?scp=84876246258&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84876246258

Research output: Contribution to journal > Article > Scientific > peer-review

### A 'clusters-in-liquid' method for calculating infrared spectra identifies the proton-transfer mode in acidic aqueous solutions

In liquid water the transfer of an excess proton between two water molecules occurs through the Zundel cation,  $H_2O \cdots H + \cdots OH_2$ . The proton-transfer mode is the asymmetric stretch of the central  $O \cdots H + \cdots O$  moiety, but there is no consensus on its identification in the infrared spectra of acidic aqueous solutions. Also, in experiments with protonated gas-phase water clusters, its position shifts with cluster size, which makes its relationship with solution spectra unclear. Here we introduce a 'clusters-in-liquid' approach for calculating the infrared spectrum from any set of charges, even single protons. We apply this procedure to multistate empirical valence-bond trajectories of protonated liquid water and to ab initio molecular dynamics of the protonated water dimer and hexamer in the gas phase. The calculated proton-transfer mode is manifested in both systems as a peak near  $1,740\text{ cm}^{-1}$ , in quantitative agreement with a band of similar frequency in the experimental infrared spectrum of protonated water clusters.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Tallinn Technical University, Institute of Chemistry, Hebrew University of Jerusalem

Contributors: Kulig, W., Agmon, N.

Number of pages: 7

Pages: 29-35

Publication date: Jan 2013

Peer-reviewed: Yes

### Publication information

Journal: Nature Chemistry

Volume: 5

Issue number: 1

ISSN (Print): 1755-4330

Ratings:

Scopus rating (2013): CiteScore 12.35 SJR 8.691 SNIP 3.666

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

DOIs:

10.1038/nchem.1503

URLs:

<http://www.scopus.com/inward/record.url?scp=84871565081&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84871565081

Research output: Contribution to journal > Article > Scientific > peer-review

### Molecular mechanism of T-cell protein tyrosine phosphatase (TCPTP) activation by mitoxantrone

T-cell protein tyrosine phosphatase (TCPTP) is a ubiquitously expressed non-receptor protein tyrosine phosphatase. It is involved in the negative regulation of many cellular signaling pathways. Thus, activation of TCPTP could have important

therapeutic applications in diseases such as cancer and inflammation. We have previously shown that the  $\alpha$ -cytoplasmic tail of integrin  $\alpha_1\beta_1$  directly binds and activates TCPTP. In addition, we have identified in a large-scale high-throughput screen six small molecules that activate TCPTP. These small molecule activators include mitoxantrone and spermidine. In this study, we have investigated the molecular mechanism behind agonist-induced TCPTP activation. By combining several molecular modeling and biochemical techniques, we demonstrate that  $\alpha_1$ -peptide and mitoxantrone activate TCPTP via direct binding to the catalytic domain, whereas spermidine does not interact with the catalytic domain of TCPTP in vitro. Furthermore, we have identified a hydrophobic groove surrounded by negatively charged residues on the surface of TCPTP as a putative binding site for the  $\alpha_1$ -peptide and mitoxantrone. Importantly, these data have allowed us to identify a new molecule that binds to TCPTP, but interestingly cannot activate its phosphatase activity. Accordingly, we describe here mechanism of TCPTP activation by mitoxantrone, the cytoplasmic tail of  $\alpha_1$ -integrin, and a mitoxantrone-like molecule at the atomic level. These data provide invaluable insight into the development of novel TCPTP activators, and may facilitate the rational discovery of small-molecule cancer therapeutics.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Jyväskylän yliopisto, Turku Centre for Biotechnology, Turun Yliopisto/Turun Biomateriaalikeskus, School of Management (JKK)

Contributors: Ylilauri, M., Mattila, E., Nurminen, E. M., Käpylä, J., Niinivehmas, S. P., Määttä, J. A., Pentikäinen, U., Ivaska, J., Pentikäinen, O. T.

Number of pages: 10

Pages: 1988-1997

Publication date: 2013

Peer-reviewed: Yes

### Publication information

Journal: Biochimica et biophysica acta: proteins and proteomics

Volume: 1834

Issue number: 10

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Scopus rating (2013): CiteScore 3.71 SJR 1.854 SNIP 1.152

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Biophysics, Biochemistry, Molecular Biology

Keywords: Differential scanning fluorimetry, Integrin, Isothermal titration calorimetry, Mitoxantrone, Molecular dynamics simulation, T-cell protein tyrosine phosphatase

DOIs:

10.1016/j.bbapap.2013.07.001

URLs:

<http://www.scopus.com/inward/record.url?scp=84884495216&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84884495216

Research output: Contribution to journal › Article › Scientific › peer-review

### New reports on anti-bacterial and anti-candidal activities of fatty acid methyl esters (FAME) obtained from *Scenedesmus bijugatus* var. *bicellularis* biomass

The present study evaluates the efficiency of fatty acid methyl esters (FAMEs) obtained from microalgal (*Scenedesmus bijugatus* var. *bicellularis*) biomass as an antimicrobial agent against *Staphylococcus aureus*, *Escherichia coli* and *Candida albicans*. The FAME profiles were determined through Gas Chromatography (GC) with a Flame Ionization detector (FID). The FAMEs showed inhibitory activity against all three microorganisms and thereby exhibited both anti-bacterial and anti-candidal activity. GC-FID analysis reveals about 30 different FAMEs. Out of these, various pharmacologically active FAMEs like stearic acid methyl ester (C18:0) (0.6% w/w), oleic acid methyl ester (C18:1) (1% w/w), linoleic acid methyl ester (C18:2) (1.40% w/w), linolenic acid methyl ester (C18:3) (6.26%), eicosapentanoic acid methyl ester (C20:5) (1.13% w/w), erucic acid methyl ester (C22:1) (1.03% w/w) and docosahexenoic acid methyl ester (C22:6) (2.27% w/w) were detected, which accounted for the bioactivity. These results clearly indicate that the FAMEs of *S. bijugatus* var. *bicellularis* have strong antimicrobial properties and could thus be used as an effective source against microbial diseases.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), Bharathidasan University, King Saud University College of Science

Contributors: Mubarakali, D., Praveenkumar, R., Shenbagavalli, T., Mari Nivetha, T., Parveez Ahamed, A., Al-Dhabi, N. A., Thajuddin, N.

Number of pages: 5

Pages: 11552-11556

Publication date: 28 Nov 2012

Peer-reviewed: Yes

### Publication information

Journal: RSC Advances

Volume: 2

Issue number: 30

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2012): CiteScore 2.4 SJR 0.872 SNIP 0.619

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all)

DOIs:

10.1039/c2ra21130k

Source: Scopus

Source ID: 84868128339

Research output: Contribution to journal > Article > Scientific > peer-review

### Semiclassical hybrid approach to condensed phase molecular dynamics: Application to the $I_2Kr_{17}$ cluster

We study the vibrational decoherence dynamics of an iodine molecule in a finite krypton cluster comprising the first solvation shell. A normal mode analysis allows us to successively increase the complexity of the description. For the ground state dynamics, comparison with experimental matrix results shows that already four degrees of freedom are sufficient to capture the main decoherence mechanism. For electronically excited iodine, we model the vibrational dynamics of initial Schrödinger cat-like states by the semiclassical hybrid dynamics [ Grossmann, F.J. Chem. Phys. 2006, 125, 014111 ] and full quantum calculations, where available. Good agreement of the results is found for a reduced model with three degrees of freedom. We find non-Gaussian distortions of the bath density matrix, which is a necessary condition, if Schrödinger catlike states in the bath are to be identified. However, in contrast to the experiment [ Segale, D.; et al. J. Chem. Phys. 2005, 122, 111104 ], we observe only incoherent superpositions of bath vibrational states.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Vodafone Department of Mobile Communications Systems, Freie Universität Berlin, Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Buchholz, M., Goletz, C. M., Grossmann, F., Schmidt, B., Heyda, J., Jungwirth, P.

Number of pages: 12

Pages: 11199-11210

Publication date: 26 Nov 2012

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physical Chemistry A

Volume: 116

Issue number: 46

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.119

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1021/jp305084f

URLs:

<http://www.scopus.com/inward/record.url?scp=84870038667&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84870038667

Research output: Contribution to journal > Article > Scientific > peer-review

### Peptide salt bridge stability: From gas phase via microhydration to bulk water simulations

The salt bridge formation and stability in the terminated lysine-glutamate dipeptide is investigated in water clusters of increasing size up to the limit of bulk water. Proton transfer dynamics between the acidic and basic side chains is described by DFT-based Born-Oppenheimer molecular dynamics simulations. While the desolvated peptide prefers to be in its neutral state, already the addition of a single water molecule can trigger proton transfer from the glutamate side chain to the lysine side chain, leading to a zwitterionic salt bridge state. Upon adding more water molecules we find that stabilization of the zwitterionic state critically depends on the number of hydrogen bonds between side chain termini, the

water molecules, and the peptidic backbone. Employing classical molecular dynamics simulations for larger clusters, we observed that the salt bridge is weakened upon additional hydration. Consequently, long-lived solvent shared ion pairs are observed for about 30 water molecules while solvent separated ion pairs are found when at least 40 or more water molecules hydrate the dipeptide. These results have implications for the formation and stability of salt bridges at partially dehydrated surfaces of aqueous proteins.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Freie Universität Berlin

Contributors: Pluhaová, E., Marsalek, O., Schmidt, B., Jungwirth, P.

Publication date: 14 Nov 2012

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chemical Physics

Volume: 137

Issue number: 18

Article number: 185101

ISSN (Print): 0021-9606

Ratings:

Scopus rating (2012): CiteScore 2.86 SJR 1.832 SNIP 1.16

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry, Medicine(all)

DOIs:

10.1063/1.4765052

URLs:

<http://www.scopus.com/inward/record.url?scp=84876463177&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84876463177

Research output: Contribution to journal > Article > Scientific > peer-review

#### Search for global minimum geometries of medium sized Cd<sub>n</sub>Te<sub>n</sub> clusters (n = 15, 16, 20, 24 and 28)

Following our recent work which revealed the lowest-energy structures of Cd<sub>n</sub>Te<sub>n</sub> (n = 1-14) clusters follow the hollow cage and the endohedral cage structural growth patterns, we extend the search for the most stable structures to some larger clusters, i.e., Cd<sub>n</sub>Te<sub>n</sub> (n = 15, 16, 20, 24 and 28). Within the size range studied, the endohedral cages are more stable than the hollow cages. The endohedral atoms increase as the cluster size increases. The computed dipole moments and polarizabilities show a clear dependence on the cluster geometry and symmetry. The hollow cage isomers possess smaller dipole moments and larger polarizabilities than the endohedral ones.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Northwest University China, National Laboratory of Solid State Microstructures, Nanjing University, Institute of Photonics and Photo-technology

Contributors: Ma, L., Wang, J., Wang, G.

Number of pages: 5

Pages: 73-77

Publication date: 12 Nov 2012

Peer-reviewed: Yes

#### Publication information

Journal: Chemical Physics Letters

Volume: 552

ISSN (Print): 0009-2614

Ratings:

Scopus rating (2012): CiteScore 2.2 SJR 1.104 SNIP 0.901

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1016/j.cplett.2012.09.036

URLs:

<http://www.scopus.com/inward/record.url?scp=84868208985&partnerID=8YFLogxK> (Link to publication in Scopus)



Source: Scopus

Source ID: 84868208985

Research output: Contribution to journal › Article › Scientific › peer-review

### **Transforming anion instability into stability: Contrasting photoionization of three protonation forms of the phosphate ion upon moving into water**

We use photoelectron emission spectroscopy with vacuum microjet technique and quantum chemistry calculations to investigate electronic structure and stability of aqueous phosphate anions. On the basis of the measured photoelectron spectra of sodium phosphates at different pH, we report the lowest vertical ionization energies of monobasic (9.5 eV), dibasic (8.9 eV), and tribasic (8.4 eV) anions. Electron binding energies were in tandem modeled with ab initio methods, using a mixed dielectric solvation model together with up to 64 explicitly solvating water molecules. We demonstrate that two solvation layers of explicit water molecules are needed to obtain converged values of vertical ionization energies (VIEs) within this mixed solvation model, leading to very good agreement with experiment. We also show that the highly charged  $\text{PO}_4^{3-}$  anion, which is electronically unstable in the gas phase, gains the electronic stability with about 16 water molecules, while only 2-3 water molecules are sufficient to stabilize the doubly charged phosphate anion. We also investigate the effect of ion pairing on the vertical ionization energy. In contrast to protonation (leading to a formation of covalent O-H bond), sodiation (leading to an anion $\cdots\text{Na}^+$  ion pair) has only a weak effect on the electron binding energy.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Department of Physical Chemistry, University of Southern California, Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, J. Heyrovský Institute of Physical Chemistry

Contributors: Pluhařová, E., Ončák, M., Seidel, R., Schroeder, C., Schroeder, W., Winter, B., Bradforth, S. E., Jungwirth, P., Slavíček, P.

Number of pages: 11

Pages: 13254-13264

Publication date: 8 Nov 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry Part B

Volume: 116

Issue number: 44

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2012): CiteScore 3.66 SJR 1.943 SNIP 1.243

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/jp306348b

URLs:

<http://www.scopus.com/inward/record.url?scp=84868554130&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84868554130

Research output: Contribution to journal › Article › Scientific › peer-review

### **Influence of ionic liquids on the dielectric relaxation behavior of CNT based elastomer nanocomposites**

The influence of an imidazolium type ionic liquid (IL) on the relaxation behavior of carbon-nanotube (CNT) based polychloroprene nanocomposites prepared by melt mixing has been investigated by broadband dielectric spectroscopy. It is demonstrated that the presence of the ionic liquid modifies the relaxation behavior of the pure rubber matrix and leads to a significant increase of the conductivity for the CNT/rubber composites. For the unfilled rubber, a distinct glass transition of the IL is observed for high concentrations demonstrating that the IL forms a separate phase. The increased conductivity of the CNT-filled rubber composites is related to a physical coupling between CNTs and rubber matrix mediated by IL leading to a better dispersion of the CNTs.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Deutsches Institut für Kautschuktechnologie e.V., Leibniz-Institut für Polymerforschung Dresden E.V., Technische Universität Dresden, Vodafone Department of Mobile Communications Systems

Contributors: Steinhauser, D., Subramaniam, K., Das, A., Heinrich, G., Klüppel, M.

Number of pages: 10  
Pages: 927-936  
Publication date: Nov 2012  
Peer-reviewed: Yes

#### Publication information

Journal: Express Polymer Letters  
Volume: 6

Issue number: 11  
ISSN (Print): 1788-618X

Ratings:

Scopus rating (2012): CiteScore 2.1 SJR 0.915 SNIP 1.597

Original language: English

ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry, Chemical Engineering(all), Organic Chemistry, Physical and Theoretical Chemistry

Keywords: Dielectric spectroscopy, Ionic liquid, Nanocomposites, Relaxation dynamics, Rubber

DOIs:

10.3144/expresspolymlett.2012.98

URLs:

<http://www.scopus.com/inward/record.url?scp=84866131281&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84866131281

Research output: Contribution to journal > Article > Scientific > peer-review

#### Azobenzene photomechanics: Prospects and potential applications

The change in shape inducible in some photo-reversible molecules using light can effect powerful changes to a variety of properties of a host material. This class of reversible light-switchable molecules includes molecules that photodimerize, such as coumarins and anthracenes; those that allow intra-molecular photo-induced bond formation, such as fulgides, spiro-pyrans, and diarylethenes; and those that exhibit photo-isomerization, such as stilbenes, crowded alkenes, and azobenzenes. The most ubiquitous natural molecule for reversible shape change, however, and perhaps the inspiration for all artificial bio-mimics, is the rhodopsin/retinal protein system that enables vision, and this is the quintessential reversible photo-switch for performance and robustness. Here, the small retinal molecule embedded in a cage of rhodopsin helices isomerizes from a cis geometry to a trans geometry around a C=C double bond with the absorption of just a single photon. The modest shape change of just a few angstroms is quickly amplified and sets off a cascade of larger shape and chemical changes, eventually culminating in an electrical signal to the brain of a vision event, the energy of the input photon amplified many thousands of times in the process. Complicated biochemical pathways then revert the trans isomer back to cis, and set the system back up for another cascade upon subsequent absorption. The reversibility is complete, and many subsequent cycles are possible. The reversion mechanism back to the initial cis state is complex and enzymatic, hence direct application of the retinal/rhodopsin photo-switch to engineering systems is difficult. Perhaps the best artificial mimic of this strong photo-switching effect however in terms of reversibility, speed, and simplicity of incorporation, is azobenzene. Trans and cis states can be switched in microseconds with low-power light, reversibility of  $10^5$  and  $10^6$  cycles is routine before chemical fatigue, and a wide variety of molecular architectures is available to the synthetic materials chemist, permitting facile anchoring and compatibility, as well as chemical and physical amplification of the simple geometric change. This review article focuses on photo-mechanical effect taking place in various material systems incorporating azobenzene. The photo-mechanical effect can be defined as reversible change in shape by absorption of light, which results in a significant macroscopic mechanical deformation, and reversible mechanical actuation, of the host material. Thus, we exclude simple thermal expansion effects, reversible but non-mechanical photo-switching or photo-chemistry, as well as the wide range of optical and electro-optical switching effects for which good reviews exist elsewhere. Azobenzene-based material systems are also of great interest for light energy harvesting applications across much of the solar spectrum, yet this emerging field is still in an early enough stage of research output as to not yet warrant review, but we hope that some of the ideas put forward here toward promising future directions of research, will help guide the field.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, McGill University, Brookhaven National Laboratory, Tokyo Institute of Technology, Aalto University

Contributors: Mahimwalla, Z., Yager, K. G., Mamiya, J. I., Shishido, A., Priimagi, A., Barrett, C. J.

Number of pages: 40

Pages: 967-1006

Publication date: Nov 2012

Peer-reviewed: Yes

#### Publication information

Journal: Polymer Bulletin  
Volume: 69  
Issue number: 8  
ISSN (Print): 0170-0839  
Ratings:

Scopus rating (2012): CiteScore 1.49 SJR 0.559 SNIP 1.027

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Polymers and Plastics, Materials Chemistry

Keywords: Azobenzene, Light harvesting, Liquid crystals, Photochemistry, Photomechanics, Thin films

DOIs:

10.1007/s00289-012-0792-0

URLs:

<http://www.scopus.com/inward/record.url?scp=84868637316&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84868637316

Research output: Contribution to journal > Article > Scientific > peer-review

### **Superquenching of SYBRGreen dye fluorescence in complex with DNA by gold nanoparticles**

The influence of gold nanoparticles (diameter of about 2.5 nm) on the complex between the SYBRGreen dye and double-stranded DNA in solutions has been investigated by fluorescence spectroscopy. Strong quenching of dye fluorescence by nanosized gold particles ("superquenching"), characterized by a high Stern-Volmer constant of  $K_{SV} = 3.3 \times 10^7$  L/mol, has been found. The superquenching effect in the test system is explained in terms of contribution of several processes: electron transfer, formation of aggregates of gold nanoparticles involving dye dications, and enhancement of intersystem crossing by a heavy atom (gold atoms of nanoparticles).

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Russian Academy of Sciences, Emanuel Institute of Biochemical Physics

Contributors: Lisitsyna, E. S., Lygo, O. N., Durandin, N. A., Dement'eva, O. V., Rudoi, V. M., Kuzmin, V. A.

Number of pages: 5

Pages: 363-367

Publication date: Nov 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: HIGH ENERGY CHEMISTRY

Volume: 46

Issue number: 6

ISSN (Print): 0018-1439

Ratings:

Scopus rating (2012): CiteScore 0.46 SJR 0.296 SNIP 0.443

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1134/S0018143912060057

URLs:

<http://www.scopus.com/inward/record.url?scp=84870905943&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84870905943

Research output: Contribution to journal > Article > Scientific > peer-review

### **Fabrication of ssDNA/oligo(ethylene glycol) monolayers and complex nanostructures by an irradiation-promoted exchange reaction**

Creative design: An approach to preparing mixed monolayers of thiolated single-stranded DNA (ssDNA) and oligo(ethylene glycol)s (OEG-AT) in a broad range of compositions as well as ssDNA/OEG-AT patterns of any required shape (see top figure) has been shown. A combination of this approach with surface-initiated enzymatic polymerization allows complex 3D DNA nanostructures to be sculpted with high spatial precision (bottom).

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Universitat Heidelberg, Duke University

Contributors: Khan, M. N., Tjong, V., Chilkoti, A., Zharnikov, M.  
Number of pages: 4  
Pages: 10303-10306  
Publication date: 8 Oct 2012  
Peer-reviewed: Yes

#### Publication information

Journal: Angewandte Chemie (International Edition)

Volume: 51

Issue number: 41

ISSN (Print): 1433-7851

Ratings:

Scopus rating (2012): CiteScore 10.55 SJR 6.407 SNIP 2.329

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis

Keywords: chemical lithography, DNA structures, monolayers, nanostructures, polymer brushes

DOIs:

10.1002/anie.201204245

URLs:

<http://www.scopus.com/inward/record.url?scp=84867091572&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84867091572

Research output: Contribution to journal > Article > Scientific > peer-review

#### Kinetics of filler wetting and dispersion in carbon nanotube/rubber composites

The effects of the surface modification of multi-walled carbon nanotubes (MWCNTs) by an ionic liquid, 1-butyl 3-methylimidazolium bis(trifluoromethyl- sulphonyl)imide (BMI) on the kinetics of filler wetting and dispersion as well as resulting electrical conductivity of polychloroprene (CR) composites were studied. Two different MWCNTs were used, Baytubes and Nanocyl, which differ in their structure, purity and compatibility to CR and BMI. The results showed that BMI can significantly improve the macrodispersion of Baytubes, and increases the electrical conductivity of the uncured BMI-Baytube/CR composites up to five orders of magnitude. In contrast, the use of BMI slows the dispersion process and the development of conductivity of BMI-Nanocyl/CR composites. Our wetting concept was further developed for the quantification of the bound polymer on the CNT surface. We found that the bonded BMI on the CNT surface is replaced by the CR molecules during mixing as a result of the concentration compensation effect. The de- and re-agglomeration processes of CNTs taking place during the subsequent curing process can increase or decrease the electrical conductivity significantly. The extent of the conductivity changes is strongly determined by the composition of the bound polymer and the curing technique used.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Martin-Luther-University Halle-Wittenberg, University of Technology - National University, Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems, Nepal Polymer Institute (NPI)

Contributors: Le, H. H., Hoang, X. T., Das, A., Gohs, U., Stoeckelhuber, K. W., Boldt, R., Heinrich, G., Adhikari, R., Radosch, H. J.

Number of pages: 14

Pages: 4543-4556

Publication date: Oct 2012

Peer-reviewed: Yes

#### Publication information

Journal: Carbon

Volume: 50

Issue number: 12

ISSN (Print): 0008-6223

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Scopus rating (2012): CiteScore 5.95 SJR 2.518 SNIP 2.118

Original language: English

ASJC Scopus subject areas: Chemistry(all)

DOIs:

10.1016/j.carbon.2012.05.039

URLs:

<http://www.scopus.com/inward/record.url?scp=84863715656&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84863715656

Research output: Contribution to journal › Article › Scientific › peer-review

### **Biomimetic surface modification of polycarbonateurethane film via phosphorylcholine-graft for resisting platelet adhesion**

Phosphorylcholine groups were covalently introduced onto a polycarbonateurethane (PCU) surface in order to create a biomimetic structure on the polymer surfaces. After introducing primary amine groups onto the polymer surface by 1,6-hexanediamine, phosphorylcholine groups were covalently linked onto the surface by the reductive amination between the amino group and the aldehyde group of phosphorylcholine glyceraldehyde (PCGA). The results of water contact angle test, X-ray photoelectron spectroscopy (XPS), and X-ray fluorescence spectrometer (XRF) analysis of the modified films indicated that PCGA had already been covalently linked to the PCU surface. The topographies and surface roughnesses were both imaged and measured by atomic force microscopy (AFM). Scanning electron microscopy (SEM) observation of the PCU films after treatment with platelet-rich plasma demonstrated that platelets had rarely adhered to the surface of the PCGA-grafted PCU films but had mainly adhered to the surface of the blank PCU films. The platelet adhesion result indicated that the PC modified PCU films could resist platelet adhesion after grafting with PCGA, and that these PCGA-grafted PCU materials, potentially, might be applied as blood-contacting materials.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Tianjin University, School of Chemical Engineering and Technology

Contributors: Gao, W., Feng, Y., Lu, J., Khan, M., Guo, J.

Number of pages: 7

Pages: 1063-1069

Publication date: Oct 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Macromolecular Research

Volume: 20

Issue number: 10

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Ratings:

Scopus rating (2012): CiteScore 1.44 SJR 0.569 SNIP 0.801

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Chemical Engineering(all)

Keywords: Biomimetic, Phosphorylcholine glyceraldehydes, Platelet adhesion, Polycarbonateurethane, Surface modification

DOIs:

10.1007/s13233-012-0152-9

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<http://www.scopus.com/inward/record.url?scp=84867230066&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84867230066

Research output: Contribution to journal › Article › Scientific › peer-review

### **Affine-response model of molecular solvation of ions: Accurate predictions of asymmetric charging free energies**

Two mechanisms have been proposed to drive asymmetric solvent response to a solute charge: a static potential contribution similar to the liquid-vapor potential, and a steric contribution associated with a water molecules structure and charge distribution. In this work, we use free-energy perturbation molecular-dynamics calculations in explicit water to show that these mechanisms act in complementary regimes; the large static potential ( $\sim 44$  kJ/mol/e) dominates asymmetric response for deeply buried charges, and the steric contribution dominates for charges near the solute-solvent interface. Therefore, both mechanisms must be included in order to fully account for asymmetric solvation in general. Our calculations suggest that the steric contribution leads to a remarkable deviation from the popular linear response model in which the reaction potential changes linearly as a function of charge. In fact, the potential varies in a piecewise-linear fashion, i.e., with different proportionality constants depending on the sign of the charge. This discrepancy is significant even when the charge is completely buried, and holds for solutes larger than single atoms. Together, these mechanisms suggest that implicit-solvent models can be improved using a combination of affine response (an offset due to the static potential) and piecewise-linear response (due to the steric contribution).

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Northeastern University, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic  
Contributors: Bardhan, J. P., Jungwirth, P., Makowski, L.  
Publication date: 28 Sep 2012  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chemical Physics

Volume: 137

Issue number: 12

Article number: 124101

ISSN (Print): 0021-9606

Ratings:

Scopus rating (2012): CiteScore 2.86 SJR 1.832 SNIP 1.16

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1063/1.4752735

URLs:

<http://www.scopus.com/inward/record.url?scp=84867017908&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84867017908

Research output: Contribution to journal > Article > Scientific > peer-review

#### Effect of sol-gel derived in situ silica on the morphology and mechanical behavior of natural rubber and acrylonitrile butadiene rubber blends

Silica particles were generated and grown in situ by sol-gel method into rubber blends comprised of natural rubber (NR) and acrylonitrile butadiene rubber (NBR) at various blend ratios. Silica formed into rubber matrix was amorphous in nature. Amount of in situ silica increased with increase in natural rubber proportion in the blends during the sol-gel process. Morphology studies showed that the generated in situ silica were nanoparticles of different shapes and sizes mostly grown into the NR phase of the blends. In situ silica filled NR/NBR blend composites showed improvement in the mechanical and dynamic mechanical behaviors in comparison to those of the unfilled and externally filled NR/ NBR blend composites. For the NR/NBR blend at 40/60 composition, in particular, the improvement was appreciable where size and dispersion of the silica particles into the rubber matrix were found to be more uniform. Dynamic mechanical analysis revealed a strong rubber-in situ silica interaction as indicated by a positive shift of the glass transition temperature of both the rubber phases in the blends.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Visvesvaraya National Institute of Technology, Leibniz-Institut für Polymerforschung Dresden E.V.

Contributors: Kapgata, B. P., Das, C., Das, A., Basu, D., Reuter, U., Heinrich, G.

Number of pages: 9

Pages: 501-509

Publication date: Sep 2012

Peer-reviewed: Yes

#### Publication information

Journal: JOURNAL OF SOL-GEL SCIENCE AND TECHNOLOGY

Volume: 63

Issue number: 3

ISSN (Print): 0928-0707

Ratings:

Scopus rating (2012): CiteScore 1.82 SJR 0.732 SNIP 1.122

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Biomaterials, Ceramics and Composites, Electronic, Optical and Magnetic Materials, Materials Chemistry

Keywords: In situ silica, Reinforcement, Rubber blend, Rubber-filler interaction, Sol-gel

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10.1007/s10971-012-2812-9

URLs:

<http://www.scopus.com/inward/record.url?scp=84875426374&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84875426374

Research output: Contribution to journal › Article › Scientific › peer-review

### **Solvation and ion-pairing properties of the aqueous sulfate anion: Explicit versus effective electronic polarization**

We assessed the relative merits of two approaches for including polarization effects in classical force fields for the sulfate anion. One of the approaches is the explicit shell model for atomic polarization and the other is an implicit dielectric continuum representation of the electronic polarization, wherein the polarizability density is spatially uniform. Both the solvation and ion association properties of sulfate were considered. We carried out an ab initio molecular dynamics simulation for a single sulfate anion in aqueous solution to obtain a benchmark for the solvation structure. For the ion-pairing properties, the models were compared to experimental thermodynamic data through Kirkwood-Buff theory, which relates the integrals of the pair correlation functions to measurable properties. While deficiencies were found for both of the approaches, the continuum polarization model was not systematically worse than the shell model. The shell model was found to give a more structured solution than the continuum polarization model, both with respect to solvation and ion pairing.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Paul Scherrer Institut, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Lund University

Contributors: Pegado, L., Marsalek, O., Jungwirth, P., Wernersson, E.

Number of pages: 10

Pages: 10248-10257

Publication date: 7 Aug 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Physical Chemistry Chemical Physics

Volume: 14

Issue number: 29

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.164

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1039/c2cp40711f

URLs:

<http://www.scopus.com/inward/record.url?scp=84863652661&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84863652661

Research output: Contribution to journal › Article › Scientific › peer-review

### **Impact of biodiesel application at various blending ratios on passenger cars of different fueling technologies**

The effect of biodiesel on emissions of diesel passenger cars is a combination of the fuel properties, the blending ratio, and the vehicle technology. In this study, saturated and unsaturated biodiesel fuels were tested neat (B100) and in 30% blend with fossil diesel (B30) on two Euro 3 diesel passenger cars of different engine technologies, namely common rail and unit injector. The measured dataset is enlarged by introducing B10 results from an earlier study [15] in order to produce generalized conclusions over a wider range of blends. None of these vehicles was equipped with a particle filter and different conclusions might be reached for filter-equipped vehicles. The results indicate that the influence of biodiesel on pollutant emissions primarily depends on the blending ratio and secondly on the level of unsaturation and engine technology. Tailpipe CO<sub>2</sub>, NO<sub>x</sub> and PM emissions with biodiesel varied from -1% to +3%, -1% to 14%, and -18% to -35%, respectively, compared to fossil diesel. The difference over fossil diesel generally increased with an increasing blending ratio. CO and HC emissions increased over the fossil diesel but remained at low levels and did not threaten the compliance of the vehicles with their respective emission limits. Use of biodiesel on the common rail vehicle led to a smaller NO<sub>x</sub> increase and a higher PM reduction than in the unit-injector case. The unsaturated fuel generally led to higher NO<sub>x</sub> emissions from both engine technologies. However, the maximum blending ratio of saturated biodiesel is limited to around B30 due to cold-flow limitations. Hence, the saturated vs. unsaturated species ratio should be carefully designed in market fuels in order to optimize environmental and operational benefits. Overall, it appears that blends up to 10% v/v may be introduced with limited urban air quality implications.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), Aristotle University of Thessaloniki, Laboratory of Applied Thermodynamics, European Commission-JRC  
Contributors: Kousoulidou, M., Ntziachristos, L., Fontaras, G., Martini, G., Dilara, P., Samaras, Z.  
Number of pages: 7  
Pages: 88-94  
Publication date: Aug 2012  
Peer-reviewed: Yes

#### Publication information

Journal: Fuel  
Volume: 98  
ISSN (Print): 0016-2361  
Ratings:  
Scopus rating (2012): CiteScore 3.99 SJR 1.813 SNIP 2.387  
Original language: English  
ASJC Scopus subject areas: Chemical Engineering(all), Fuel Technology, Energy Engineering and Power Technology, Organic Chemistry  
Keywords: Biodiesel, Fuel injection technology, Unsaturation level, Vehicle emissions  
DOIs:  
10.1016/j.fuel.2012.03.038  
URLs:  
<http://www.scopus.com/inward/record.url?scp=84861986728&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 84861986728  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Accurate description of aqueous carbonate ions: An effective polarization model verified by neutron scattering

The carbonate ion plays a central role in the biochemical formation of the shells of aquatic life, which is an important path for carbon dioxide sequestration. Given the vital role of carbonate in this and other contexts, it is imperative to develop accurate models for such a high charge density ion. As a divalent ion, carbonate has a strong polarizing effect on surrounding water molecules. This raises the question whether it is possible to describe accurately such systems without including polarization. It has recently been suggested the lack of electronic polarization in nonpolarizable water models can be effectively compensated by introducing an electronic dielectric continuum, which is with respect to the forces between atoms equivalent to rescaling the ionic charges. Given how widely nonpolarizable models are used to model electrolyte solutions, establishing the experimental validity of this suggestion is imperative. Here, we examine a stringent test for such models: a comparison of the difference of the neutron scattering structure factors of  $K_2CO_3$  vs  $KNO_3$  solutions and that predicted by molecular dynamics simulations for various models of the same systems. We compare standard nonpolarizable simulations in SPC/E water to analogous simulations with effective ion charges, as well as simulations in explicitly polarizable POL3 water (which, however, has only about half the experimental polarizability). It is found that the simulation with rescaled charges is in a very good agreement with the experimental data, which is significantly better than for the nonpolarizable simulation and even better than for the explicitly polarizable POL3 model.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic  
Contributors: Mason, P. E., Wernersson, E., Jungwirth, P.  
Number of pages: 9  
Pages: 8145-8153  
Publication date: 19 Jul 2012  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B  
Volume: 116  
Issue number: 28  
ISSN (Print): 1520-6106  
Ratings:  
Scopus rating (2012): CiteScore 3.66 SJR 1.943 SNIP 1.243  
Original language: English  
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films  
DOIs:  
10.1021/jp3008267



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Source: Scopus

Source ID: 84863696122

Research output: Contribution to journal › Article › Scientific › peer-review

### **Nematicons in azobenzene liquid crystals**

We review our comprehensive investigation of light self-localization phenomena in planarly configured azobenzene liquid crystals. Cis-trans isomerization of azobenzene molecules and related changes in the order parameter of the liquid crystals support a high nonlinear response and the formation of optical spatial solitons at microwatt excitations. We describe bright soliton angular steering, deflection, interleaving and merging, as well as dark solitons.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Beam Engineering for Advanced Measurements Co, Nonlinear Optics and OptoElectronics Lab

Contributors: Serak, S. V., Tabiryán, N. V., Assanto, G.

Number of pages: 12

Pages: 202-213

Publication date: 19 Jul 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Molecular Crystals and Liquid Crystals

Volume: 559

ISSN (Print): 1542-1406

Ratings:

Scopus rating (2012): CiteScore 0.44 SJR 0.246 SNIP 0.379

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Science(all)

Keywords: Cis-trans isomerization, laser, liquid crystals, solitons

DOIs:

10.1080/15421406.2012.658710

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Source: Scopus

Source ID: 84861494448

Research output: Contribution to journal › Article › Scientific › peer-review

### **Molecular mechanisms of ion-specific effects on proteins**

The specific binding sites of Hofmeister ions with an uncharged 600-residue elastin-like polypeptide, (VPGVG)<sub>120</sub>, were elucidated using a combination of NMR and thermodynamic measurements along with molecular dynamics simulations. It was found that the large soft anions such as SCN<sup>-</sup> and I<sup>-</sup> interact with the polypeptide backbone via a hybrid binding site that consists of the amide nitrogen and the adjacent  $\alpha$ -carbon. The hydrocarbon groups at these sites bear a slight positive charge, which enhances anion binding without disrupting specific hydrogen bonds to water molecules. The hydrophobic side chains do not contribute significantly to anion binding or the corresponding salting-in behavior of the biopolymer. Cl<sup>-</sup> binds far more weakly to the amide nitrogen/ $\alpha$ -carbon binding site, while SO<sub>4</sub><sup>2-</sup> is repelled from both the backbone and hydrophobic side chains of the polypeptide. The Na<sup>+</sup> counterions are also repelled from the polypeptide. The identification of these molecular-level binding sites provides new insights into the mechanism of peptide-anion interactions.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Texas A and M University, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Rembert, K. B., Paterová, J., Heyda, J., Hilty, C., Jungwirth, P., Cremer, P. S.

Number of pages: 8

Pages: 10039-10046

Publication date: 20 Jun 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of the American Chemical Society

Volume: 134

Issue number: 24

ISSN (Print): 0002-7863

Ratings:

Scopus rating (2012): CiteScore 10.37 SJR 6.211 SNIP 2.374

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis, Biochemistry, Colloid and Surface Chemistry

DOIs:

10.1021/ja301297g

URLs:

<http://www.scopus.com/inward/record.url?scp=84862532625&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84862532625

Research output: Contribution to journal › Article › Scientific › peer-review

### **Halogen bonding versus hydrogen bonding in driving self-assembly and performance of light-responsive supramolecular polymers**

Halogen bonding is arguably the least exploited among the many non-covalent interactions used in dictating molecular self-assembly. However, its directionality renders it unique compared to ubiquitous hydrogen bonding. Here, the role of this directionality in controlling the performance of light-responsive supramolecular polymers is highlighted. In particular, it is shown that light-induced surface patterning, a unique phenomenon occurring in azobenzene-containing polymers, is more efficient in halogen-bonded polymer-azobenzene complexes than in the analogous hydrogen-bonded complexes. A systematic study is performed on a series of azo dyes containing different halogen or hydrogen bonding donor moieties, complexed to poly(4-vinylpyridine) backbone. Through single-atom substitution of the bond-donor, control of both the strength and the nature of the noncovalent interaction between the azobenzene units and the polymer backbone is achieved. Importantly, such substitution does not significantly alter the electronic properties of the azobenzene units, hence providing us with unique tools in studying the structure-performance relationships in the light-induced surface deformation process. The results represent the first demonstration of light-responsive halogen-bonded polymer systems and also highlight the remarkable potential of halogen bonding in fundamental studies of photoresponsive azobenzene-containing polymers.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Tokyo Institute of Technology, Politecnico di Milano, Università degli Studi di Milano, Aalto University, VTT Technical Research Centre of Finland

Contributors: Priimagi, A., Cavallo, G., Forni, A., Gorynsztejn-Leben, M., Kaivola, M., Metrangolo, P., Milani, R., Shishido, A., Pilati, T., Resnati, G., Terraneo, G.

Number of pages: 8

Pages: 2572-2579

Publication date: 20 Jun 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Advanced Functional Materials

Volume: 22

Issue number: 12

ISSN (Print): 1616-301X

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Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Biomaterials, Condensed Matter Physics, Electrochemistry

Keywords: halogen bonding, optically active materials, self-assembly, supramolecular polymers, surface relief gratings

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10.1002/adfm.201200135

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<http://www.scopus.com/inward/record.url?scp=84862000539&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84862000539

Research output: Contribution to journal › Article › Scientific › peer-review

### Behavior of 4-hydroxynonenal in phospholipid membranes

Under conditions of oxidative stress, 4-hydroxy-2-nonenal (4-HNE) is commonly present in vivo. This highly reactive and cytotoxic compound is generated by oxidation of lipids in membranes and can be easily transferred from a membrane to both cytosol and the extracellular space. Employing time-dependent fluorescence shift (TDFS) method and molecular dynamics simulations, we found that 4-HNE is stabilized in the carbonyl region of a 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) bilayer. 4-HNE is thus able to react with cell membrane proteins and lipids. Stabilization in the membrane is, however, moderate and a transfer of 4-HNE to either extra- or intracellular space occurs on a microsecond time scale. These molecular-level details of 4-HNE behavior in the lipid membrane rationalize the experimentally observed reactivity of 4-HNE with proteins inside and outside the cell. Furthermore, these results support the view that 4-HNE may play an active role in cell signaling pathways.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Center for Biomolecules and Complex Molecular Systems, Division of Organic Chemistry and Biochemistry, Rudjer Bošković Institute, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, V.v.i.

Contributors: Vazdar, M., Jurkiewicz, P., Hof, M., Jungwirth, P., Cwiklik, L.

Number of pages: 5

Pages: 6411-6415

Publication date: 7 Jun 2012

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 116

Issue number: 22

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2012): CiteScore 3.66 SJR 1.943 SNIP 1.243

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/jp3044219

URLs:

<http://www.scopus.com/inward/record.url?scp=84861861948&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84861861948

Research output: Contribution to journal > Article > Scientific > peer-review

### Elemental and mixed actinide dioxides: An ab initio study

We present a systematic study of the electronic, geometric, and magnetic properties of the actinide dioxides,  $\text{UO}_2$ ,  $\text{PuO}_2$ ,  $\text{AmO}_2$ ,  $\text{U}_{0.5}\text{Pu}_{0.5}\text{O}_2$ ,  $\text{U}_{0.5}\text{Am}_{0.5}\text{O}_2$  and  $\text{Pu}_{0.5}\text{Am}_{0.5}\text{O}_2$ . For  $\text{UO}_2$ ,  $\text{PuO}_2$  and  $\text{AmO}_2$ , both density functional and hybrid density functional theory (DFT and HDFT) have been used. The fractions of exact HartreeFock (HF) exchange chosen were 25% and 40% for the hybrid density functional. For  $\text{U}_{0.5}\text{Pu}_{0.5}\text{O}_2$ ,  $\text{U}_{0.5}\text{Am}_{0.5}\text{O}_2$  and  $\text{Pu}_{0.5}\text{Am}_{0.5}\text{O}_2$ , only HDFT with 40% exact HF exchange was used. Each compound has been studied at the nonmagnetic, ferromagnetic and anti-ferromagnetic configurations, with and without spinorbit coupling (SOC). The lattice parameters, magnetic structures, bulk moduli, band gaps and density of states have been computed and compared to available experimental data and other theoretical results. Pure DFT fails to provide a satisfactory qualitative description of the electronic and magnetic structures of the actinide dioxides. On the other hand, HDFT performs very well in the prediction and description of the properties of the actinide dioxides. Our total energy calculations clearly indicate that the ground-state structures are anti-ferromagnetic for all actinide dioxides considered here. The lattice constants and the band gaps expand with an increase of HF exchange in HDFT. The influence of SOC is found to be significant.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Texas at Arlington, Pacific Northwest National Laboratory

Contributors: Ma, L., Atta-Fynn, R., Ray, A. K.

Number of pages: 19

Pages: 611-629

Publication date: Jun 2012

Peer-reviewed: Yes

### Publication information

Journal: Journal of Theoretical and Computational Chemistry

Volume: 11

Issue number: 3

ISSN (Print): 0219-6336

Ratings:

Scopus rating (2012): CiteScore 0.69 SJR 0.315 SNIP 0.304

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Computational Theory and Mathematics, Computer Science Applications

Keywords: Actinide dioxides, hybrid density functional theory, mixed actinide oxides

DOIs:

10.1142/S021963361250040X

URLs:

<http://www.scopus.com/inward/record.url?scp=84862874223&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84862874223

Research output: Contribution to journal > Article > Scientific > peer-review

### Structural characteristics and flammability of fire retarding EPDM/layered double hydroxide (LDH) nanocomposites

A high performance elastomeric flame retardant nanocomposite was prepared which was based on maleic anhydride grafted ethylene-propylene-diene terpolymer (mEPDM), a one-step synthesised organo-layered double hydroxide (LDH), and an intumescent flame retardant (FR) comprised of pentaerythritol (PER), ammonium polyphosphate (APP) and methyl cyanoacetate (MCA). The morphology, fire behavior and mechanical properties of the flame-retarded mEPDM/LDH nanocomposite have been studied in detail. Wide angle X-ray scattering (WAXS), small angle X-ray scattering (SAXS) and TEM observation confirmed an exfoliated structure of LDH in a particular composite containing 2 phr (parts per hundred) LDH and 38 phr FR. As an effective flame retardant synergistic agent, MgAl-LDH shows a significant decrease in the heat release rate (HRR), low mass loss (ML) and low fire growth rate (FIGRA) of the nanocomposite. The flame retardant mechanism has been proposed, which is mainly due to the condensed phase flame retardant mechanism to form reinforced char layers during combustion, leading to the low volatiles produced. Moreover, as far as the mechanical properties of the vulcanizates are concerned, in all cases of flame retardant mEPDM and flame retarded mEPDM/LDH nanocomposites, they exhibit superior values compared to the gum compound.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems

Contributors: Wang, D. Y., Das, A., Leuteritz, A., Mahaling, R. N., Jehnichen, D., Wagenknecht, U., Heinrich, G.

Number of pages: 7

Pages: 3927-3933

Publication date: 21 Apr 2012

Peer-reviewed: Yes

### Publication information

Journal: RSC Advances

Volume: 2

Issue number: 9

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2012): CiteScore 2.4 SJR 0.872 SNIP 0.619

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all)

DOIs:

10.1039/c2ra20189e

URLs:

<http://www.scopus.com/inward/record.url?scp=84863098130&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84863098130

Research output: Contribution to journal > Article > Scientific > peer-review

**Highly exfoliated natural rubber/Clay composites by "propping-open procedure": The influence of fatty-acid chain length on exfoliation**

A high degree of exfoliation of MMT in NR is achieved by using the so-called "propping-open approach" in which a stepwise expansion of the interlayer spacing of MMT takes place. The nanostructure is characterized by WAXD and TEM which indicate different extents of clay dispersion depending on the fatty-acid chain length. Curing kinetics of different nanocomposites is studied and interestingly low activation energies of the vulcanization process are observed in the case of NR/EMMT nanocomposites. The incorporation of EMMT dramatically affects composite properties whereas DMA indicates significant reduction of  $\tan \delta$  peak height and the tensile strength approximately doubles from 14 to 30 MPa with only 5 phr EMMT.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems

Contributors: Rooj, S., Das, A., Stöckelhuber, K. W., Reuter, U., Heinrich, G.

Number of pages: 15

Pages: 369-383

Publication date: Apr 2012

Peer-reviewed: Yes

#### Publication information

Journal: Macromolecular Materials and Engineering

Volume: 297

Issue number: 4

ISSN (Print): 1438-7492

Ratings:

Scopus rating (2012): CiteScore 2.34 SJR 0.963 SNIP 1.187

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Organic Chemistry, Polymers and Plastics, Materials Chemistry

Keywords: curing kinetics, exfoliation, Mooney-Rivlin equation, nanocomposites, propping-open approach

DOIs:

10.1002/mame.201100185

URLs:

<http://www.scopus.com/inward/record.url?scp=84859811037&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84859811037

Research output: Contribution to journal > Article > Scientific > peer-review

#### Excited-state polarizability in crystalline sexithiophene: Charge-transfer and vibronic effects

A model of vibronic coupling in a manifold of coupled Frenkel and charge transfer states is applied to evaluate the electric-field-induced shifts of lowest vibronic levels deriving from the lower Davydov component of the Frenkel exciton in sexithiophene. With respect to the isolated-molecule value, vibronic terms combined with the mixing between Frenkel and CT configurations amplify the field-induced shift by the factor of seven for the 0-0 line and by further 60% for the vibronic replica in the main progression-forming mode. Confirmation is found in the existing experimental literature.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Groningen, K. Gumiński Department of Theoretical Chemistry, Uniwersytet Jagiellonski w Krakowie

Contributors: Stradomska, A., Kulig, W., Slawik, M., Petelenz, P.

Number of pages: 4

Pages: 27-30

Publication date: 9 Mar 2012

Peer-reviewed: Yes

#### Publication information

Journal: Chemical Physics Letters

Volume: 529

ISSN (Print): 0009-2614

Ratings:

Scopus rating (2012): CiteScore 2.2 SJR 1.104 SNIP 0.901

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1016/j.cplett.2012.01.038

URLs:

<http://www.scopus.com/inward/record.url?scp=84857532168&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84857532168

Research output: Contribution to journal > Article > Scientific > peer-review

### **A novel thermotropic elastomer based on highly-filled LDH-SSB composites**

Elastomeric composites are prepared based on solution styrene butadiene elastomer and zinc-aluminium layered double hydroxides (LDH), using a conventional sulphur cure system. Up to 100 parts per hundred rubber of LDH are incorporated into the elastomer matrix. The composites exhibit an interesting phenomenon of thermoreversible transparency, i.e. the transparent sample becomes opaque at warm condition and restores the transparency at room temperature. The transparency is found to be increased as the amount of LDH was increased. The addition of LDH gradually improved the mechanical, dynamic mechanical performance and thermal stability of the base elastomer. These developed elastomers could be utilised as smart materials in different applications

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems

Contributors: Das, A., George, J. J., Kutlu, B., Leuteritz, A., Wang, D. Y., Rooj, S., Jurk, R., Rajeshbabu, R., Stöckelhuber, K. W., Galiatsatos, V., Heinrich, G.

Number of pages: 6

Pages: 337-342

Publication date: 27 Feb 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Macromolecular Rapid Communications

Volume: 33

Issue number: 4

ISSN (Print): 1022-1336

Ratings:

Scopus rating (2012): CiteScore 4.7 SJR 2.096 SNIP 1.251

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics

DOIs:

10.1002/marc.201100735

URLs:

<http://www.scopus.com/inward/record.url?scp=84863149624&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84863149624

Research output: Contribution to journal > Article > Scientific > peer-review

### **Glycerol mediated synthesis of 5-substituted 1H-tetrazole under catalyst free conditions**

We have developed simple, cost effective and environmentally benign protocol for the synthesis of 5-substituted 1H-tetrazoles via [2,3] cycloaddition reaction from organic nitriles and sodium azide in glycerol under catalyst free condition. The corresponding 5-substituted 1H-tetrazoles were obtained with good to excellent yields (68-95%).

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: North Maharashtra University, N Maharashtra Univ, North Maharashtra University, Dept Organ Chem

Contributors: Nandre, K. P., Salunke, J. K., Nandre, J. P., Patil, V. S., Borse, A. U., Bhosale, S. V.

Number of pages: 4

Pages: 161-164

Publication date: Feb 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Chinese Chemical Letters

Volume: 23

Issue number: 2

ISSN (Print): 1001-8417

Ratings:

Scopus rating (2012): CiteScore 1.21 SJR 0.419 SNIP 0.759

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: 5-Substituted 1H-tetrazole, [3+2] Cycloaddition, Catalyst free, Glycerol, Nitriles

DOIs:

10.1016/j.ccllet.2011.11.019

### Bibliographical note

EXT="Salunke, Jagadish"

Source: Scopus

Source ID: 84855928133

Research output: Contribution to journal > Article > Scientific > peer-review

### Surface-relief gratings and stable birefringence inscribed using light of broad spectral range in supramolecular polymer-bisazobenzene complexes

We report on phenol-pyridine hydrogen-bonded supramolecular polymer-azobenzene complexes made from a newly designed polar bisazobenzene chromophore. Because of the substitution with a polar nitro group, the chromophore possesses an extremely broad absorption band, spanning from near-UV up to 650 nm. Moreover, the inclusion of two methoxy groups to the central benzene ring prevents excessive chromophore-chromophore intermolecular interactions and provides advantageous size-related properties. Together, these features of the prepared photoresponsive polymer materials enable efficient inscription of (i) photoinduced birefringence with outstanding stability at various chromophore concentrations and (ii) surface-relief grating formation over a wide range of writing wavelengths from 405 to 633 nm. The photoresponsive behavior is compared to that of Disperse Yellow 7-based supramolecular complexes.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Applied Physics, Aalto University, Tokyo Institute of Technology, University of Bristol

Contributors: Koskela, J. E., Vapaavuori, J., Hautala, J., Priimagi, A., Faul, C. F. J., Kaivola, M., Ras, R. H. A.

Number of pages: 8

Pages: 2363-2370

Publication date: 26 Jan 2012

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physical Chemistry C

Volume: 116

Issue number: 3

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

10.1021/jp210706n

URLs:

<http://www.scopus.com/inward/record.url?scp=84856360260&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84856360260

Research output: Contribution to journal > Article > Scientific > peer-review

### Structure, dynamics, and reactivity of hydrated electrons by Ab initio molecular dynamics

Understanding the properties of hydrated electrons, which were first observed using pulse radiolysis of water in 1962, is crucial because they are key species in many radiation chemistry processes. Although time-resolved spectroscopic studies and molecular simulations have shown that an electron in water (prepared, for example, by water photoionization) relaxes quickly to a localized, cavity-like structure  $\sim 2.5$  Å in radius, this picture has recently been questioned. In another experimental approach, negatively charged water clusters of increasing size were studied with photoelectron and IR spectroscopies. Although small water clusters can bind an excess electron, their character is very different from bulk hydrated species. As data on electron binding in liquid water have become directly accessible experimentally, the cluster-to-bulk extrapolations have become a topic of lively debate. Quantum electronic structure calculations addressing experimental measurables have, until recently, been largely limited to small clusters; extended systems were approached mainly with pseudopotential calculations combining a classical description of water with a quantum mechanical treatment

of the excess electron. In this Account, we discuss our investigations of electrons solvated in water by means of ab initio molecular dynamics simulations. This approach, applied to a model system of a negatively charged cluster of 32 water molecules, allows us to characterize structural, dynamical, and reactive aspects of the hydrated electron using all of the system's valence electrons. We show that under ambient conditions, the electron localizes into a cavity close to the surface of the liquid cluster. This cavity is, however, more flexible and accessible to water molecules than an analogous area around negatively charged ions. The dynamical process of electron attachment to a neutral water cluster is strongly temperature dependent. Under ambient conditions, the electron relaxes in the liquid cluster and becomes indistinguishable from an equilibrated, solvated electron on a picosecond time scale. In contrast, for solid, cryogenic systems, the electron only partially localizes outside of the cluster, being trapped in a metastable, weakly bound "cushion-like" state. Strongly bound states under cryogenic conditions could only be prepared by cooling equilibrated, liquid, negatively charged clusters. These calculations allow us to rationalize how different isomers of electrons in cryogenic clusters can be observed experimentally. Our results also bring into question the direct extrapolation of properties of cryogenic, negatively charged water clusters to those of electrons in the bulk liquid. Ab initio molecular dynamics represents a unique computational tool for investigating the reactivity of the solvated electron in water. As a prototype, the electron-proton reaction was followed in the 32-water cluster. In accord with experiment, the molecular mechanism is a proton transfer process that is not diffusion limited, but rather controlled by a proton-induced deformation of the excess electron's solvent shell. We demonstrate the necessary ingredients of a successful density functional methodology for the hydrated electron that avoids potential pitfalls, such as self-interaction error, insufficient basis set, or lack of dispersion interactions. We also benchmark the density functional theory methods and outline the path to faithful ab initio simulations of dynamics and reactivity of electrons solvated in extended aqueous systems.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, University of Zurich, Center for Biomolecules

Contributors: Marsalek, O., Uhlig, F., Vandevondele, J., Jungwirth, P.

Number of pages: 10

Pages: 23-32

Publication date: 17 Jan 2012

Peer-reviewed: Yes

### Publication information

Journal: Accounts of Chemical Research

Volume: 45

Issue number: 1

ISSN (Print): 0001-4842

Ratings:

Scopus rating (2012): CiteScore 21.17 SJR 12.299 SNIP 5.413

Original language: English

ASJC Scopus subject areas: Chemistry(all)

DOIs:

10.1021/ar200062m

URLs:

<http://www.scopus.com/inward/record.url?scp=84855914692&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84855914692

Research output: Contribution to journal › Article › Scientific › peer-review

### Layered Double Hydroxides (LDH): A multifunctional versatile system for nanocomposites

Layered Double Hydroxides gained tremendous research efforts in the last years as a filler for polymer nanocomposites similar to montmorillonite in order to increase barrier properties, improve mechanical properties and reduce flammability. Due to its broad variety in composition and possibility to organically modify the layers LDH might be used in very different applications. This summary intends to show possibilities of integration of additional functionalities apart from the benefits of LDH as platelet decomposing like the classical flame retardant magnesium hydroxide, by selecting a specific metal combination, by fine tuning structural features and by selecting an organic modification with a functionality thus providing a true added value to filler for nanocomposite applications.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V.

Contributors: Leuteritz, A., Kutlu, B., Meinel, J., Wang, D., Das, A., Wagenknecht, U., Heinrich, G.

Number of pages: 7

Pages: 107-113



Publication date: 2012

Peer-reviewed: Yes

#### Publication information

Journal: Molecular Crystals and Liquid Crystals

Volume: 556

ISSN (Print): 1542-1406

Ratings:

Scopus rating (2012): CiteScore 0.44 SJR 0.246 SNIP 0.379

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Science(all)

Keywords: Conductivity, Flame retardancy, Layered double hydroxide, Photostability, Vulcanization

DOIs:

10.1080/15421406.2012.635923

URLs:

<http://www.scopus.com/inward/record.url?scp=84861542986&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84861542986

Research output: Contribution to journal > Article > Scientific > peer-review

#### Location of the Azobenzene moieties within the cross-linked liquid-crystalline polymers can dictate the direction of photoinduced bending

We present a simple way to control the photoinduced bending direction of azobenzene-containing cross-linked liquidcrystalline polymers. By changing the location of the photoactive azobenzene moieties from cross-links to side-chains, the bending direction of the sample is reversed under identical irradiation conditions. In addition to providing a versatile route toward directionality control of the photoinduced macroscopic motions, this observation highlights the complicated nature of the photomechanical response of azobenzene-containing cross-linked liquidcrystalline polymers, showing that the photomobile behavior can be determined by seemingly small details on the materials design.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Aalto University, Tokyo Institute of Technology, University of Hyogo, Kobe, Tohoku University, Chuo University

Contributors: Priimagi, A., Shimamura, A., Kondo, M., Hiraoka, T., Kubo, S., Mamiya, J. I., Kinoshita, M., Ikeda, T., Shishido, A.

Number of pages: 4

Pages: 96-99

Publication date: 2012

Peer-reviewed: Yes

#### Publication information

Journal: ACS Macro Letters

Volume: 1

Issue number: 1

ISSN (Print): 2161-1653

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry

DOIs:

10.1021/mz200056w

URLs:

<http://www.scopus.com/inward/record.url?scp=84861898337&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84861898337

Research output: Contribution to journal > Article > Scientific > peer-review

#### Chasing charge localization and chemical reactivity following photoionization in liquid water

The ultrafast dynamics of the cationic hole formed in bulk liquid water following ionization is investigated by ab initio molecular dynamics simulations and an experimentally accessible signature is suggested that might be tracked by femtosecond pump-probe spectroscopy. This is one of the fastest fundamental processes occurring in radiation-induced chemistry in aqueous systems and biological tissue. However, unlike the excess electron formed in the same process, the nature and time evolution of the cationic hole has been hitherto little studied. Simulations show that an initially partially delocalized cationic hole localizes within ~30 fs after which proton transfer to a neighboring water molecule proceeds practically immediately, leading to the formation of the OH radical and the hydronium cation in a reaction which can be formally written as  $\text{H}_2\text{O}^+ + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_3\text{O}^+$ . The exact amount of initial spin delocalization is, however, somewhat

method dependent, being realistically described by approximate density functional theory methods corrected for the self-interaction error. Localization, and then the evolving separation of spin and charge, changes the electronic structure of the radical center. This is manifested in the spectrum of electronic excitations which is calculated for the ensemble of ab initio molecular dynamics trajectories using a quantum mechanics/molecular mechanics (QM/MM) formalism applying the equation of motion coupled-clusters method to the radical core. A clear spectroscopic signature is predicted by the theoretical model: as the hole transforms into a hydroxyl radical, a transient electronic absorption in the visible shifts to the blue, growing toward the near ultraviolet. Experimental evidence for this primary radiation-induced process is sought using femtosecond photoionization of liquid water excited with two photons at 11 eV. Transient absorption measurements carried out with ~40 fs time resolution and broadband spectral probing across the near-UV and visible are presented and direct comparisons with the theoretical simulations are made. Within the sensitivity and time resolution of the current measurement, a matching spectral signature is not detected. This result is used to place an upper limit on the absorption strength and/or lifetime of the localized  $\text{H}_2\text{O}^+$  (aq) species.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, University of Kansas Lawrence, University of Wisconsin-Madison, HCl e 486.1, University of Southern California

Contributors: Marsalek, O., Elles, C. G., Pieniazek, P. A., Pluhaov, E., Vandevondele, J., Bradforth, S. E., Jungwirth, P.

Publication date: 14 Dec 2011

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chemical Physics

Volume: 135

Issue number: 22

Article number: 224510

ISSN (Print): 0021-9606

Ratings:

Scopus rating (2011): CiteScore 3.07 SJR 1.845 SNIP 1.231

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry, Medicine(all)

DOIs:

10.1063/1.3664746

URLs:

<http://www.scopus.com/inward/record.url?scp=83755182728&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 83755182728

Research output: Contribution to journal > Article > Scientific > peer-review

#### The Discovery of Compounds That Stimulate the Activity of Kallikrein-Related Peptidase3 (KLK3)

Kallikrein-related peptidase3 (KLK3), also known as prostate-specific antigen (PSA), is the most useful biomarker for prostate cancer (PCa). KLK3 is suggested to play a role in regulating cancer growth through anti-angiogenic activity *in vivo* and *in vitro*. This feature, together with its specificity for prostate tissue, makes KLK3 an intriguing target for the design of new therapies for PCa. 3D pharmacophores for KLK3-stimulating compounds were generated based on peptides that bind specifically to KLK3 and increase its enzymatic activity. As a result of pharmacophore-based virtual screening, four small, drug-like compounds with affinity for KLK3 were discovered and validated by capillary differential scanning calorimetry. One of the compounds also stimulated the activity of KLK3, and is therefore the first published small molecule with such an activity. Target specificity: Successful 3D pharmacophore-based virtual screening resulted in the first small, drug-like molecule that stimulates the activity of kallikrein-related peptidase3 (KLK3, PSA). The compound discovered can be applied to the design of novel KLK3-stimulating compounds with the potential to inhibit tumor angiogenesis and progression of prostate cancer.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Ita-Suomen yliopisto, Helsinki University Central Hospital, Tampere University Hospital, Kobenhavns Universitet, European ScreeningPort GmbH

Contributors: Härkönen, H. H., Mattsson, J. M., Määttä, J. A. E., Stenman, U. H., Koistinen, H., Matero, S., Windshügel, B., Poso, A., Lahtela-Kakkonen, M.

Number of pages: 9

Pages: 2170-2178

Publication date: 9 Dec 2011

Peer-reviewed: Yes

### Publication information

Journal: CHEMMEDCHEM

Volume: 6

Issue number: 12

ISSN (Print): 1860-7179

Ratings:

Scopus rating (2011): CiteScore 3.24 SJR 1.267 SNIP 0.933

Original language: English

ASJC Scopus subject areas: Molecular Medicine, Pharmacology, Toxicology and Pharmaceutics(all), Organic Chemistry

Keywords: Angiogenesis, Kallikrein, Molecular modeling, Peptides, Virtual screening

DOIs:

10.1002/cmdc.201100349

URLs:

<http://www.scopus.com/inward/record.url?scp=82955165662&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 82955165662

Research output: Contribution to journal > Article > Scientific > peer-review

### Cholesterol driven alteration of the conformation and dynamics of phospholamban in model membranes

The effects of cholesterol on various membrane proteins are of long-standing interest in membrane biophysics. Here we present systematic molecular dynamics simulations (totaling 1.4  $\mu$ s) of integral protein phospholamban incorporated in POPC/cholesterol bilayers (containing 0, 11.11, 22.03, 33.33, and 50 mol% of cholesterol). Phospholamban is a key regulator of cardiac contractility and has recently emerged as a potential drug target. In agreement with experiments, our results show that in a cholesterol-free pure POPC bilayer, phospholamban exhibits broad conformational distribution, ranging from the closed T-state to the extended R-state, crucial for its functionality. Increasing cholesterol concentration progressively stabilizes the bent conformers of phospholamban over open structures, and favors extensive interactions of its amphipathic N-terminal helix with the bilayer surface. The interaction energies between the N-terminal helix of PLB and different POPC/cholesterol bilayers quantitatively confirm its stronger interaction with a higher cholesterol-containing membrane. Simulation with 50 mol% of cholesterol further supports the above conclusions, where phospholamban undergoes rapid conformational transition from extended to closed form, which remains stable for the rest of the simulation time and exhibits the strongest interaction with the membrane. Cholesterol participates in hydrogen-bonding and  $\pi$ -stacking interactions with polar and/or aromatic residues and favors membrane association of phospholamban. We observed cholesterol-enrichment in the neighborhood of phospholamban. Moreover, as a modulator of membrane biophysical properties, cholesterol modifies the hydrophobic matching and trans-membrane tilting of phospholamban and also hinders its 2D-lateral mobility. Altogether, our results highlight atomistic details of protein-lipid interplay and provide new insights into the possible effects of cholesterol on conformational dynamics of phospholamban in membrane bilayers.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Calcutta

Contributors: Manna, M., Mukhopadhyay, C.

Number of pages: 11

Pages: 20188-20198

Publication date: 7 Dec 2011

Peer-reviewed: Yes

### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 13

Issue number: 45

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.184

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1039/c1cp21793c

URLs:

<http://www.scopus.com/inward/record.url?scp=81255129160&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 81255129160

Research output: Contribution to journal > Article > Scientific > peer-review

### **Effect of ionic liquid on dielectric, mechanical and dynamic mechanical properties of multi-walled carbon nanotubes/polychloroprene rubber composites**

This paper focuses on the influence of ionic liquid on carbon nanotube based elastomeric composites. Multi-walled carbon nanotubes (MWCNTs) are modified using an ionic liquid at room temperature, 1-butyl 3-methyl imidazolium bis (trifluoromethylsulphonyl) imide (BMI) and modified MWCNTs exhibit physical (cation- $\pi/\pi-\pi$ ) interaction with BMI. The polychloroprene rubber (CR) composites are prepared using unmodified and BMI modified MWCNTs. The presence of BMI not only increases the alternating current (AC) electrical conductivity and polarisability of the composites but also improves the state of dispersion of the tubes as observed from dielectric spectroscopy and transmission electron microscopy respectively. In addition to the hydrodynamic reinforcement, the formation of improved filler-filler networks is reflected in the dynamic storage modulus ( $E'$ ) for modified MWCNTs/CR composites in amplitude sweep measurement upon increasing the proportion of BMI. Hardness and mechanical properties are also studied for the composites as a function of BMI.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V., Deutsches Institut für Kautschuktechnologie e.V., Vodafone Department of Mobile Communications Systems

Contributors: Subramaniam, K., Das, A., Steinhauser, D., Klüppel, M., Heinrich, G.

Number of pages: 10

Pages: 2234-2243

Publication date: Dec 2011

Peer-reviewed: Yes

#### **Publication information**

Journal: European Polymer Journal

Volume: 47

Issue number: 12

ISSN (Print): 0014-3057

Ratings:

Scopus rating (2011): CiteScore 3.03 SJR 1.109 SNIP 1.822

Original language: English

ASJC Scopus subject areas: Polymers and Plastics, Physics and Astronomy(all), Organic Chemistry

Keywords: Carbon nanotubes, Electrical conductivity, Ionic liquids, Polychloroprene rubber

DOIs:

10.1016/j.eurpolymj.2011.09.021

URLs:

<http://www.scopus.com/inward/record.url?scp=81155135001&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 81155135001

Research output: Contribution to journal > Article > Scientific > peer-review

### **Arrhenius analysis of anisotropic surface self-diffusion on the prismatic facet of ice**

We present an Arrhenius analysis of self-diffusion on the prismatic surface of ice calculated from molecular dynamics simulations. The six-site water model of Nada and van der Eerden was used in combination with a structure-based criterion for determining the number of liquid-like molecules in the quasi-liquid layer. Simulated temperatures range from 230 K-287 K, the latter being just below the melting temperature of the model, 289 K. Calculated surface diffusion coefficients agree with available experimental data to within quoted precision. Our results indicate a positive Arrhenius curvature, implying a change in the mechanism of self-diffusion from low to high temperature, with a concomitant increase in energy of activation from 29.1 kJ mol<sup>-1</sup> at low temperature to 53.8 kJ mol<sup>-1</sup> close to the melting point. In addition, we find that the surface self-diffusion is anisotropic at lower temperatures, transitioning to isotropic in the temperature range of 240-250 K. We also present a framework for self-diffusion in the quasi-liquid layer on ice that aims to explain these observations.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, University of Puget Sound

Contributors: Gladich, I., Pfalzgraff, W., Maršálek, O., Jungwirth, P., Roeselová, M., Neshyba, S.

Number of pages: 10

Pages: 19960-19969

Publication date: 28 Nov 2011

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 13

Issue number: 44

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.184

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1039/c1cp22238d

URLs:

<http://www.scopus.com/inward/record.url?scp=80455123676&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 80455123676

Research output: Contribution to journal › Article › Scientific › peer-review

#### Detection and verification of glycosylation patterns of glycoproteins from clinical specimens using lectin microarrays and lectin-based immunosorbent assays

Aberrant glycosylation is a fundamental characteristic of progression of diseases such as cancer. Therefore, characterization of glycosylation patterns of proteins from disease tissues may identify changes specific to the disease development and improve diagnostic performance. Thus, analysis strategies with sufficient sensitivity for evaluation of glycosylation patterns in clinical specimens are needed. Here, we describe an analytical strategy for detection and verification of glycosylation patterns. It is based on a two-phase platform including a pattern discovery phase to identify the glycosylation changes using high-density lectin microarrays and a verification phase by developing lectin-based immunosorbent assays using the identified lectins. We evaluated the analytical performance of the platform using the glycoprotein standard and found that the lectin microarray could detect specific bindings of glycoprotein to lectins at the nanogram level and the lectin-based immunosorbent assay could be used for verification of protein glycosylation. We then applied the approach to the analysis of glycosylation patterns of two glycoproteins, which are highly expressed in prostate cancer in our prior studies, prostate specific antigen (PSA) and membrane metallo-endopeptidase (MME), from aggressive (AC) and nonaggressive prostate cancer (NAC) tissues. The observed differences in glycosylation patterns of PSA and MME may represent a significant clinical importance and could be used to develop multiplex assays for diagnosis of aggressive prostate cancer.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Prostate cancer research center (PCRC), Institute of Biophysics Chinese Academy of Sciences, Shanghai Jiaotong University, Johns Hopkins University, Visiting Graduate Student in Department of Urban Design and Planning, University of Washington, Seattle, USA 1.1.2012-15.6.2012 (12.9.2011 alkaen)

Contributors: Li, Y., Tao, S. C., Bova, G. S., Liu, A. Y., Chan, D. W., Zhu, H., Zhang, H.

Number of pages: 8

Pages: 8509-8516

Publication date: 15 Nov 2011

Peer-reviewed: Yes

#### Publication information

Journal: Analytical Chemistry

Volume: 83

Issue number: 22

ISSN (Print): 0003-2700

Ratings:

Scopus rating (2011): CiteScore 5.86 SJR 2.616 SNIP 1.658

Original language: English

ASJC Scopus subject areas: Analytical Chemistry

DOIs:

10.1021/ac201452f

URLs:

<http://www.scopus.com/inward/record.url?scp=81255146498&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 81255146498

Research output: Contribution to journal › Article › Scientific › peer-review

### **Orientational dependence of the affinity of guanidinium ions to the water surface**

The behavior of guanidinium chloride at the surface of aqueous solutions is investigated using classical molecular dynamics (MD) simulations. It is found that the population of guanidinium ions oriented parallel to the interface is greater in the surface region than in bulk. The opposite is true for ions in other orientations. Overall, guanidinium chloride is depleted in the surface region, in agreement with the fact that the addition of guanidinium chloride increases the surface tension of water. The orientational dependence of the surface affinity of the guanidinium cation is related to its anisotropic hydration. To bring the ion to the surface in the parallel orientation does not require hydrogen bonds to be broken, in contrast to other orientations. The surface enrichment of parallel-oriented guanidinium indicates that its solvation is more favorable near the surface than in bulk solution for this orientation. The dependence of the bulk and surface properties of guanidinium on the force field parameters is also investigated. Despite significant quantitative differences between the force fields, the surface behavior is qualitatively robust. The implications for the orientations of the guanidinium groups of arginine side chains on protein surfaces are also outlined.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Division of Organic Chemistry and Biochemistry, Bijienska Cesta 54, Lund University, Crop and Soil Sciences, Cornell Univ.

Contributors: Wernersson, E., Heyda, J., Vazdar, M., Lund, M., Mason, P. E., Jungwirth, P.

Number of pages: 6

Pages: 12521-12526

Publication date: 3 Nov 2011

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry Part B

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ISSN (Print): 1520-6106

Ratings:

Scopus rating (2011): CiteScore 3.62 SJR 1.801 SNIP 1.223

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

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URLs:

<http://www.scopus.com/inward/record.url?scp=80054988916&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 80054988916

Research output: Contribution to journal > Article > Scientific > peer-review

### **The effect of lipid oxidation on the water permeability of phospholipids bilayers**

The effect of lipid oxidation on water permeability of phosphatidylcholine membranes was investigated by means of both scattering stopped flow experiments and atomistic molecular dynamics simulations. Formation of water pores followed by a significant enhancement of water permeability was observed. The molecules of oxidized phospholipids facilitate pore formation and subsequently stabilize water in the membrane interior. A wide range of oxidation ratios, from 15 to 100 mol%, was considered. The degree of oxidation was found to strongly influence the time needed for the opening of a pore. In simulations, the oxidation ratio of 75 mol% was found to be a threshold for spontaneous pore formation in the tens of nanosecond timescale, whereas 15 mol% of oxidation led to significant water permeation in the timescale of seconds. Once a pore was formed, the water permeability was found to be virtually independent of the oxidation ratio. This journal is

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Wrocław University of Technology, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, J. Heyrovský Institute of Physical Chemistry

Contributors: Lis, M., Wizert, A., Przybylo, M., Langner, M., Swiatek, J., Jungwirth, P., Cwiklik, L.

Number of pages: 9

Pages: 17555-17563

Publication date: 21 Oct 2011

Peer-reviewed: Yes

### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 13

Issue number: 39

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.184

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

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10.1039/c1cp21009b

URLs:

<http://www.scopus.com/inward/record.url?scp=80053535630&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 80053535630

Research output: Contribution to journal > Article > Scientific > peer-review

### Efficient surface structuring and photoalignment of supramolecular polymer-azobenzene complexes through rational chromophore design

Rational selection of the para-substituent of azobenzene chromophores in supramolecular polymeric complexes is exploited to control the chromophore-chromophore intermolecular interactions occurring in the material system. This allows optimizing the material system for either efficient surface-relief formation or for high and stable photoalignment. The surface-relief gratings can be subsequently coated with amorphous TiO<sub>2</sub> using atomic layer deposition, resulting in high-quality and high-index organic-inorganic gratings with vastly improved thermal stability compared to all-polymeric gratings.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Frontier Photonics, Department of Applied Physics, Aalto University, Tokyo Institute of Technology

Contributors: Vapaavuori, J., Valtavirta, V., Alasaarela, T., Mamiya, J. I., Priimagi, A., Shishido, A., Kaivola, M.

Number of pages: 5

Pages: 15437-15441

Publication date: 21 Oct 2011

Peer-reviewed: Yes

### Publication information

Journal: Journal of Materials Chemistry

Volume: 21

Issue number: 39

ISSN (Print): 0959-9428

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Scopus rating (2011): SJR 2.614 SNIP 1.539

Original language: English

ASJC Scopus subject areas: Materials Chemistry, Chemistry(all)

DOIs:

10.1039/c1jm12642c

URLs:

<http://www.scopus.com/inward/record.url?scp=80053301644&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 80053301644

Research output: Contribution to journal > Article > Scientific > peer-review

### Like-charge guanidinium pairing from molecular dynamics and ab initio calculations

Pairing of guanidinium moieties in water is explored by molecular dynamics simulations of short arginine-rich peptides and ab initio calculations of a pair of guanidinium ions in water clusters of increasing size. Molecular dynamics simulations show that, in an aqueous environment, the diarginine guanidinium like-charged ion pairing is sterically hindered, whereas in the Arg-Ala-Arg tripeptide, this pairing is significant. This result is supported by the survey of protein structure databases, where it is found that stacked arginine pairs in dipeptide fragments exist solely as being imposed by the protein structure. In contrast, when two arginines are separated by a single amino acid, their guanidinium groups can freely approach each other and they frequently form stacked pairs. Molecular dynamics simulations results are also supported by ab initio calculations, which show stabilization of stacked guanidinium pairs in sufficiently large water clusters.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Division of Organic Chemistry and Biochemistry, Bijičnická Cesta 54

Contributors: Vazdar, M., Vymětal, J., Heyda, J., Vondrášek, J., Jungwirth, P.

Number of pages: 9

Pages: 11193-11201

Publication date: 20 Oct 2011

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physical Chemistry A

Volume: 115

Issue number: 41

ISSN (Print): 1089-5639

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Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1021/jp203519p

URLs:

<http://www.scopus.com/inward/record.url?scp=80054686180&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 80054686180

Research output: Contribution to journal > Article > Scientific > peer-review

### Versatile bio-ink for covalent immobilization of chimeric avidin on sol-gel substrates

A bio-ink for covalent deposition of thermostable, high affinity biotin-binding chimeric avidin onto sol-gel substrates was developed. The bio-ink was prepared from heterobifunctional crosslinker 6-maleimido-hexanoic acid N-hydroxysuccinimide which was first reacted either with 3-aminopropyltriethoxysilane or 3-aminopropyltrimethylethoxysilane to form silane linkers 6-maleimide- N-(3-(triethoxysilyl)propyl)hexanamide or -(ethoxydimethylsilyl)propyl)-hexanamide. C-terminal cysteine genetically engineered to chimeric avidin was reacted with the maleimide group of silane linker in methanol/PBS solution to form a suspension, which was printed on sol-gel modified PMMA film. Different concentrations of chimeric avidin and ratios between silane linkers were tested to find the best properties for the bio-ink to enable gravure or inkjet printing. Bio-ink prepared from 3-aminopropyltriethoxysilane was found to provide the highest amount of active immobilized chimeric avidin. The developed bio-ink was shown to be valuable for automated fabrication of avidin-functionalized polymer films.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Univ of Oulu, VTT Technical Research Centre of Finland, Tampere University Hospital

Contributors: Heikkinen, J. J., Kivimäki, L., Määttä, J. A. E., Mäkelä, I., Hakalahti, L., Takkinen, K., Kulomaa, M. S., Hytönen, V. P., Hormi, O. E. O.

Number of pages: 6

Pages: 409-414

Publication date: 15 Oct 2011

Peer-reviewed: Yes

### Publication information

Journal: Colloids and Surfaces B: Biointerfaces

Volume: 87

Issue number: 2

ISSN (Print): 0927-7765

Ratings:

Scopus rating (2011): CiteScore 3.49 SJR 1.051 SNIP 1.27

Original language: English

ASJC Scopus subject areas: Biotechnology, Colloid and Surface Chemistry, Physical and Theoretical Chemistry, Surfaces and Interfaces

Keywords: Avidin-biotin technology, Biomolecule immobilization, Biosensing, Chimeric avidin, Maleimide, Printing, Sol-gel

DOIs:

10.1016/j.colsurfb.2011.05.052



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Source: Scopus

Source ID: 79960384544

Research output: Contribution to journal › Article › Scientific › peer-review

### **Quantitative glycoproteomic analysis of optimal cutting temperature-embedded frozen tissues identifying glycoproteins associated with aggressive prostate cancer**

Prostate cancer is the most common malignancy in men in the United States, and one in seven men with prostate cancer dies of the disease. A major issue of prostate diagnosis is that there is no good method to reliably distinguish aggressive prostate cancer from nonaggressive prostate cancer. This leads to significant unnecessary suffering among prostate cancer patients and massive unnecessary health care expenditures. In this study, we aim to identify glycoproteins associated with aggressive prostate cancer using optimal cutting temperature (OCT)-embedded frozen tissues obtained from patients with known clinical outcome. To eliminate the interference of mass spectrometric analysis by the compounds in OCT and identify extracellular proteins that are likely to serve as biomarkers in body fluids, we employed glycoproteomic analysis using solid-phase extraction of glycopeptides, which allowed the immobilization of glycopeptides to solid support and removal of OCT from sample proteins before releasing the glycopeptides from the solid support for mass spectrometry analysis. Tumor tissues were cryostat microdissected from four cases of aggressive and four cases of nonaggressive prostate tumors, and glycopeptides were isolated and labeled with iTRAQ reagents before the samples were analyzed with LTQ Orbitrap Velos. From the aggressive prostate cancer tissues, we identified the overexpression of three glycoproteins involved in an extracellular matrix remodeling and further examined two glycoproteins, cathepsin L and periostin, using Western blot and immunohistochemistry analyses. This is the first proteomic study to identify proteins potentially associated with aggressive prostate cancer using OCT-embedded frozen tissues. Further study of these proteins will be needed to understand the roles of extracellular matrix proteins in cancer progression and their potential clinical utility in improving diagnosis of aggressive prostate cancer.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Prostate cancer research center (PCRC), Johns Hopkins University

Contributors: Tian, Y., Bova, G. S., Zhang, H.

Number of pages: 7

Pages: 7013-7019

Publication date: 15 Sep 2011

Peer-reviewed: Yes

#### **Publication information**

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Volume: 83

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ISSN (Print): 0003-2700

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Original language: English

ASJC Scopus subject areas: Analytical Chemistry

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Source: Scopus

Source ID: 80052805542

Research output: Contribution to journal › Article › Scientific › peer-review

### **Tube-like natural halloysite/fluoroelastomer nanocomposites with simultaneous enhanced mechanical, dynamic mechanical and thermal properties**

A novel kind of fluoroelastomer nanocomposites based on tube-like halloysite clay mineral were successfully prepared using a bis-phenol curing system, which resulted in prominent improvements in mechanical and dynamic mechanical properties and in the elevation as high as 30 K of the thermal decomposition temperature. Wide-angle X-ray scattering and transmission electron microscopy techniques were employed to assess the morphology developed in the nanocomposites, while stress strain diagrams were used to evaluate the mechanical properties. These nanocomposites were further characterized by moving die rheometer, dynamic mechanical properties and thermo-gravimetric analysis. Structure-properties relationship and the improvement of the mechanical, dynamic mechanical and thermal properties of fluoroelastomers are reported in the present study. Increasing amount of the filler reduced the curing efficiency of the bis-phenol curing system, which was evident from the rheometric and physical properties of the resulting composites. A sort of filler-filler interaction was perceived during the strain sweep analysis of the composites. The polymer-filler interaction was

reflected in the improved mechanical and thermal properties which were the consequence of proper dispersion of the nanotubes in the polymer matrix; whereas the intercalation of macromolecular chains into the nanotubes was not reflected in the X-ray diffraction analysis.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems

Contributors: Rooj, S., Das, A., Heinrich, G.

Number of pages: 10

Pages: 1746-1755

Publication date: Sep 2011

Peer-reviewed: Yes

#### Publication information

Journal: European Polymer Journal

Volume: 47

Issue number: 9

ISSN (Print): 0014-3057

Ratings:

Scopus rating (2011): CiteScore 3.03 SJR 1.109 SNIP 1.822

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Polymers and Plastics, Organic Chemistry

Keywords: Curing chemistry, Fluoroelastomers, Halloysite nanotube, Nanocomposites, Thermal stability

DOIs:

10.1016/j.eurpolymj.2011.06.007

URLs:

<http://www.scopus.com/inward/record.url?scp=80052038140&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 80052038140

Research output: Contribution to journal > Article > Scientific > peer-review

#### Towards universal enrichment nanocoating for IR-ATR waveguides

Polymer multilayered nanocoating capable of concentrating various chemical substances at IR-ATR waveguide surfaces is described. The coating affinity to an analyte played a pivotal role in sensitivity enhancement of the IR-ATR measurements, since the unmodified waveguide did not show any analyte detection.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Clemson University, School of Materials Science and Engineering/COMSET, University of Delaware, Massachusetts Institute of Technology

Contributors: Giammarco, J., Zdyrko, B., Petit, L., Musgraves, J. D., Hu, J., Agarwal, A., Kimerling, L., Richardson, K., Luzinov, I.

Number of pages: 3

Pages: 9104-9106

Publication date: 28 Aug 2011

Peer-reviewed: Yes

#### Publication information

Journal: Chemical Communications

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Issue number: 32

ISSN (Print): 1359-7345

Ratings:

Scopus rating (2011): CiteScore 5.96 SJR 2.889 SNIP 1.326

Original language: English

ASJC Scopus subject areas: Catalysis, Electronic, Optical and Magnetic Materials, Ceramics and Composites, Chemistry(all), Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry

DOIs:

10.1039/c1cc12780b

URLs:

<http://www.scopus.com/inward/record.url?scp=79961012632&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79961012632

Research output: Contribution to journal › Article › Scientific › peer-review

### From a localized H<sub>3</sub>O radical to a delocalized H<sub>3</sub>O<sup>+</sup>·e<sup>-</sup> solvent-separated pair by sequential hydration

The impact of microhydration on the electronic structure and reactivity of the H<sub>3</sub>O moiety is investigated by ab initio calculations. In the gas phase, H<sub>3</sub>O is a radical with spin density localized on its hydrogen end, which is only kinetically stable and readily decomposes into a water molecule and a hydrogen atom. When solvated by a single water molecule, H<sub>3</sub>O preserves to a large extent its radical character, however, two water molecules are already capable to shift most of the spin density to the solvent. With three solvating water molecules this shift is practically completed and the system is best described as a solvent-separated pair of a hydronium cation and a hydrated electron. The electronic structure of this system and its proton transfer reactivity leading to formation of a hydrogen atom already resemble those of a proton-electron pair in bulk water.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Uhlig, F., Marsalek, O., Jungwirth, P.

Number of pages: 7

Pages: 14003-14009

Publication date: 21 Aug 2011

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

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URLs:

<http://www.scopus.com/inward/record.url?scp=79960952162&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79960952162

Research output: Contribution to journal › Article › Scientific › peer-review

### Urea and guanidinium induced denaturation of a Trp-cage miniprotein

Using a combination of experimental techniques (circular dichroism, differential scanning calorimetry, and NMR) and molecular dynamics simulations, we performed an extensive study of denaturation of the Trp-cage miniprotein by urea and guanidinium. The experiments, despite their different sensitivities to various aspects of the denaturation process, consistently point to simple, two-state unfolding process. Microsecond molecular dynamics simulations with a femtosecond time resolution allow us to unravel the detailed molecular mechanism of Trp-cage unfolding. The process starts with a destabilizing proline shift in the hydrophobic core of the miniprotein, followed by a gradual destruction of the hydrophobic loop and the  $\alpha$ -helix. Despite differences in interactions of urea vs guanidinium with various peptide moieties, the overall destabilizing action of these two denaturants on Trp-cage is very similar.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, University of Leeds

Contributors: Heyda, J., Kožíšek, M., Bednářová, L., Thompson, G., Konvalinka, J., Vondrášek, J., Jungwirth, P.

Number of pages: 15

Pages: 8910-8924

Publication date: 21 Jul 2011

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 115

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ISSN (Print): 1520-6106

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/jp200790h

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<http://www.scopus.com/inward/record.url?scp=79960344032&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79960344032

Research output: Contribution to journal › Article › Scientific › peer-review

### **Defined-size DNA triple crossover construct for molecular electronics: Modification, positioning and conductance properties**

We present a novel, defined-size, small and rigid DNA template, a so-called B-A-B complex, based on DNA triple crossover motifs (TX tiles), which can be utilized in molecular scale patterning for nanoelectronics, plasmonics and sensing applications. The feasibility of the designed construct is demonstrated by functionalizing the TX tiles with one biotin-triethylene glycol (TEG) and efficiently decorating them with streptavidin, and furthermore by positioning and anchoring single thiol-modified B-A-B complexes to certain locations on a chip via dielectrophoretic trapping. Finally, we characterize the conductance properties of the non-functionalized construct, first by measuring DC conductivity and second by utilizing AC impedance spectroscopy in order to describe the conductivity mechanism of a single B-A-B complex using a detailed equivalent circuit model. This analysis also reveals further information about the conductivity of DNA structures in general.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Jyväskylän yliopisto, Adult Stem Cells, School of Management (JKK)

Contributors: Linko, V., Leppiniemi, J., Paasonen, S. T., Hytönen, V. P., Jussi Toppari, J.

Publication date: 8 Jul 2011

Peer-reviewed: Yes

#### **Publication information**

Journal: Nanotechnology

Volume: 22

Issue number: 27

Article number: 275610

ISSN (Print): 0957-4484

Ratings:

Scopus rating (2011): CiteScore 3.86 SJR 1.899 SNIP 1.471

Original language: English

ASJC Scopus subject areas: Bioengineering, Chemistry(all), Electrical and Electronic Engineering, Mechanical Engineering, Mechanics of Materials, Materials Science(all)

DOIs:

10.1088/0957-4484/22/27/275610

URLs:

<http://www.scopus.com/inward/record.url?scp=79957825438&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79957825438

Research output: Contribution to journal › Article › Scientific › peer-review

### **Internal structure, hygroscopic and reactive properties of mixed sodium methanesulfonate-sodium chloride particles**

Internal structures, hygroscopic properties and heterogeneous reactivity of mixed  $\text{CH}_3\text{SO}_3\text{Na}/\text{NaCl}$  particles were investigated using a combination of computer modeling and experimental approaches. Surfactant properties of  $\text{CH}_3\text{SO}_3^-$  ions and their surface accumulation in wet, deliquesced particles were assessed using molecular dynamics (MD) simulations and surface tension measurements. Internal structures of dry  $\text{CH}_3\text{SO}_3\text{Na}/\text{NaCl}$  particles were investigated using scanning electron microscopy (SEM) assisted with X-ray microanalysis mapping, and time-of-flight secondary ion mass spectrometry (TOF-SIMS). The combination of these techniques shows that dry  $\text{CH}_3\text{SO}_3\text{Na}/\text{NaCl}$  particles are composed of a NaCl core surrounded by a  $\text{CH}_3\text{SO}_3\text{Na}$  shell. Hygroscopic growth, deliquescence and efflorescence phase

transitions of mixed  $\text{CH}_3\text{SO}_3\text{Na}/\text{NaCl}$  particles were determined and compared to those of pure  $\text{NaCl}$  particles. These results indicate that particles undergo a two step deliquescence transition: first at ~69% relative humidity (RH) the  $\text{CH}_3\text{SO}_3\text{Na}$  shell takes up water, and then at ~75% RH the  $\text{NaCl}$  core deliquesces. Reactive uptake coefficients for the particle- $\text{HNO}_3$  heterogeneous reaction were determined at different  $\text{CH}_3\text{SO}_3\text{Na}/\text{NaCl}$  mixing ratios and RH. The net reaction probability decreased notably with increasing  $\text{CH}_3\text{SO}_3\text{Na}$  and at lower RH.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Colorado at Denver, Kyushu University, Colorado State University, University of Southern California, Pacific Northwest National Laboratory, Defence Science and Technology Laboratory, Lawrence Berkeley National Laboratory, Department of Aerospace and Mechanical Engineering, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Liu, Y., Minofar, B., Desyaterik, Y., Dames, E., Zhu, Z., Cain, J. P., Hopkins, R. J., Gilles, M. K., Wang, H., Jungwirth, P., Laskin, A.

Number of pages: 12

Pages: 11846-11857

Publication date: 7 Jul 2011

Peer-reviewed: Yes

#### Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 13

Issue number: 25

ISSN (Print): 1463-9076

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Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

DOIs:

10.1039/c1cp20444k

URLs:

<http://www.scopus.com/inward/record.url?scp=79960772846&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79960772846

Research output: Contribution to journal > Article > Scientific > peer-review

#### Steric and electronic effects in the host-guest hydrogen bonding in clathrate hydrates

Clathrate hydrates with polar guest molecules (dimethyl ether, ethylene oxide, trimethylene oxide, tetrahydrofuran, and tetrahydropyran) were studied by means of the density functional theory. A model of a large cage of structure-I clathrate was employed. Optimal configurations of encaged guests were investigated with a focus on the host-guest hydrogen bond formation. Weak hydrogen bonds were found to be formed by each guest, while for THP a strong hydrogen bond and formation of L-defect was also observed. This is in accord with previous computational and experimental studies. Steric factors were shown to play a key role for the strength of the hydrogen bond formed. Interestingly, the host-guest binding is influenced not only by the size of a guest molecule but also by its shape. This work demonstrates that both electronic and steric properties of a polar guest should be considered for a full description of clathrate systems.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), K. Gumiński Department of Theoretical Chemistry, Uniwersytet Jagiellonski w Krakowie, J. Heyrovský Institute of Physical Chemistry, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Kulig, W., Kubisiak, P., Cwiklik, L.

Number of pages: 6

Pages: 6149-6154

Publication date: 16 Jun 2011

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry A

Volume: 115

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ISSN (Print): 1089-5639

Ratings:

Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

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10.1021/jp111245z

URLs:

<http://www.scopus.com/inward/record.url?scp=79959539436&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79959539436

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Behavior of $\beta$ -amyloid 1-16 at the air-water interface at varying pH by nonlinear spectroscopy and molecular dynamics simulations**

The adsorption and aggregation of  $\beta$ -amyloid (1-16) fragment at the air-water interface was investigated by the combination of second harmonic generation (SHG) spectroscopy, Brewster angle microscopy (BAM), and molecular dynamics simulations (MD). The Gibbs free energy of surface adsorption was measured to be -10.3 kcal/mol for bulk pHs of 7.4 and 3, but no adsorption was observed for pH 10-11. The 1-16 fragment is believed not to be involved in fibril formation of the  $\beta$ -amyloid protein, but it exhibits interesting behavior at the air-water interface, as manifested in two time scales for the observed SHG response. The shorter time scale (minutes) reflects the surface adsorption, and the longer time scale (hours) reflects rearrangement and aggregation of the peptide at the air-water interface. Both of these processes are also evidenced by BAM measurements. MD simulations confirm the pH dependence of surface behavior of the  $\beta$ -amyloid, with largest surface affinity found at pH = 7. It also follows from the simulations that phenylalanine is the most surface exposed residue, followed by tyrosine and histidine in their neutral form.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), American University, Crop and Soil Sciences, Cornell Univ., Midwest Research Institute - Kansas City, Berkeley, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

Contributors: Miller, A. E., Petersen, P. B., Hollars, C. W., Saykally, R. J., Heyda, J., Jungwirth, P.

Number of pages: 8

Pages: 5873-5880

Publication date: 16 Jun 2011

Peer-reviewed: Yes

#### **Publication information**

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Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

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<http://www.scopus.com/inward/record.url?scp=79959981055&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79959981055

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **Behavior of the eigen form of hydronium at the air/water interface**

Surface affinity of hydronium was explored using umbrella sampling molecular dynamics simulations with a refined polarizable potential. The polarizable interaction potential of  $\text{H}_3\text{O}^+$  was reparametrized against accurate ab initio calculations for geometries including a water molecule approaching the Eigen cation from its oxygen side. Although there is no true hydrogen bonding with  $\text{H}_3\text{O}^+$  acting as an acceptor, respecting in the force field the very shallow ab initio minimum corresponding to this interaction leads to a decrease in surface propensity of hydronium compared to previous results. Qualitatively, the mild surface affinity and strong surface orientation of hydronium is, nevertheless, robustly predicted by various computational approaches, as well as by spectroscopic experiments.

#### **General information**

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, J. Heyrovský Institute of Physical Chemistry  
Contributors: Jagoda-Cwiklik, B., Cwiklik, L., Jungwirth, P.  
Number of pages: 6  
Pages: 5881-5886  
Publication date: 16 Jun 2011  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry A

Volume: 115

Issue number: 23

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1021/jp110078s

URLs:

<http://www.scopus.com/inward/record.url?scp=79959934455&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79959934455

Research output: Contribution to journal > Article > Scientific > peer-review

#### Preparation of zinc oxide free, transparent rubber nanocomposites using a layered double hydroxide filler

A layered double hydroxide (LDH) mineral filler particle has been designed and employed in rubber vulcanization to prepare a more environmentally friendly rubber composite. The LDH delivers zinc ions in the vulcanization process as accelerators, stearate anions as activators and simultaneously the mineral sheets act as a nanofiller to reinforce the rubber matrix whilst totally replacing the separate zinc oxide (ZnO) and stearic acid conventionally used in the formulation of rubber. This method leads to a significant reduction (nearly 10 times) of the zinc level and yields excellent transparent properties in the final rubber product. The morphological characterization, rheometric curing behaviour, mechanical properties and uniaxial multi-hysteresis behaviours of the resultant rubber/LDH nanocomposite are studied in this paper.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V., Durham University

Contributors: Das, A., Wang, D. Y., Leuteritz, A., Subramaniam, K., Greenwell, H. C., Wagenknecht, U., Heinrich, G.

Number of pages: 7

Pages: 7194-7200

Publication date: 28 May 2011

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Materials Chemistry

Volume: 21

Issue number: 20

ISSN (Print): 0959-9428

Ratings:

Scopus rating (2011): SJR 2.614 SNIP 1.539

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Chemistry

DOIs:

10.1039/c0jm03784b

URLs:

<http://www.scopus.com/inward/record.url?scp=79955619174&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79955619174

Research output: Contribution to journal > Article > Scientific > peer-review

### Detection of DNA hybridisation in a diluted serum matrix by surface plasmon resonance and film bulk acoustic resonators

Nanomolar quantities of single-stranded DNA products ~ 100 nucleotides long can be detected in diluted 1% serum by surface plasmon resonance (SPR) and film bulk acoustic resonators (FBARs). We have used a novel FBAR sensor in parallel with SPR and obtained promising results with both the acoustic and the optical device. Oligonucleotides and a repellent lipoamide, Lipa-DEA, were allowed to assemble on the sensor chip surfaces for only 15 min by dispensing. Lipa-DEA surrounds the analyte-binding probes on the surface and effectively reduces the non-specific binding of bovine serum albumin and non-complementary strands. In a highly diluted serum matrix, the non-specific binding is, however, a hindrance, and the background response must be reduced. Nanomolar concentrations of short complementary oligos could be detected in buffer, whereas the response was too low to be measured in serum. DNA strands that are approximately 100 base pairs long at concentrations as low as 1-nM could be detected both in buffer and in 1% serum by both SPR and the FBAR resonator.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), VTT Technical Research Centre of Finland, HCl e 486.1, Siemens AG

Contributors: Auer, S., Nirschl, M., Schreiter, M., Vikholm-Lundin, I.

Number of pages: 10

Pages: 1387-1396

Publication date: May 2011

Peer-reviewed: Yes

#### Publication information

Journal: Analytical and Bioanalytical Chemistry

Volume: 400

Issue number: 5

ISSN (Print): 1618-2642

Ratings:

Scopus rating (2011): CiteScore 3.47 SJR 1.37 SNIP 1.27

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Biochemistry

Keywords: DNA hybridisation detection, DNA sensor, Film bulk acoustic resonator, Self-assembled monolayer, Serum, Surface plasmon resonance

DOIs:

10.1007/s00216-011-4871-0

URLs:

<http://www.scopus.com/inward/record.url?scp=79955562374&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79955562374

Research output: Contribution to journal > Article > Scientific > peer-review

### Energetic origin of proton affinity to the air/water interface

Recent experimental and theoretical studies showed the preference of the hydronium ion for the vapor/water interface. To investigate the mechanism responsible for the surface propensity of this ion, we performed a series of novel quantum chemical simulations combined with the theory of solutions. The solvation free energy of the  $\text{H}_3\text{O}^+$  solute placed at the interface was obtained as -97.9 kcal/mol, being more stable by 3.6 kcal/mol than that of the solute embedded in the bulk. Further, we decomposed the solvation free energies into contributions from the water molecules residing in the oxygen and the hydrogen sides of the solute to clarify the origin of the surface preference. When the solute was displaced from the bulk to the interface, it was shown that the free energy contribution from the oxygen side is destabilized by ~10 kcal/mol because of a reduction of the number of surrounding solvent water molecules. It was observed, however, that the free energy contribution due to the hydrogen side of the solute is unexpectedly stabilizing and surpasses the destabilization in the opposite side. We found that the stabilization in the hydrogen side originates from the solute-solvent interaction in the medium range beyond the nearest neighbor. It was also revealed that the free energy contribution due to the solute's electronic polarization amounts to about the half of the total free energy change associated with the solute displacement from the bulk to the interface.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Tohoku University, Osaka University, Kyoto Women's University, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Japan Science and Technology Agency



Contributors: Takahashi, H., Maruyama, K., Karino, Y., Morita, A., Nakano, M., Jungwirth, P., Matubayasi, N.  
Number of pages: 7  
Pages: 4745-4751  
Publication date: 28 Apr 2011  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 115

Issue number: 16

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2011): CiteScore 3.62 SJR 1.801 SNIP 1.223

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films  
DOIs:

10.1021/jp2015676

URLs:

<http://www.scopus.com/inward/record.url?scp=79955461660&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79955461660

Research output: Contribution to journal > Article > Scientific > peer-review

#### Molecular dynamics simulations of the interactions of kinin peptides with an anionic POPS bilayer

We have performed molecular dynamics simulations of peptide hormone bradykinin (BK) and its fragment des-Arg9-BK in the presence of an anionic lipid bilayer, with an aim toward delineating the mechanism of action related to their bioactivity. Starting from the initial aqueous environment, both of the peptides are quickly adsorbed and stabilized on the cell surface. Whereas BK exhibits a stronger interaction with the membrane and prefers to stay on the interface, des-Arg9-BK, with the loss of C-terminal Arg, penetrates further. The heterogeneous lipid-water interface induces  $\beta$ -turn-like structure in the otherwise inherently flexible peptides. In the membrane-bound state, we observed C-terminal  $\beta$ -turn formation in BK, whereas for des-Arg9-BK, with the deletion of Arg9, turn formation occurred in the middle of the peptide. The basic Arg residues anchor the peptide to the bilayer by strong electrostatic interactions with charged lipid headgroups. Simulations with different starting orientations of the peptides with respect to the bilayer surface lead to the same observations, namely, the relative positioning of the peptides on the membrane surface, deeper penetration of the des-Arg9-BK, and the formation of turn structures. The lipid headgroups adjacent to the bound peptides become substantially tilted, causing bilayer thinning near the peptide contact region and increase the degree of disorder in nearby lipids. Again, because of hydrogen bonding with the peptide, the neighboring lipid's polar heads exhibit considerably reduced flexibility. Corroborating findings from earlier experiments, our results provide important information about how the lipid environment promotes peptide orientation/conformation and how the peptide adapts to the environment.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Calcutta

Contributors: Manna, M., Mukhopadhyay, C.

Number of pages: 10

Pages: 3713-3722

Publication date: 5 Apr 2011

Peer-reviewed: Yes

#### Publication information

Journal: Langmuir

Volume: 27

Issue number: 7

ISSN (Print): 0743-7463

Ratings:

Scopus rating (2011): CiteScore 4.42 SJR 2.051 SNIP 1.341

Original language: English

ASJC Scopus subject areas: Electrochemistry, Condensed Matter Physics, Surfaces and Interfaces, Materials Science(all), Spectroscopy

DOIs:

10.1021/la104046z

URLs:

<http://www.scopus.com/inward/record.url?scp=79953236597&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79953236597

Research output: Contribution to journal › Article › Scientific › peer-review

### **Ionization of purine tautomers in nucleobases, nucleosides, and nucleotides: From the gas phase to the aqueous environment**

We have simulated ionization of purine nucleic acid components in the gas phase and in a water environment. The vertical and adiabatic ionization processes were calculated at the PMP2/aug-cc-pVDZ level with the TDDFT method applied to obtain ionization from the deeper lying orbitals. The water environment was modeled via microsolvation approach and using a nonequilibrium polarizable continuum model. We have characterized a set of guanine tautomers and investigated nucleosides and nucleotides in different conformations. The results for guanine, i.e., the nucleic acid base with the lowest vertical ionization potential, were also compared to those for the other purine base, adenine. The main findings of our study are the following: (i) Guanine remains clearly the base with the lowest ionization energy even upon aqueous solvation. (ii) Water solvent has a strong effect on the ionization energetics of guanine and adenine and their derivatives; the vertical ionization potential (VIP) is lowered by about 1 eV for guanine while it is ~1.5 eV higher in the nucleotides, overall resulting in similar VIPs for GMP<sup>-</sup>, guanosine and guanine in water. (iii) Water efficiently screens the electrostatic interactions between nucleic acid components. Consequently, ionization in water always originates from the base unit of the nucleic acid and all the information about conformational state is lost in the ionization energetics. (iv) The energy splitting between ionization of the two least bound electrons increases upon solvation. (v) Tautomerism does not contribute to the width of the photoelectron spectra in water. (vi) The effect of specific short-range interactions with individual solvent molecules is negligible for purine bases, compared to the long-range dielectric effects of the aqueous medium.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Department of Physical Chemistry, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, University of Southern California

Contributors: Pluhařová, E., Jungwirth, P., Bradforth, S. E., Slaviček, P.

Number of pages: 12

Pages: 1294-1305

Publication date: 10 Feb 2011

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry Part B

Volume: 115

Issue number: 5

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2011): CiteScore 3.62 SJR 1.801 SNIP 1.223

Original language: English

ASJC Scopus subject areas: Surfaces, Coatings and Films, Physical and Theoretical Chemistry, Materials Chemistry

DOIs:

10.1021/jp110388v

URLs:

<http://www.scopus.com/inward/record.url?scp=79952844542&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79952844542

Research output: Contribution to journal › Article › Scientific › peer-review

### **Site-specific polarizabilities as predictors of favorable adsorption sites on Nan clusters**

The adsorption of water and ammonia molecules to Na<sub>n</sub> (n = 7, 18, and 25) clusters was studied using density functional theory calculations. Calculated adsorption energies are small (

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Central Michigan University, Argonne National Laboratory

Contributors: Ma, L., Jackson, K. A., Jellinek, J.

Number of pages: 6

Pages: 80-85

Publication date: 8 Feb 2011

Peer-reviewed: Yes

### Publication information

Journal: Chemical Physics Letters

Volume: 503

Issue number: 1-3

ISSN (Print): 0009-2614

Ratings:

Scopus rating (2011): CiteScore 2.38 SJR 1.159 SNIP 1.004

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

DOIs:

10.1016/j.cplett.2010.12.049

URLs:

<http://www.scopus.com/inward/record.url?scp=79751533497&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79751533497

Research output: Contribution to journal › Article › Scientific › peer-review

### Interactions of molecular ions with model phospholipid membranes

The affinities of a series of biologically relevant ions for a hydrated phospholipid membrane were investigated using molecular dynamics simulation. Interactions of molecular ions, such as guanidinium, tetramethylammonium, and thiocyanate with the bilayer were computationally characterized for the first time. Simulations reveal strong ion specificity. On one hand, ions like guanidinium and thiocyanate adsorb relatively strongly to the headgroup region of the membrane. On the other hand, potassium or chloride interact very weakly with the phospholipids and merely act as neutralizing counterions. Calculations also show that these ions affect differently biophysical properties of the membrane, such as lipid diffusion, headgroup hydration and tilt angle.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Academy of Sciences of Czech Republic, J. Heyrovský Institute of Physical Chemistry

Contributors: Petrov, M., Cwiklik, L., Jungwirth, P.

Number of pages: 17

Pages: 695-711

Publication date: 2011

Peer-reviewed: Yes

### Publication information

Journal: Collection of Czechoslovak Chemical Communications

Volume: 76

Issue number: 6

ISSN (Print): 0010-0765

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Biophysics, Molecular dynamics, Phospholipids

DOIs:

10.1135/cccc2011026

URLs:

<http://www.scopus.com/inward/record.url?scp=79958070440&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79958070440

Research output: Contribution to journal › Article › Scientific › peer-review

### An electro-optically tunable Bragg reflector based on liquid crystals

In this paper we report the analysis of a distributed feedback guided-wave reflector in liquid crystals and we describe the main properties of the device. The device is based on a comb-shaped interdigitated electrodes and a liquid crystal slab. The device shows a wide tuning range exceeding 100 nm covering C and L bands for wavelength division multiplexing.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Sapienza University, University "Roma Tre", Dipartimento di Ingegneria dell'Informazione, Elettronica e Telecomunicazioni

Contributors: Gilardi, G., Asquini, R., D'Alessandro, A., Assanto, G.

Number of pages: 7  
Pages: 62-68  
Publication date: 2011  
Peer-reviewed: Yes

#### Publication information

Journal: Molecular Crystals and Liquid Crystals

Volume: 549

ISSN (Print): 1542-1406

Ratings:

Scopus rating (2011): CiteScore 0.53 SJR 0.288 SNIP 0.473

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Science(all)

Keywords: electro-optic effect, liquid crystals, Optical waveguides

DOIs:

10.1080/15421406.2011.581137

URLs:

<http://www.scopus.com/inward/record.url?scp=80053362957&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 80053362957

Research output: Contribution to journal > Article > Scientific > peer-review

#### Enrichment polymer layers for detection of volatile vapors by ATR FT-IR

Fourier Transformed Infrared Spectroscopy (FT-IR) is an effective analytical method for the identification of organic compounds be they man made or naturally produced. There is, however, a limitation to what a normal FT-IR can detect if an analyte is in vapor phase or in low concentration. To this end, we have applied enrichment polymer layer systems (EPLS) to an attenuated total reflection (ATR) crystal waveguide to enhance detection capability for the method. These EPLS are comprised of polymers with different functionality along the backbone and provide unique interaction capabilities that can attract volatile chemicals and concentrate them in the evanescence wave region. The thickness of the polymer layers is kept on 30-50nm level. The EPLS were characterized by atomic force microscopy, ellipsometry and FT-IR. The overall goal of this work is to construct a "universal" sensor platform capable of detecting a wide range of volatile organic chemicals via infrared spectroscopy.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Massachusetts Institute of Technology, School of Materials Science and Engineering/COMSET, Clemson University, Department of Materials Science and Engineering, University of Delaware

Contributors: Giammarco, J. M., Zdyrko, B., Hu, J., Agarwal, A., Kimerling, L., Carlie, N., Petit, L., Richardson, K., Luzinov, I.

Publication date: 2011

Peer-reviewed: Yes

#### Publication information

Journal: ACS National Meeting Book of Abstracts

ISSN (Print): 0065-7727

Original language: English

ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

URLs:

<http://www.scopus.com/inward/record.url?scp=80051876637&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 80051876637

Research output: Contribution to journal > Article > Scientific > peer-review

#### Efficient production of NV colour centres in nanodiamonds using high-energy electron irradiation

Nanodiamond powders with an average size of 50 nm have been irradiated using high-energy electron beam. After annealing and chemical treatment, nanodiamond colloidal solutions were obtained and deposited on silica coverslips by spin-coating. The fluorescence of nanodiamonds was studied by confocal microscopy together with atomic force microscopy. We evaluated the proportion of luminescent nanodiamonds as a function of the irradiation duration and showed that large quantities, exceeding hundreds of mg, of luminescent nanodiamonds can be produced within 1 h of electron irradiation.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Laboratoire de Physique Quantique et Moléculaire

Contributors: Dantelle, G., Slablab, A., Rondin, L., Lainé, F., Carrel, F., Bergonzo, P., Perruchas, S., Gacoin, T., Treussart, F., Roch, J. F.

Number of pages: 4

Pages: 1655-1658

Publication date: Sep 2010

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Luminescence

Volume: 130

Issue number: 9

ISSN (Print): 0022-2313

Ratings:

Scopus rating (2010): SJR 0.909 SNIP 1.103

Original language: English

ASJC Scopus subject areas: Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Chemistry(all), Biochemistry, Biophysics

Keywords: Diamond, Luminescence, NV centre

DOIs:

10.1016/j.jlumin.2009.12.003

URLs:

<http://www.scopus.com/inward/record.url?scp=77955274026&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 77955274026

Research output: Contribution to journal > Article > Scientific > peer-review

#### On entropy-based molecular descriptors: Statistical analysis of real and synthetic chemical structures

This paper presents an analysis of entropy-based molecular descriptors. Specifically, we use real chemical structures, as well as synthetic isomeric structures, and investigate properties of and among descriptors with respect to the used data set by a statistical analysis. Our numerical results provide evidence that synthetic chemical structures are notably different to real chemical structures and, hence, should not be used to investigate molecular descriptors. Instead, an analysis based on real chemical structures is favorable. Further, we find strong hints that molecular descriptors can be partitioned into distinct classes capturing complementary information.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: TU Vienna, Technical University Darmstadt, Computational Biology and Machine Learning, School of Medicine

Contributors: Dehmer, M., Varmuza, K., Borgert, S., Emmert-Streib, F.

Number of pages: 9

Pages: 1655-1663

Publication date: 27 Jul 2009

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Chemical Information and Modeling

Volume: 49

Issue number: 7

ISSN (Print): 1549-9596

Ratings:

Scopus rating (2009): SJR 1.039 SNIP 1.219

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Chemistry(all), Computer Science Applications, Library and Information Sciences

DOIs:

10.1021/ci900060x

URLs:

<http://www.scopus.com/inward/record.url?scp=68149167631&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 68149167631

Research output: Contribution to journal > Article > Scientific > peer-review

### **Structural information content of networks: Graph entropy based on local vertex functionals**

In this paper we define the structural information content of graphs as their corresponding graph entropy. This definition is based on local vertex functionals obtained by calculating  $j$ -spheres via the algorithm of Dijkstra. We prove that the graph entropy and, hence, the local vertex functionals can be computed with polynomial time complexity enabling the application of our measure for large graphs. In this paper we present numerical results for the graph entropy of chemical graphs and discuss resulting properties.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: TU Vienna, Department of Biostatistics, Visiting Graduate Student in Department of Urban Design and Planning, University of Washington, Seattle, USA 1.1.2012-15.6.2012 (12.9.2011 alkaen), Department of Genome Sciences

Contributors: Dehmer, M., Emmert-Streib, F.

Number of pages: 8

Pages: 131-138

Publication date: Apr 2008

Peer-reviewed: Yes

#### **Publication information**

Journal: Computational Biology and Chemistry

Volume: 32

Issue number: 2

ISSN (Print): 1476-9271

Ratings:

Scopus rating (2008): SJR 0.795 SNIP 0.687

Original language: English

ASJC Scopus subject areas: Biochemistry, Structural Biology, Analytical Chemistry, Physical and Theoretical Chemistry

Keywords: Chemical graph theory, Gene networks, Graph entropy, Information theory, Structural information content

DOIs:

10.1016/j.compbiolchem.2007.09.007

Source: Scopus

Source ID: 40049085450

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

### **The structural information content of chemical networks**

We present an information-theoretic method to measure the structural information content of networks and apply it to chemical graphs. As a result, we find that our entropy measure is more general than classical information indices known in mathematical and computational chemistry. Further, we demonstrate that our measure reflects the essence of molecular branching meaningfully by determining the structural information content of some chemical graphs numerically.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: TU Vienna, Department of Biostatistics, Visiting Graduate Student in Department of Urban Design and Planning, University of Washington, Seattle, USA 1.1.2012-15.6.2012 (12.9.2011 alkaen)

Contributors: Dehmer, M., Emmert-Streib, F.

Number of pages: 4

Pages: 155-158

Publication date: Mar 2008

Peer-reviewed: Yes

#### **Publication information**

Journal: Zeitschrift fur Naturforschung Section A: A Journal of Physical Sciences

Volume: 63

Issue number: 3-4

ISSN (Print): 0932-0784

Ratings:

Scopus rating (2008): SJR 0.318 SNIP 0.78

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

Keywords: Chemical graph theory, Graph entropy, Information theory, Structural information content

URLs:

<http://www.scopus.com/inward/record.url?scp=46649096825&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 46649096825

Research output: Contribution to journal › Article › Scientific › peer-review

### **Batch dark fermentative hydrogen production from grass silage: The effect of inoculum, pH, temperature and VS ratio**

The potential for fermentative hydrogen ( $H_2$ ) production from grass silage was evaluated in laboratory batch assays. First, two different inocula (from a dairy farm digester and digested sewage sludge) were studied with and without prior heat treatment and pH adjustment. Only the inoculum from the dairy farm digester produced  $H_2$  from grass silage. Without heat treatment, methane ( $CH_4$ ) was mainly produced, but heat treatment efficiently inhibited  $CH_4$  production. pH adjustment to 6 further increased  $H_2$  production. The effects of initial pH (4, 5 and 6), temperature (35, 55 and 70 °C) and the substrate to inoculum volatile solids (VS) ratio (henceforth VS ratio) (1:1; 1.5:1 and 2:1) on  $H_2$  production from grass silage were evaluated with heat-treated dairy farm digester sludge as inoculum. Optimal pH was found to be between 5 and 6, while at pH 4 no  $H_2$  was formed. The highest  $H_2$  yield was achieved at 70 °C.  $H_2$  production also increased when the VS ratio was increased. However, the overall energy value of  $H_2$  compared to that of  $CH_4$  production remained low.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Jyväskylän yliopisto, University of Jyväskylä

Contributors: Pakarinen, O., Lehtomäki, A., Rintala, J.

Number of pages: 8

Pages: 594-601

Publication date: Jan 2008

Peer-reviewed: Yes

#### **Publication information**

Journal: International Journal of Hydrogen Energy

Volume: 33

Issue number: 2

ISSN (Print): 0360-3199

Ratings:

Scopus rating (2008): SJR 1.389 SNIP 2.1

Original language: English

ASJC Scopus subject areas: Electrochemistry, Fuel Technology, Renewable Energy, Sustainability and the Environment

Keywords: Fermentative hydrogen production, Grass silage, Heat treatment, pH, Temperature, VS ratio

DOIs:

10.1016/j.ijhydene.2007.10.008

Source: Scopus

Source ID: 39049172869

Research output: Contribution to journal › Article › Scientific › peer-review

### **Ultrasound-assisted extraction in the determination of arsenic, cadmium, copper, lead, and silver in contaminated soil samples by inductively coupled plasma atomic emission spectrometry**

An extraction method was developed for the determination of toxic elements in contaminated soil samples by inductively coupled plasma atomic emission spectrometry (ICP-AES). The determination of arsenic, cadmium, lead, and silver in ultrasound-assisted extracts of SRM 2710 and SRM 2711 by ICP-AES was carried out with high accuracy and precision (RSD<3.7%). The certified concentrations of the SRMs were obtained for arsenic, cadmium, lead, and silver by using an ultrasound-assisted extraction method with a digestion solution of (1+1)-diluted aqua regia. The determination of copper in SRMs by the ultrasound-assisted extraction method and analysis by ICP-AES failed to obtain the certified concentrations at the 95% level of confidence using ( $\pm 2$  s) as confidence limits of the mean. However, the same results were observed with the use of the microwave digestion method and reflux, which is the ISO 11466 standard method. The analysis of the SRMs showed that the ultrasound-assisted extraction method is highly comparable with the other methods used for such purposes. The major advantages of the ultrasound-assisted extraction method compared to the microwave and reflux methods are the high treatment rate (50 samples simultaneously in nine minutes) and low reagent usage, the main benefit of which are the low chloride and nitrate concentrations in the extracts.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Jyväskylän yliopisto, University of Jyväskylä

Contributors: Väisänen, A., Suontamo, R., Silvonen, J., Rintala, J.

Number of pages: 5

Pages: 93-97  
Publication date: 2002  
Peer-reviewed: Yes

#### Publication information

Journal: Analytical and Bioanalytical Chemistry  
Volume: 373  
Issue number: 1-2  
ISSN (Print): 1618-2642  
Ratings:

Scopus rating (2002): SJR 0.72 SNIP 0.771

Original language: English

ASJC Scopus subject areas: Clinical Biochemistry, Analytical Chemistry

Keywords: Contaminated soil, Elemental analyses, ICP-AES, Toxic metals, Ultrasound-assisted extraction

DOIs:

10.1007/s00216-002-1290-2

URLs:

<http://www.scopus.com/inward/record.url?scp=0036012773&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 0036012773

Research output: Contribution to journal > Article > Scientific > peer-review

#### Control of matrix interferences by the multiple linear regression model in the determination of arsenic, antimony and tin in lead pellets by inductively coupled plasma atomic emission spectrometry

A multiple linear regression technique was used to evaluate the matrix interferences in the determination of hydride-forming elements in lead shotgun pellets by inductively coupled plasma atomic emission spectrometry. The determination of arsenic, antimony, and tin in SRM C2416 (Bullet Lead) by ICP-AES failed to obtain the certified concentrations at the 95% level of confidence using the t-test. However, it proved possible, by using the multiple linear regression technique, to correct the concentrations of all three elements to a statistically acceptable level. This method of correction is based on the multiple regression line obtained from the analysis of 19 synthetic mixtures of matrix elements (arsenic, antimony, bismuth, copper, silver, and tin) in five levels of concentrations. The direct determination of bismuth, copper and silver in SRM C2416 was performed with high accuracy and precision (RSD < 2.2%) as was the determination of arsenic, antimony, and tin after the correction. Total element recovery varied from 95.6% to 101.8% in the SRM sample analyzed.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Jyväskylä

Contributors: Väisänen, A., Suontamo, R., Rintala, J.

Number of pages: 3

Pages: 274-276

Publication date: 2002

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Analytical Atomic Spectrometry

Volume: 17

Issue number: 3

ISSN (Print): 0267-9477

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Original language: English

ASJC Scopus subject areas: Spectroscopy

DOIs:

10.1039/b108543n

URLs:

<http://www.scopus.com/inward/record.url?scp=0036009258&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 0036009258

Research output: Contribution to journal > Article > Scientific > peer-review

#### Vilsmeier formylation of 2-carboxyindoles and preparation of O-benzylhydroxyureas on solid phase

The Vilsmeier formylation has been introduced for the solid-phase functionalization of five different 2-carboxyindoles. The aldehyde functionality has been utilized in the preparation of O-benzylhydroxyureas.



### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Helsinki University, Department of Pharmacy, Division of Pharmaceutical Chemistry, Division of Pharmacognosy, Viikki Drug Discov. Technol. Center, University of Tokyo  
Contributors: Tois, J., Franzén, R., Aitio, O., Laakso, I., Kylänlahti, I.  
Number of pages: 4  
Pages: 542-545  
Publication date: Nov 2001  
Peer-reviewed: Yes

### Publication information

Journal: Journal of Combinatorial Chemistry  
Volume: 3  
Issue number: 6  
ISSN (Print): 1520-4766  
Original language: English  
ASJC Scopus subject areas: Chemistry(all), Organic Chemistry, Discrete Mathematics and Combinatorics, Drug Discovery  
DOIs:  
10.1021/cc010004f  
Source: Scopus  
Source ID: 0035514539  
Research output: Contribution to journal > Article > Scientific > peer-review

### Solid-phase bromination and Suzuki coupling of 2-carboxyindoles

As part of an ongoing lead discovery project we have developed a convenient method for the modification and substitution of indole moieties at the 3-position. Selective bromination of three different 2-carboxyindoles was followed by Suzuki cross-coupling with aryl and heteroaryl boronic acids on a Merrifield resin solid-phase. After column chromatography, yields of the 3- substituted indoles ranged from 42-98%.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: University of Helsinki, Department of Pharmacy  
Contributors: Tois, J., Franzén, R., Aitio, O., Laakso, I., Huuskonen, J., Taskinen, J.  
Number of pages: 4  
Pages: 521-524  
Publication date: 2001  
Peer-reviewed: Yes

### Publication information

Journal: Combinatorial Chemistry and High Throughput Screening  
Volume: 4  
Issue number: 6  
ISSN (Print): 1386-2073  
Ratings:  
Scopus rating (2001): SJR 0.78 SNIP 0.872  
Original language: English  
ASJC Scopus subject areas: Clinical Biochemistry, Chemistry (miscellaneous), Pharmacology  
DOIs:  
10.2174/1386207013330887  
URLs:  
<http://www.scopus.com/inward/record.url?scp=0034861953&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 0034861953  
Research output: Contribution to journal > Article > Scientific > peer-review

### Computational studies for the interpretation of gas response of SnO<sub>2</sub>(110) surface

Tin dioxide is a widely used material in gas sensing applications. This is partly due to its stable surface structure and high sensitivity to many gases. The interaction of different gas components with an oxide surface may lead to changes in the lattice oxygen content at the surface in addition to changes in the amount of adsorbed species. The electronic and atomic structures of the surface change with the changes in the lattice oxygen content. This leads to surface relaxation and changes in the surface dipole layer of the ionic surface in addition to changes in the Schottky barrier which is a result of the charge accumulation onto the surface from the bulk of the semiconducting oxide. Changes in both the dipole layer and the Schottky barrier change the work function of the semiconductor and may reflect in its electrical conductivity. Here we

have used first-principles calculations based on LDA-SCF to study changes in the electronic and atomic structures of the SnO<sub>2</sub>(110) surface as a result of oxygen exchange between the lattice and the ambient gas. The transducer function relating the changes at the surface to the changes in the conductivity of a ceramic microstructure is also described by an example.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: University of Oulu, Department of Physical Sciences  
Contributors: Rantala, T. S., Rantala, T. T., Lantto, V.  
Number of pages: 4  
Pages: 375-378  
Publication date: 30 Jun 2000  
Peer-reviewed: Yes

#### Publication information

Journal: Sensors and Actuators B: Chemical  
Volume: 65  
Issue number: 1  
ISSN (Print): 0925-4005  
Ratings:  
Scopus rating (2000): SJR 0.952 SNIP 1.337  
Original language: English  
ASJC Scopus subject areas: Analytical Chemistry, Electrochemistry, Electrical and Electronic Engineering  
DOIs:  
10.1016/S0925-4005(99)00292-0  
Source: Scopus  
Source ID: 0034733267  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Preparation of 5-substituted 2-carboxyindoles on solid support

The preparation of 5-substituted 2-carboxyindoles on solid support is reported. In the approach, the indole moiety is synthesized in solution phase, followed by nitro-group reduction, reductive amination and alkylation on solid support. The method provides a simple and convenient route for the preparation of 5-substituted 2-carboxyindoles with high purity and good yield. (C) 2000 Elsevier Science Ltd.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Div. Pharmaceutical Chem., Dept. P., University of Helsinki, Helsinki University  
Contributors: Tois, J., Franzén, R., Aitio, O., Huikko, K., Taskinen, J.  
Number of pages: 4  
Pages: 2443-2446  
Publication date: 1 Apr 2000  
Peer-reviewed: Yes

#### Publication information

Journal: Tetrahedron Letters  
Volume: 41  
Issue number: 14  
ISSN (Print): 0040-4039  
Ratings:  
Scopus rating (2000): SJR 1.626 SNIP 0.962  
Original language: English  
ASJC Scopus subject areas: Biochemistry, Organic Chemistry, Drug Discovery  
DOIs:  
10.1016/S0040-4039(00)00151-9  
URLs:  
<http://www.scopus.com/inward/record.url?scp=0034175579&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 0034175579  
Research output: Contribution to journal > Article > Scientific > peer-review

## The Suzuki, the Heck, and the Stille reaction - Three versatile methods, for the introduction of new C-C bonds on solid support

Metal-catalyzed coupling reactions are very efficient and reliable methods for the introduction of new carbon-carbon bonds onto molecules attached to a solid support. This review summarizes recent advances in utilizing the three most used methods, the Suzuki reaction, the Heck reaction, and the Stille reaction, in the field of solid phase organic synthesis resulting in small organic molecule libraries.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: University of Helsinki  
Contributors: Franzén, R.  
Number of pages: 6  
Pages: 957-962  
Publication date: 2000  
Peer-reviewed: Yes

### Publication information

Journal: Canadian Journal of Chemistry - Revue Canadienne de Chimie  
Volume: 78  
Issue number: 7  
ISSN (Print): 0008-4042  
Ratings:  
Scopus rating (2000): SJR 0.628 SNIP 0.672  
Original language: English  
ASJC Scopus subject areas: Chemistry(all)  
Keywords: Carbon-carbon bonds, Combinatorial chemistry, Drug discovery, Metal-catalyzed coupling reactions, Solid phase synthesis  
DOIs:  
10.1139/v00-089  
URLs:  
<http://www.scopus.com/inward/record.url?scp=0033843143&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 0033843143  
Research output: Contribution to journal › Article › Scientific › peer-review

## Experimental and theoretical study of the spin-spin coupling tensors in methylsilane

The experimental and theoretical  $^{13}\text{C}$ - $^{29}\text{Si}$  spin-spin coupling tensors,  $^1J_{\text{C}_{\text{Si}}}$ , are reported for methylsilane,  $^{13}\text{CH}_3\text{ }^{29}\text{SiH}_3$ . The experiments are performed by applying the liquid crystal NMR (LC NMR) method. The data obtained by dissolving  $\text{CH}_3\text{SiH}_3$  in nematic phases of two LC's is analyzed by taking into account harmonic and anharmonic vibrations, internal rotation, and solvent-induced anisotropic deformation of the molecule. The necessary parameters describing the relaxation of the molecular geometry during the internal rotation, as well as the harmonic force field, are produced theoretically with semiempirical (AM1 and PM3) and ab initio (MP2) calculations. A quantum mechanical approach has been taken to treat the effects arising from internal rotation. All the J tensors are determined theoretically by ab initio MCSCF linear response calculations. The theoretical and experimental J coupling anisotropies,  $\Delta^1J_{\text{C}_{\text{Si}}} = -59.3$  Hz and  $-89 \pm 10$  Hz, respectively, are in fair mutual agreement. These results indicate that the indirect contribution has to be taken into account when experimental  $^1D_{\text{C}_{\text{Si}}}^{\text{exp}}$  couplings are to be applied to the determination of molecular geometry and orientation. The theoretically determined J tensors are found to be qualitatively similar to what was found in our previous calculations for ethane, which suggests that the indirect contributions can be partially corrected for by transferring the corresponding J tensors from a model molecule to another.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: University of Oulu, Oulu Polytechnic, Raahe Institute of Computer Engineering, Max-Planck-Institut für Festkörperforschung  
Contributors: Kaski, J., Lantto, P., Rantala, T. T., Schroderus, J., Vaara, J., Jokisaari, J.  
Number of pages: 9  
Pages: 9669-9677  
Publication date: 2 Dec 1999  
Peer-reviewed: Yes

### Publication information

Journal: Journal of Physical Chemistry A  
Volume: 103

Issue number: 48  
ISSN (Print): 1089-5639  
Ratings:

Scopus rating (1999): SJR 1.443 SNIP 1.592  
Original language: English  
ASJC Scopus subject areas: Physical and Theoretical Chemistry  
DOIs:

10.1021/jp9920491  
Source: Scopus  
Source ID: 0001687009  
Research output: Contribution to journal > Article > Scientific > peer-review

### Surface relaxation of the (110) face of rutile SnO<sub>2</sub>

Surface relaxation of the stoichiometric and reduced SnO<sub>2</sub> (110) surfaces is studied with first-principles calculations. Calculations are carried out with two different self-consistent ab initio LDA methods, which lead to similar results. The most prominent feature in the relaxation is that the surface layer oxygens of the reduced surface move outwards about 0.4 Å with respect to the surface tin atoms. The stoichiometric (oxidized) surface is stabilized by the "bridging" oxygen atoms, and therefore, relaxes less. The valence band density-of-states is similar at both surfaces, except that removing bridging oxygens leaves behind electrons that occupy gap states formed at the reduced tin atoms.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Department of Physical Sciences, University of Oulu  
Contributors: Rantala, T. T., Rantala, T. S., Lantto, V.  
Number of pages: 7  
Pages: 103-109  
Publication date: 11 Jan 1999  
Peer-reviewed: Yes

### Publication information

Journal: Surface Science  
Volume: 420  
Issue number: 1  
ISSN (Print): 0039-6028  
Ratings:  
Scopus rating (1999): SJR 1.752 SNIP 0.974  
Original language: English  
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Condensed Matter Physics, Surfaces and Interfaces  
Keywords: Density functional calculations, Semiconducting surfaces, Single crystal surfaces, Surface relaxation and reconstruction, Tin oxides  
DOIs:  
10.1016/S0039-6028(98)00833-4  
Source: Scopus  
Source ID: 0032784368  
Research output: Contribution to journal > Article > Scientific > peer-review

### Effect of nitro groups and alkyl chain length on the negative ion tandem mass spectra of alkyl 3-hydroxy-5-(4'-nitrophenoxy) and alkyl 3-hydroxy-5-(2', 4'-dinitrophenoxy) benzoates

Tandem mass spectrometric behaviour was studied for a small combinatorial library of alkyl 3-hydroxy-5-(4'-nitrophenoxy) benzoates (A1-A5) and alkyl 3-hydroxy-5-(2', 4'-dinitrophenoxy) benzoates (B1-B5). The spectra were recorded by negative ion electrospray low-energy collision induced dissociation (CID) tandem mass spectrometry. The product ion spectra of  $[M - H]^-$  of the benzoates A1-A5 are similar, as are those of benzoates B1-B5. However, the spectra of the B series compounds differ significantly from those of the A series owing to the second electron-withdrawing nitro substituent in the B compounds. In addition, the length of the alkyl chain has an effect on the fragmentation. However, both series of compounds exhibit an abundant nitrophenoxy ion formed by the loss of 3-hydroxybenzoate. This is at  $m/z$  138 in A1-A5 and at  $m/z$  183 in B1-B5. A precursor ion scan of the nitrophenoxy ion provides a rapid method to identify the synthesised compounds in this type of combinatorial mixture.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Division of Pharmaceutical Chemistry, University of Helsinki, Department of Pharmacy  
Contributors: Kangas, H., Franzén, R., Tois, J., Taskinen, J., Kostianen, R.

Number of pages: 5  
Pages: 1680-1684  
Publication date: 1999  
Peer-reviewed: Yes

#### Publication information

Journal: Rapid Communications in Mass Spectrometry

Volume: 13

Issue number: 16

ISSN (Print): 0951-4198

Ratings:

Scopus rating (1999): SJR 1.379 SNIP 1.096

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Spectroscopy

DOIs:

10.1002/(SICI)1097-0231(19990830)13:16<1680::AID-RCM698>3.0.CO;2-R

URLs:

<http://www.scopus.com/inward/record.url?scp=0032814434&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 0032814434

Research output: Contribution to journal › Article › Scientific › peer-review

#### Computational approaches to the chemical sensitivity of semiconducting tin dioxide

Some computational approaches to the chemical sensitivity of semiconducting tin dioxide are presented. Chemical sensitivity is often observed using conductance measurement. Therefore, the potential energy barriers in grain contacts between adjacent grains of a polycrystalline semiconductor are the key parameters for transducing the chemical surface sensitivity into the conductance response. The rate equation model describes the electronic exchange between the adsorbed oxygen species and the bulk conduction band of a semiconductor. It predicts the type of the major negative oxygen ion ( $O_2^-$  or  $O^-$ ) at the surface as a function of temperature in agreement with experimental findings. The grain geometry has only a small effect on the potential energy barrier at the surface of finite grains. Even a small neck contact between grains, in the case of mobile donors, decreases strongly the potential energy barrier between grains compared to that in the case of an open grain contact. Results from Monte Carlo simulations with random barrier networks reveal that the current-voltage characteristic of a polycrystalline semiconductor is non-linear at higher voltages and the non-linearity of the network increases with increasing width of the barrier distributions. Electronic-structure calculations with clusters give qualitative information on the role of oxygen vacancies in different atomic planes in  $SnO_2$  and its unrelaxed and unreconstructed (110) surface.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Oulu, Department of Physical Sciences, Chalmers University of Technology, State University of New York

Contributors: Rantala, T., Lantto, V., Rantala, T.

Number of pages: 6

Pages: 59-64

Publication date: 1 Jan 1998

Peer-reviewed: Yes

#### Publication information

Journal: Sensors and Actuators B: Chemical

Volume: 47

Issue number: 1-3

ISSN (Print): 0925-4005

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Electrochemistry, Electrical and Electronic Engineering

Keywords: Electronic structure, Grain contact, Mobile donor, Surface energy barrier

DOIs:

10.1016/S0925-4005(98)00007-0

Source: Scopus

Source ID: 0032041202

Research output: Contribution to journal › Article › Scientific › peer-review

#### Investigation of the adducts formed by reaction of butenedioic acids with adenosine

Several genotoxic butenedioic acids present in chlorine-disinfected drinking water were allowed to react with adenosine, guanosine, and cytidine in aqueous solution. HPLC analyses, with detection at 254 and 310 nm, showed that clearly

detectable products were formed only in the reactions with adenosine. The major products from the reactions between either 2-chloro-3-methyl-2-butenedioic acid (ox-MCF) or 2-chloro-3-(chloromethyl)-2-butenedioic acid (ox-CMCF) and adenosine were the same. This substance was isolated by C18 column chromatography and characterized by UV absorbance,  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy, and mass spectrometry. It was identified as 3-( $\beta$ -D-ribofuranosyl)-7-carboxy-7-formyl-8-[9'-( $\beta$ -D-ribofuranosyl)-N<sup>6</sup>-adenosinyl]-1,N<sup>6</sup>-ethanoadenosine (cf&A,A). The yields of cf&A,A in reactions performed at pH 7.4 and 37 °C were 0.7% and 0.3% with ox-MCF and ox-CMCF, respectively.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Natl. Inst. for Environ. Studies  
Contributors: Franzén, R., Morita, M., Tanabe, K., Takagi, H., Shibata, Y.  
Number of pages: 6  
Pages: 1186-1191  
Publication date: Oct 1997  
Peer-reviewed: Yes

#### Publication information

Journal: Chemical Research in Toxicology  
Volume: 10  
Issue number: 10  
ISSN (Print): 0893-228X  
Original language: English  
ASJC Scopus subject areas: Drug Discovery, Organic Chemistry, Chemistry(all), Toxicology, Health, Toxicology and Mutagenesis  
DOIs:  
10.1021/tx970036d  
URLs:  
<http://www.scopus.com/inward/record.url?scp=0030778905&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 0030778905  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Calculation of the molecular ordering parameters of ( $\pm$ )-3-butyn-2-ol dissolved in an organic solution of poly( $\gamma$ -benzyl-L-glutamate)

The proton and natural abundance carbon-13 NMR spectra of ( $\pm$ )-3-butyn-2-ol enriched in the S enantiomer (ee = 72%) and oriented in the chiral nematic liquid crystalline phase of [poly( $\gamma$ -benzyl-L-glutamate)/deuteriochloroform] have been obtained and analyzed. The residual  $^1\text{H}$ - $^1\text{H}$  and  $^1\text{H}$ - $^{13}\text{C}$  dipolar couplings were corrected for the effects of molecular harmonic vibrational motions and used to determine the  $r_a$  structure and the five independent order parameters,  $S_{\alpha\beta}$ , for each enantiomer. It is shown that the data is consistent with the two enantiomers having an identical  $r_a$  structure, but the order matrices differ in both the magnitudes of their elements and the orientation of their principal axes.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Université de Paris-Sud, University of Southampton, United Kingdom, Dept. of Physical Sciences Linnanmaa, University of Oulu  
Contributors: Lesot, P., Merlet, D., Courtieu, J., Emsley, J. W., Rantala, T. T., Jokisaari, J.  
Number of pages: 6  
Pages: 5719-5724  
Publication date: 31 Jul 1997  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry A  
Volume: 101  
Issue number: 31  
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Original language: English  
ASJC Scopus subject areas: Physical and Theoretical Chemistry  
DOIs:  
10.1021/jp9709262  
URLs:  
<http://www.scopus.com/inward/record.url?scp=0031175387&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 0031175387

Research output: Contribution to journal > Article > Scientific > peer-review

### **Inequivalence of single CH<sub>a</sub> and CH<sub>b</sub> methylene bonds in the interior of a diunsaturated lipid bilayer from a molecular dynamics simulation**

Orientational order parameters for individual CH<sub>a</sub> and CH<sub>b</sub> bonds are local measures for the alignment of the bonds in a membrane interior. Experimental values exist for some lipid systems but no results are available from molecular dynamics (MD) simulations, although they are increasingly used to study biomembranes. We present such detailed analysis of a one nanosecond MD simulation for a PLPC (16:0/18:2<sup>Δ9,12</sup>) bilayer. The results show marked inequivalence for the CH<sub>a</sub> and CH<sub>b</sub> bonds of the methylene segments in the beginning and in the double bond region of the diunsaturated sn-2 chain. They also suggest slight inequivalences in the saturated chain.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Ita-Suomen yliopisto, University of Oulu, Department of Physical Sciences

Contributors: Hyvönen, M., Ala-Korpela, M., Vaara, J., Rantala, T. T., Jokisaari, J.

Number of pages: 6

Pages: 55-60

Publication date: 4 Apr 1997

Peer-reviewed: Yes

#### **Publication information**

Journal: Chemical Physics Letters

Volume: 268

Issue number: 1-2

ISSN (Print): 0009-2614

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Spectroscopy, Atomic and Molecular Physics, and

Optics

DOIs:

10.1016/S0009-2614(97)00171-1

Source: Scopus

Source ID: 0031552317

Research output: Contribution to journal > Article > Scientific > peer-review

### **Start-up and Operation of Laboratory-Scale Thermophilic Upflow Anaerobic Sludge Blanket Reactors Treating Vegetable Processing Wastewaters**

Thermophilic anaerobic treatment of hot vegetable processing wastewaters was studied in laboratory-scale UASB reactors at 55°C. The high-strength wastewater streams, deriving from steam peeling and blanching of carrot, potato and swede were used. The reactors were inoculated with mesophilic granular sludge. Stable thermophilic methanogenesis with about 60% COD removal was reached within 28 days. During the 134 day study period the loading rate was increased up to 24 kg COD m<sup>-3</sup> day<sup>-1</sup>. High treatment efficiency of more than 90% COD removal and concomitant methane production of 7.3 m<sup>3</sup> CH<sub>4</sub> m<sup>-3</sup> day<sup>-1</sup> were achieved. The anaerobic process performance was not affected by the changes in the wastewater due to the different processed vegetables. The results demonstrated the feasibility of thermophilic anaerobic treatment of vegetable processing wastewaters in UASB reactors.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Science and Environmental Engineering, Tampere University of Technology, University of

Jyväskylä, Jyväskylän yliopisto, Aalto University

Contributors: Lepistö, S. S., Rintala, J. A.

Number of pages: 9

Pages: 331-339

Publication date: Mar 1997

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Chemical Technology and Biotechnology

Volume: 68

Issue number: 3

ISSN (Print): 0268-2575

Original language: English

ASJC Scopus subject areas: Biotechnology, Chemical Engineering(all), Bioengineering, Chemistry(all)  
Keywords: Anaerobic treatment, Food industry, Granular sludge, Start-up, Thermophilic, Vegetable processing wastewater  
DOIs:

10.1002/(SICI)1097-4660(199703)68:3<331::AID-JCTB657>3.0.CO;2-Z

URLs:

<http://www.scopus.com/inward/record.url?scp=0030616058&partnerID=8YFLogxK> (Link to publication in Scopus)

#### **Bibliographical note**

Contribution: organisation=bio,FACT1=1

Source: researchoutputwizard

Source ID: 30520

Research output: Contribution to journal › Article › Scientific › peer-review

#### **Surface relaxation of the (1010) face of wurtzite CdS**

Atomic geometry and electronic density of states of the wurtzite CdS (1010) cleavage surface have been calculated. Calculations were carried out with two different self-consistent ab initio LDA methods leading to similar results. Surface relaxation is found to be strong: cations relax towards bulk and anions outwards from the surface. This is in accordance with experimental observations and other published calculations.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physical Sciences, University of Oulu

Contributors: Rantala, T. T., Rantala, T. S., Lantto, V., Vaara, J.

Number of pages: 6

Pages: 77-82

Publication date: 15 May 1996

Peer-reviewed: Yes

#### **Publication information**

Journal: Surface Science

Volume: 352-354

ISSN (Print): 0039-6028

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Condensed Matter Physics, Surfaces and Interfaces

Keywords: Cadmium sulphide, Density-functional calculation, Semiconducting surfaces, Single crystal surfaces, Surface electronic phenomena, Surface relaxation and reconstruction

DOIs:

10.1016/0039-6028(95)01094-7

Source: Scopus

Source ID: 0030147848

Research output: Contribution to journal › Article › Scientific › peer-review

#### **Mutational spectra of Salmonella typhimurium revertants induced by chlorohydroxyfuranones, byproducts of chlorine disinfection of drinking water**

The base substitution specificities of 3-chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone (MX), 3-chloro-4-(chloromethyl)-5-hydroxy-2(SH)-furanone (CMCF), 3,4-dichloro-5-hydroxy-2(5H)-furanone (MCA), and chloromalonaldehyde (CMA), a putative breakdown product of MCA, were examined in the hisG46 gene and in the hisG428 gene of *Salmonella typhimurium* using allele specific oligonucleotide hybridization. Although the compounds are structurally closely related, they induced substantially different mutation spectra: MCA and CMA caused primarily GC → AT transitions in the hisG46 allele (target sequence CCC), in particular, at the second position of the codon in strain TA100. In TA100 the mutation spectrum of MCA was similar to that of CMA. The mutational specificity of MCA can be explained as a consequence of misincorporation opposite to cyclic ethene adducts identical to those formed by the carcinogen vinyl chloride. The spectra induced by MX and CMCF in TA100 were almost identical but distinctively different from the spectra of MCA and CMA. Both compounds induced primarily GC → TA transversions, in particular, at the second position of the codon, and to a lesser extent in the first position of the codon. An identical site bias is induced by carcinogens such as polycyclic aromatic hydrocarbons and heterocyclic amines as a consequence of formation of (noncyclic) guanosine adducts. In hisG428 (target sequence TAA) MX induced again primarily GC → TA transversions in Tyr tRNA genes (supC/M) and, to a lesser extent, intragenic AT → TA transversions (TAA → AAA). The possible involvement of guanosine and adenosine adducts in the mutational specificity of MX is addressed.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed



Organisations: Der Technischen Universität Wien Fakultät für Elektrotechnik und Informationstechnik, Tumor Biology/Cancer Research Inst., University of Vienna, Abo Akademi University  
Contributors: Knasmüller, S., Zöhrer, E., Kronberg, L., Kundi, M., Franzen, R., Schulte-Hermann, R.  
Number of pages: 8  
Pages: 374-381  
Publication date: 1996  
Peer-reviewed: Yes

#### Publication information

Journal: Chemical Research in Toxicology  
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Issue number: 2  
ISSN (Print): 0893-228X  
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ASJC Scopus subject areas: Drug Discovery, Organic Chemistry, Chemistry(all), Toxicology, Health, Toxicology and Mutagenesis  
DOIs:  
10.1021/tx9500686  
Source: Scopus  
Source ID: 0029882809  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Effects of two double bonds on the hydrocarbon interior of a phospholipid bilayer

A phospholipid bilayer was modelled by duplicating a monolayer system of 36 1-palmitoyl-2-linoleoyl-sn-glycero-3-phosphatidylcholine (PLPC) molecules ( 16:0 18:2) plus 1368 water molecules and simulated using molecular dynamics. The analyses revealed distinct characteristics in the membrane structure due to polyunsaturation. The orientational behaviour of the fatty acid chains in the PLPC bilayer was found to be seemingly different from that in monounsaturated or in saturated phospholipid bilayers. The specific attributes responsible for the observed behaviour of the saturated and polyunsaturated chains are discussed and their relative importance assessed.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: University of Oulu, Hammersmith Hospital, Department of Physical Sciences  
Contributors: Hyvönen, M., Ala-Korpela, M., Vaara, J., Rantala, T. T., Jokisaari, J.  
Number of pages: 7  
Pages: 300-306  
Publication date: 24 Nov 1995  
Peer-reviewed: Yes

#### Publication information

Journal: Chemical Physics Letters  
Volume: 246  
Issue number: 3  
ISSN (Print): 0009-2614  
Original language: English  
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)  
DOIs:  
10.1016/0009-2614(95)01113-N  
Source: Scopus  
Source ID: 4243491046  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Synthesis of chlorinated 5-hydroxy 4-methyl-2(5H)-furanones and mucochloric acid

An improved procedure for the synthesis of chlorinated 5-hydroxy-4-methyl-2(5H)-furanones is described. By this method also carbon-labelled ( $^{13}\text{C}$  and  $^{14}\text{C}$  at C-3) hydroxyfuranones, including mucochloric acid, can be prepared. Each step of the method was examined in an effort to optimize both the yield and the purity of the compounds.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Abo Akademi University  
Contributors: Franzén, R., Kronberg, L.  
Number of pages: 4

Pages: 3905-3908  
Publication date: 29 May 1995  
Peer-reviewed: Yes

#### Publication information

Journal: Tetrahedron Letters  
Volume: 36  
Issue number: 22  
ISSN (Print): 0040-4039  
Original language: English  
ASJC Scopus subject areas: Biochemistry, Organic Chemistry, Drug Discovery  
DOIs:  
10.1016/0040-4039(95)00638-S  
URLs:  
<http://www.scopus.com/inward/record.url?scp=0029012567&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 0029012567  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Si<sub>10</sub> and photoabsorption spectra of mid-sized silicon clusters

The photoabsorption spectra of various isomers of Si<sub>10</sub>, Si<sub>9</sub>, Si<sub>11</sub> and other silicon clusters are calculated using a tight-binding method. Remarkable similarities between the calculated results and the experimental spectra for mid-sized clusters are noted. It is suggested that the mid-sized clusters are composed of aggregates of smaller clusters.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: University of Oulu, College at Fredonia, Washington State University Pullman  
Contributors: Rantala, T. T., Jelski, D. A., George, T. F.  
Number of pages: 6  
Pages: 215-220  
Publication date: 13 Jan 1995  
Peer-reviewed: Yes

#### Publication information

Journal: Chemical Physics Letters  
Volume: 232  
Issue number: 3  
ISSN (Print): 0009-2614  
Original language: English  
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)  
DOIs:  
10.1016/0009-2614(94)01342-S  
Source: Scopus  
Source ID: 4243879058  
Research output: Contribution to journal › Article › Scientific › peer-review

#### A cluster approach for the SnO<sub>2</sub> (110) face

Some results are given from a cluster approach for the electronic structure of the SnO<sub>2</sub> (110) face together with some oxygen vacancies and 'adsorbates'. Computations are based on ab initio methods, the local-density approximation and atomic orbitals as a basis set. Solutions were calculated self-consistently, but also using a composition of atomic potentials (for some smaller clusters). The atomic-orbital nature (origin) of the cluster levels was traced by projection onto the atomic bases set. The results here refer to a basic cluster [SnO<sub>213</sub> with 17 surface atoms modelling the SnO<sub>2</sub> (110) face and the other 22 atoms in the next five surface layers. The effect of oxygen 'adsorbates' and oxygen vacancies in the few uppermost subsurface layers on the electronic structure was considered. In particular, the focus was on the levels related to oxygen vacancies and originating from Sn 5s orbitals, which are well-known donor levels in the deep bulk, making SnO<sub>2</sub> an n-type semiconductor. The results support some other theoretical and experimental predictions that oxygen vacancies behave as neutral defects at or near SnO<sub>2</sub> surfaces.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Microelectronics Laboratory, University of Oulu  
Contributors: Rantala, T. S., Lantto, V., Rantala, T. T.

Number of pages: 4  
Pages: 716-719  
Publication date: 1994  
Peer-reviewed: Yes

#### Publication information

Journal: Sensors and Actuators B: Chemical  
Volume: 19  
Issue number: 1-3  
ISSN (Print): 0925-4005  
Original language: English  
ASJC Scopus subject areas: Analytical Chemistry, Electrochemistry, Electrical and Electronic Engineering  
DOIs:  
10.1016/0925-4005(93)01220-X  
Source: Scopus  
Source ID: 0028407824  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Rate equation simulation of the height of Schottky barriers at the surface of oxidic semiconductors

Rate equation simulation is used in the present computational approach in order to study the role of different adsorbed oxygen ions ( $O_2^-$  and  $O^-$ ) in controlling the height of the Schottky barrier at the surface of  $SnO_2$ , a key material in the field of semiconductor gas sensors. Computations are based on the adsorption/desorption model and consider the electron transfer between different oxygen species on the surface and the bulk conduction band. Different values have been tested for both the frequency factors and the activation energies of the rate constants in order to consider the relative population between the  $O^-$  and  $O_2^-$  ions on the surface at different temperatures, the dependence of the height of the surface Schottky barrier on temperature and oxygen partial pressure, and also the response and recovery times of the barrier heights as a consequence of rapid temperature changes. Comparisons of calculated barrier heights with some empirical values are also given at different temperatures and oxygen partial pressures.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: University of Oulu  
Contributors: Rantala, T. S., Lantto, V., Rantala, T. T.  
Number of pages: 4  
Pages: 234-237  
Publication date: 1993  
Peer-reviewed: Yes

#### Publication information

Journal: Sensors and Actuators B: Chemical  
Volume: 13  
Issue number: 1-3  
ISSN (Print): 0925-4005  
Original language: English  
ASJC Scopus subject areas: Analytical Chemistry, Electrochemistry, Electrical and Electronic Engineering  
DOIs:  
10.1016/0925-4005(93)85369-L  
Source: Scopus  
Source ID: 0027590715  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Electronic and structural properties of Si<sub>10</sub> cluster

Possible structures for Si<sub>10</sub> cluster are considered using a tight-binding model and drawing on significant work done in the past. It is shown that the tight-binding parametrization, fitted to the bulk, is also valid for smaller systems. This model is found to essentially reproduce other published results, but requires much less effort than ab initio techniques—thus, allowing the study of a wide variety of structures and their ions. However, unlike classical force-field calculations, it yields information about the electronic structure of clusters. A new geometric structure for Si<sub>10</sub> is found, which is not only of lowest energy, but which also matches the experimental photoelectron band gap and explains the experimental reactivity data. Because of the Jahn-Teller effect, the photoelectron spectrum is very sensitive to geometry. Also, ionization of the cluster alters the geometry slightly.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Departments of Chemistry, and Physics and Astronomy, 239 Fronczak Hall, State University of New York, College at Fredonia

Contributors: Rantala, T. T., Jelski, D. A., George, T. F.

Number of pages: 12

Pages: 189-200

Publication date: Jun 1990

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Cluster Science

Volume: 1

Issue number: 2

ISSN (Print): 1040-7278

Original language: English

ASJC Scopus subject areas: Inorganic Chemistry

Keywords: Silicon clusters, tight-binding model

DOIs:

10.1007/BF00702719

Source: Scopus

Source ID: 21544431551

Research output: Contribution to journal > Article > Scientific > peer-review

#### Morphological and structural changes in laser CVD of silicon: comparison of theoretical temperature calculations with experimental results

The paper considers to what extent theoretical calculation of the laser induced temperature profile in a substrate can be used to predict the morphology and structure of silicon tracks deposited by pyrolytic LCVD. The micron scale tracks are deposited from silane using a focussed argon ion laser onto a substrate consisting of 1000 Å SiO<sub>2</sub> upon a 300 μm thick, 100 mm diameter, [100] silicon wafer. The influence of various experimental parameters such as scan speed, laser power, gas pressure and gas composition on the temperature profile and on the deposited silicon track is investigated. Temperature profiles and their time evolution are simulated by numerically solving the heat diffusion equation using a finite difference approach. The track deposition is simulated using experimental temperature and pressure dependent growth rates. Gaussian shaped low laser power track profiles are well reproduced but the volcano like structures of high power deposition are not explained by the present model alone. The calculations are found to explain, at least qualitatively, the observed relationships between various experimental parameters.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Herriot-Watt University, Microelectronics and Materials Physics Laboratories, University of Oulu

Contributors: Miine, D., Wilson, J. I. B., Rantala, T. T., Lenkkeri, J.

Number of pages: 6

Pages: 81-86

Publication date: 2 Dec 1989

Peer-reviewed: Yes

#### Publication information

Journal: Applied Surface Science

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ISSN (Print): 0169-4332

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Condensed Matter Physics

DOIs:

10.1016/0169-4332(89)90194-3

Source: Scopus

Source ID: 0024900802

Research output: Contribution to journal > Article > Scientific > peer-review

#### Sorption and retention of ethylene glycol monoethyl ether (EGME) on silicas

Sorption of ethylene glycol monoethyl ether (EGME) was studied gravimetrically and correlated with the results of retention experiments where samples wetted with EGME were evacuated. If a sorption measurement is done conventionally by increasing the vapor pressure slowly by small steps, molecules are packed smoothly along the surface, and a fairly flat isotherm is obtained. If the sample is directly exposed to a high vapor pressure or the normal sorption

mode is disturbed by directly reducing the pressure, more EGME is sorbed. Then some of the molecules may be fixed only at their hydroxy ends. The evacuation curves are best interpreted in a semilogarithmic form, by which the value of the monolayer capacity can be estimated. EGME can be used for surface area measurements of silicas, but with porous samples areas that are too large are probably obtained. When EGME is packed smoothly on standard silica TK 800, one molecule occupies an area of  $0.44 \text{ nm}^2$ , computed by the BET equation with three parameters, or 1 mg of EGME covers  $3.0 \text{ m}^2$ .

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Rakennetekniikka, Tampere University of Technology, University of Tampere

Contributors: Kellomäki, A., Kuula-Väisänen, P., Nieminen, P.

Number of pages: 6

Pages: 373-378

Publication date: 1989

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Colloid and Interface Science

Volume: 129

Issue number: 2

ISSN (Print): 0021-9797

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ASJC Scopus subject areas: Colloid and Surface Chemistry, Physical and Theoretical Chemistry, Surfaces and Interfaces

DOIs:

10.1016/0021-9797(89)90450-5

URLs:

<http://www.scopus.com/inward/record.url?scp=45149145866&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 45149145866

Research output: Contribution to journal > Article > Scientific > peer-review

#### Numerical simulation of temperature distributions in layered structures during laser processing

A numerical simulation approach for the evaluation of temperature distribution in layer structured substrates during laser processing is introduced. The explicit finite-difference solution of the heat equation is used and the full non-linearity of the heat diffusion is taken into account by temperature dependent substrate parameters. The heat equations for layered structures are solved using both rectangular and cylindrical coordinate systems. The method is applied to CW  $\text{Ar}^+$  laser-induced temperature distributions in some commonly used layer structures in microelectronics, such as silicon on sapphire (SOS) and  $\text{SiO}_2$  coated silicon. Results are compared with experiments.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Oulu, Microelectronics and Materials Physics Laboratories

Contributors: Levoska, J., Rantala, T. T., Lenkkeri, J.

Number of pages: 11

Pages: 12-22

Publication date: 1989

Peer-reviewed: Yes

#### Publication information

Journal: Applied Surface Science

Volume: 36

Issue number: 1-4

ISSN (Print): 0169-4332

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Condensed Matter Physics

DOIs:

10.1016/0169-4332(89)90895-7

Source: Scopus

Source ID: 0024301353

Research output: Contribution to journal > Article > Scientific > peer-review

### Potential energy curves for diatomic molecules calculated with numerical basis functions

A computational scheme for molecules is presented for the evaluation of total energy properties such as potential energy curves and vibrational frequencies. The calculations are performed within the local density approximation utilizing the LCAO MO scheme with numerical basis functions, and multipole expansion of the molecular charge density is used to obtain the molecular potential. The total energy expression is written in terms of matrix elements already used for solving one-electron equations, and hence any evaluation of explicit integrals over charge density is avoided. The accuracy of the method and the effect of basis set incompleteness are studied for the CO and N<sub>2</sub> molecules and compared with fully numerical (basis-free) results.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Chalmers University of Technology  
Contributors: Rantala, T. T., Wästberg, B., Rosén, A.  
Number of pages: 8  
Pages: 261-268  
Publication date: 15 Nov 1986  
Peer-reviewed: Yes

#### Publication information

Journal: Chemical Physics  
Volume: 109  
Issue number: 2-3  
ISSN (Print): 0301-0104  
Original language: English  
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Spectroscopy, Atomic and Molecular Physics, and Optics  
DOIs:  
10.1016/0301-0104(86)87056-2  
Source: Scopus  
Source ID: 2842530832  
Research output: Contribution to journal › Article › Scientific › peer-review

### A finite cluster approach to the electron-hole pair damping of the adsorbate vibration: CO adsorbed on Cu(100)

A finite cluster method is applied to describe the energy transfer from the adsorbate vibrations to the electron-hole pair excitations. For CO stretch vibration on Cu(100) surface a value of 0.5 meV is found for the consequent damping (corresponding to the lifetime of  $1.3 \cdot 10^{-12}$  s) in an agreement with a recently measured vibrational line width. The mechanism behind the electron-hole pair excitations is found to be charge oscillations between the molecular  $2\pi^*$  resonance and the substrate, caused by the molecular vibration. Cluster size effects have been found to be negligible.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Chalmers University of Technology, University of California, Santa Barbara  
Contributors: Rantala, T. T., Rosén, A., Hellsing, B.  
Number of pages: 9  
Pages: 173-181  
Publication date: 1986  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Electron Spectroscopy and Related Phenomena  
Volume: 39  
Issue number: C  
ISSN (Print): 0368-2048  
Original language: English  
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Spectroscopy, Atomic and Molecular Physics, and Optics, Surfaces and Interfaces  
DOIs:  
10.1016/0368-2048(86)85045-9  
Source: Scopus  
Source ID: 0001168090  
Research output: Contribution to journal › Article › Scientific › peer-review

### A Finite Cluster Approach to the Electron-Hole Pair Damping of the Adsorbate Vibration: CO Adsorbed on Cu(100)

Abstract: A finite cluster method is applied to describe the energy transfer from the adsorbate vibrations to the electron-hole pair excitations. For CO stretch vibration on Cu(100) surface a value of 0.5 meV is found for the consequent damping (corresponding to the lifetime of  $1.3 \cdot 10^{-12}$  s) in an agreement with a recently measured vibrational line width. The mechanism behind the electron-hole pair excitations is found to be charge oscillations between the molecular  $2\pi$  resonance and the substrate, caused by the molecular vibration. Cluster size effects have been found to be negligible.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chalmers University of Technology, University of California, Santa Barbara

Contributors: Rantala, T. T., Rosén, A., Helsing, B.

Number of pages: 9

Pages: 173-181

Publication date: 1986

Peer-reviewed: Yes

#### Publication information

Journal: Studies in Surface Science and Catalysis

Volume: 26

Issue number: C

ISSN (Print): 0167-2991

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Catalysis, Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

DOIs:

10.1016/S0167-2991(09)61238-6

Source: Scopus

Source ID: 77956976821

Research output: Contribution to journal > Article > Scientific > peer-review

### Anomalous Auger-electron spectra of metallic calcium

A1 K $\alpha$ -excited L<sub>2,3</sub> MM and L<sub>2,3</sub> MV Auger-electron spectra of Ca have been measured in ultrahigh vacuum from a metallic sample evaporated onto an Ag substrate. An interpretation of the spectra is made by applying a line-fitting procedure. The lineshape and the solid-state-free-atom kinetic-energy shift are also studied. The extrinsic loss structure in the L<sub>2,3</sub> MM Auger-electron emission is found to be similar to that in 2p photoelectron emission. Spin-density-functional (SDF) calculations for the singularity index describing the intrinsic lineshape give a value of  $\sim 0.35$  for both processes. Thus the experimental 2p<sub>3/2</sub> photoelectron line broadened from 1.2 to  $\sim 5$  eV FWHM has been used as a standard line in the line fitting of the L<sub>2,3</sub> MM transitions. The term splitting of the L<sub>2,3</sub> M<sub>2,3</sub> M<sub>2,3</sub> transition is larger than in the corresponding free-atom spectrum. This result is also supported by the SDF calculations. The L<sub>2,3</sub> M<sub>2,3</sub> V spectrum is anomalously sharp, probably both because of the structure of the local density of states at the site of the core-ionized atom and because of differences in the transition probabilities into the different parts of the band. The experimental solid-state shift is 20.3 eV for the L<sub>2,3</sub> M<sub>2,3</sub> M<sub>2,3</sub>:<sup>1</sup>D transition, and the binding-energy shifts are 8.3 and 6.1 eV for the 2p and 3p levels, respectively. The SDF shifts for the above transitions are 19.9 (configurational average), 9.4 and 8.0 eV, consecutively, in agreement with the experimental values. The calculations also show a localized d-type (atomic-like) structure for the screening of the initial- and final-state core hole (s). This is the origin of the large values of both the singularity index and the solid-state shift.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, University of Oulu, University of Turku

Contributors: Väyrynen, J., Rantala, T. T., Minni, E., Suoninen, E.

Number of pages: 13

Pages: 293-305

Publication date: 1983

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Electron Spectroscopy and Related Phenomena

Volume: 31

Issue number: 3

ISSN (Print): 0368-2048

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Spectroscopy, Atomic and Molecular Physics, and Optics, Surfaces and Interfaces

DOIs:

10.1016/0368-2048(83)85077-4

Source: Scopus

Source ID: 0342803978

Research output: Contribution to journal › Article › Scientific › peer-review

### **Direct measurement of the kinetic energy shift between the molecular and atomic $M_{4.5}N_{4.5}N_{4.5}$ Auger spectra of iodine**

The  $M_{4.5}N_{4.5}N_{4.5}$  Auger electron spectrum of iodine has been measured from molecular and atomic iodine vapours. The energy shift of  $3.25 \pm 0.10$  eV between molecular and atomic Auger spectra has been determined using a least-squares fitting procedure to spectra containing both molecular and atomic contributions. Different initial and final state splittings for atomic and molecular spectra, as well as the extra-atomic relaxation energy, are discussed.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Oulu

Contributors: Rantala, T., Väyrynen, J., Kumpula, R., Aksela, S.

Number of pages: 3

Pages: 384-386

Publication date: 1 Oct 1979

Peer-reviewed: Yes

#### **Publication information**

Journal: Chemical Physics Letters

Volume: 66

Issue number: 2

ISSN (Print): 0009-2614

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DOIs:

10.1016/0009-2614(79)85040-X

URLs:

<http://www.scopus.com/inward/record.url?scp=49249145180&partnerID=8YFLogxK> (Link to publication in Scopus)

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Source ID: 49249145180

Research output: Contribution to journal › Article › Scientific › peer-review