Production of long chain alkyl esters from carbon dioxide and electricity by a two-stage bacterial process

Microbial electrosynthesis (MES) is a promising technology for the reduction of carbon dioxide into value-added multicarbon molecules. In order to broaden the product profile of MES processes, we developed a two-stage process for microbial conversion of carbon dioxide and electricity into long chain alkyl esters. In the first stage, the carbon dioxide is reduced to organic compounds, mainly acetate, in a MES process by Sporomusa ovata. In the second stage, the liquid end-products of the MES process are converted to the final product by a second microorganism, Acinetobacter baylyi in an aerobic bioprocess. In this proof-of-principle study, we demonstrate for the first time the bacterial production of long alkyl esters (wax esters) from carbon dioxide and electricity as the sole sources of carbon and energy. The process holds potential for the efficient production of carbon-neutral chemicals or biofuels.

General information
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Authors: Lehtinen, T., Efimova, E., Tremblay, P. L., Santala, S., Zhang, T., Santala, V.
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Scopus rating (2011): 2.314 2.508
Scopus rating (2010): 2.086 2.355
Scopus rating (2009): 1.912 2.231
Scopus rating (2008): 1.734 2.732
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Scopus rating (2006): 1.315 1.98
Scopus rating (2005): 1.269 2.006
Scopus rating (2004): 1.197 1.659
Scopus rating (2003): 0.948 1.639
Scopus rating (2002): 0.882 1.3
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Comparison of liposomal drug formulations for transdermal iontophoretic drug delivery

This study was aimed to evaluate the in vitro transdermal direct/pulsed current iontophoretic delivery of an amphiphilic model compound from various lipid vesicle-encapsulated formulations compared to free-drug formulation. Conventional, pegylated, ultraformable liposomes (transfersomes) and ethosomes loaded with a negatively charged drug diclofenac sodium (DS) were prepared and characterized. All the liposomes possessed an average size of ≈ 100–150 nm and negative zeta potential. No changes in colloidal stability were detected after 8 h incubation of any vesicle formulation under constant or pulsed iontophoretic current. DS was released from all the liposome formulations with a similar, limited rate (= 50% in 24 h), leading therefore to significantly lower transdermal fluxes across full-thickness porcine skin compared to the respective free drug formulation. From the tested lipid vesicle formulations, the transfersomes resulted in the highest passive flux and the ethosomes in the highest iontophoretic flux under direct constant current treatment. Higher negative surface charge of the vesicle led to better transport efficiency due to the higher mobility of the drug carrier under electric field. Pulsed current iontophoresis had no advantage over constant current treatment in combination with any type of lipid vesicular nanocarriers, in contrast to what has been described earlier with drug-loaded polymeric nanocarriers.

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Authors: Malinovskaja-Gomez, K., Espuelas, S., Garrido, M. J., Hirvonen, J., Laaksonen, T.
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Scopus rating (2015): 1.156 1.415
Web of Science (2015): 3.773 3.752 6.6 0.561 0.01365 0.802
Publication Forum (2015): 2
Scopus rating (2014): 0.994 1.247
Web of Science (2014): 3.35 3.463 6.6 0.776 0.01296 0.764
Publication Forum (2014): 3
Scopus rating (2013): 1.038 1.287
Publication Forum (2013): 3
Scopus rating (2012): 1.254 1.425
Publication Forum (2012): 3
Scopus rating (2011): 1.236 1.428
Scopus rating (2010): 1.289 1.283
Scopus rating (2009): 1.169 1.465
Scopus rating (2008): 1.015 1.265
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Scopus rating (2005): 0.93 1.409
Scopus rating (2004): 0.873 1.367
Scopus rating (2003): 0.964 1.4
Scopus rating (2002): 0.791 1.167
Scopus rating (2001): 0.694 0.969
Effects of different nickel species on autotrophic denitrification driven by thiosulfate in batch tests and a fluidized-bed reactor

Nickel is a common heavy metal and often occurs with nitrate (NO₃⁻) in effluents from mining and metal-finishing industry. The present study investigates the effects of increasing concentrations (5–200 mg Ni/L) of NiEDTA₂⁻ and NiCl₂ on autotrophic denitrification with thiosulfate (S₂O₃²⁻) in batch tests and a fluidized-bed reactor (FBR). In batch bioassays, 50 and 100 mg Ni/L of NiEDTA₂⁻ only increased the transient accumulation of NO₂⁻, whereas 25–100 mg Ni/L of NiCl₂ inhibited denitrification by 9–19%. NO₃⁻ and NO₂⁻ were completely removed in the FBR at feed NiEDTA₂⁻ and NiCl₂ concentrations as high as 100 and 200 mg Ni/L, respectively. PCR-DGGE revealed the dominance of Thiobacillus denitrificans and the presence of the sulfate-reducing bacterium Desulfovibrio putealis in the FBR microbial community at all feed nickel concentrations investigated. Nickel mass balance, thermodynamic modeling and solid phase characterization indicated that nickel sulfide, phosphate and oxide precipitated in the FBR during NiCl₂ injection.

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Scopus rating (2014): 2.41 2.104
Web of Science (2014): 4.494 5.33 4.6 0.822 0.12645 1.042
Publication Forum (2014): 2
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Publication Forum (2013): 2
Scopus rating (2012): 2.389 2.465
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Scopus rating (2009): 1.912 2.231
Scopus rating (2008): 1.734 2.732
Scopus rating (2007): 1.529 2.423
Scopus rating (2006): 1.315 1.98
Effect of alkylaminophenols on growth inhibition and apoptosis of bone cancer cells

In this work, we report the anticancer properties of a series of 11 chemically synthesized alkylaminophenols against human osteosarcoma U2OS tumor cell line. Several assays including cytotoxicity, inhibitor kinetic study, cell migration, Annexin-V/PI double staining, reactive oxygen species (ROS) and caspase 3/7 assays were conducted on this cell line. Cytotoxic 2-((3,4-dihydroquinolin-1(2H)-yl)(p-tolyl)methyl)phenol was determined to have an IC50 value of 36.6μM against U2OS cells and it also inhibits the cell growth in time-dependent manner. The potent activity of lead compound against the growth of multiple cell lines, U2OS, MG-65 and HEK-293T, confirms the osteosarcoma cell specific inhibition. Further studies indicated that such compound is an inhibitor of metastatic property of tumor cells and inducing apoptosis agent. The ability of increasing ROS and inducing caspases 3 and 7 further confirm the contribution of programmed cell death in U2OS and HEK-293T cells. Additionally, four compounds based on the 2-(indolin-1-yl(aryl)methyl)-4-nitrophenol core were also identified to be cytotoxic with IC50 values in the 66-88μM range. This work further demonstrates the anticancer properties of phenol derivatives, adding one more entry to the collection of promising chemotherapeutic agents for cancer treatment.
Self-Regulating Iris Based on Light-Actuated Liquid Crystal Elastomer

The iris, found in many animal species, is a biological tissue that can change the aperture (pupil) size to regulate light transmission into the eye in response to varying illumination conditions. The self-regulation of the eye lies behind its autofocusing ability and large dynamic range, rendering it the ultimate "imaging device" and a continuous source of inspiration in science. In optical imaging devices, adjustable apertures play a vital role as they control the light exposure, the depth of field, and optical aberrations of the systems. Tunable irises demonstrated to date require external control through mechanical actuation, and are not capable of autonomous action in response to changing light intensity without control circuitry. A self-regulating artificial iris would offer new opportunities for device automation and stabilization. Here, this paper reports the first iris-like, liquid crystal elastomer device that can perform automatic shape-adjustment by reacting to the incident light power density. Similar to natural iris, the device closes under increasing light intensity, and upon reaching the minimum pupil size, reduces the light transmission by a factor of seven. The light-responsive materials design, together with photoalignment-based control over the molecular orientation, provides a new approach to automatic, self-regulating optical systems based on soft smart materials.
Comparison of Scenedesmus acuminatus and Chlorella vulgaris cultivation in liquid digestates from anaerobic digestion of pulp and paper industry and municipal wastewater treatment sludge

Two microalgae, Chlorella vulgaris and Scenedesmus acuminatus, were batch cultivated separately in two types of diluted liquid digestates. The first digestate (ADPP) was obtained from a mesophilic laboratory digester treating biosludge from a pulp and paper industry wastewater treatment plant. The second digestate (ADMW) was collected from a full-scale mesophilic anaerobic digester treating mixed municipal wastewater treatment sludge. The highest biomass production (as volatile suspended solids, VSS), 8.2–9.4 g L⁻¹, was obtained with S. acuminatus in ADPP. C. vulgaris in ADMW had the lowest biomass production, reaching 2.0 g L⁻¹. Both microalgae removed ammonium efficiently from ADPP (99.9% removal) while the final ammonium removal efficiencies from ADMW with S. acuminatus and C. vulgaris were only 44.0 and 23.8%, respectively. The phosphate removal efficiencies from both ADPP and ADMW were higher than 96.9% with both microalgae. The highest carbohydrate content (60.5%) was obtained with S. acuminatus cultivated in ADPP. Scenedesmus acuminatus in ADPP showed one of the highest biomass production yields that have been reported for microalgae in real wastewater-derived nutrient sources. Consequently, this combination is promising for developing biorefinery and biofuel applications in the pulp and paper industry.

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This work presents a methodology that combines experimental measurements and Computational Fluid Dynamics (CFD) modeling to determine the global reaction kinetics of high heating rate biomass devolatilization. Three particle size ranges of woody biomass are analyzed: small (SF), medium (MF) and large (LF) fractions. Devolatilization mass loss is measured for each fraction in a laminar Drop-Tube Reactor (DTR) in nitrogen atmosphere, using two nominal reactor temperatures of 873 and 1173 K. Single First Order Reaction (SFOR) kinetics are determined by coupling an optimization routine with CFD models of the DTR. The global pre-exponential factors and activation energies for the SF, MF and LF particles are 5880 1/s and 42.7 kJ/mol, 48.1 1/s and 20.2 kJ/mol, and 102 1/s and 24.8 kJ/mol, respectively. These parameters are optimized for the isothermal heat transfer model available in CFD programs, and it is recommended that the specific heat capacity that was used in the optimization (1500 J/kgK) is used together with the parameters. Using the SF kinetics for small wood particles and either of the MF or LF kinetics for large particles, it is expected that more accurate devolatilization predictions can be obtained for the whole fuel size distribution in large scale CFD simulations.
Uniform and pinhole-free electron selective TiO$_2$ layers are of utmost importance for efficient perovskite solar cells. Here we used a scalable and low-cost dip coating method to prepare uniform and ultra-thin (5−50 nm) compact TiO$_2$ films on fluorine doped tin oxide (FTO) glass substrates. The thickness of the film was tuned by changing the TiCl$_4$ precursor concentration. The formed TiO$_2$ follows the texture of the underlying FTO substrates, but at higher TiCl$_4$ concentrations, the surface roughness is substantially decreased. This change occurs at a film thickness close to 20–30 nm. A similar TiCl$_4$ concentration is needed to produce crystalline TiO$_2$ films. Furthermore, below this film thickness, the underlying FTO might be exposed resulting in pinholes in the compact TiO$_2$ layer. When integrated into mesoscopic perovskite solar cells, there appears to be a similar critical compact TiO$_2$ layer thickness above which the devices perform more optimally. The power conversion efficiency was improved by more than 50% (from 5.5% to ~8.6%) when inserting a compact TiO$_2$ layer. Devices without or with very thin compact TiO$_2$ layers display J-V curves with an “s-shaped” feature in the negative voltage range, which could be attributed to immobilized negative ions at the electron-extracting interface. A strong correlation between the magnitude of the s-shape feature and the exposed FTO seen in the x-ray photoelectron spectroscopy measurements indicates that the s-shape is related to pinholes in the compact TiO$_2$ layer when it is too thin.
Molding Optical Waveguides with Nematicons

Optical waveguides are usually fabricated by top-down methods. Hereby, this study demonstrates a bottom-up approach based on nonlinear optics in reorientational nematic liquid crystals with polymerizable materials. Near-infrared optical spatial solitons—nematicons—in conjunction with UV exposure are employed in order to achieve (i) real-time signal waveguiding for point-to-point beam-induced interconnects by effectively quenching the fluctuations of nematicon trajectories through polymer stabilization; (ii) the molding of permanent channel waveguides in a crosslinked polymer network, so that they persist after turning off the soliton beam and confine signals of various wavelengths and intensities. These findings introduce a novel, highly versatile platform and a wealth of possibilities for guided-wave photonics, signal addressing, and processing in liquid crystalline soft matter.

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Authors: Karimi, N., Virkki, M., Alberucci, A., Buchnev, O., Kauranen, M., Priimägi, A., Assanto, G.
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Publication Forum (2015): 1
Scopus rating (2014): 1.818 1.707
Charge Carrier Dynamics in Solar Water Oxidation
The search for sustainable energy sources is one of the greatest problems facing mankind in the 21st century. Most renewable sources do not have adequate potential to cover the growing need for energy in order to sustain economic and population growth. Solar power is a plausible way to fully cover mankind’s continuously growing need for energy. However, sunlight is diurnal, and the amount of sunlight received at different latitudes of the Earth varies drastically. Harnessing solar energy into chemical bonds is an attractive approach to enable the storage of energy for transportation and later use. Direct photoelectrochemical water splitting produces only oxygen and hydrogen, of which hydrogen can be used to sustain a possible hydrogen based economy. The materials used in this Thesis are metal oxide semiconductors that act as photoanodes, performing the water oxidation reaction on their surface and supplying electrons for the water reduction reaction.

Hematite is an n-type metal oxide semiconductor that has a band gap suitable for the absorption of a noticeable fraction of solar radiation. The absorption of light leads to the generation of electron-hole pairs that are separated due to a built-in electric field. However, the conduction band level of hematite is not suitable for unassisted water splitting and it suffers from poor intrinsic charge transport properties. For this reason the photoanodes studied in this Thesis have been modified with doping and by forming heterojunctions with other metal oxide semiconductors, namely titanium dioxide.

This Thesis studies the evolution of the primary charge carriers responsible for water splitting in modified hematite photoanodes. The method selected to probe the charge carrier dynamics is transient absorption spectroscopy that enables the monitoring of charge carriers from the subpicosecond timescale up to seconds. The measurements were performed in a three electrode photoelectrochemical cell to see the effects of additional bias voltage on the charge carrier dynamics and how the recombination and oxygen evolution reaction are changed when a photocurrent is generated.

The results of this Thesis indicate that the modification of hematite has a profound effect on the charge carrier behaviour. The observed effects range from changes in recombination on the picosecond timescale, to nanosecond timescale trapping of electrons into intraband or surface states, and all the way to changes in the reaction rates of long-lived holes in the hundreds of milliseconds timescale.

Biohydrogen production from xylose by fresh and digested activated sludge at 37, 55 and 70 °C
Two heat–treated inocula, fresh and digested activated sludge from the same municipal wastewater treatment plant, were compared for their H₂ production via dark fermentation at mesophilic (37 °C), thermophilic (55 °C) and hyperthermophilic (70 °C) conditions using xylose as the substrate. At both 37 and 55 °C, the fresh activated sludge yielded more H₂ than
the digested sludge, whereas at 70 °C, neither of the inocula produced H₂ effectively. A maximum yield of 1.85 mol H₂ per mol of xylose consumed was obtained at 55 °C. H₂ production was linked to acetate and butyrate production, and there was a linear correlation (R² = 0.96) between the butyrate and H₂ yield for the fresh activated sludge inoculum at 55 °C. Approximately 2.4 mol H₂ per mol of butyrate produced were obtained against a theoretical maximum of 2.0, suggesting that H₂ was produced via the acetate pathway prior to switching to the butyrate pathway due to the increased H₂ partial pressure. Clostridia sp. were the prevalent species at both 37 and 55 °C, irrespective of the inoculum type. Although the two inocula originated from the same plant, different thermophilic microorganisms were detected at 55 °C. Thermoanaerobacter sp., detected only in the fresh activated sludge cultures, may have contributed to the high H₂ yield obtained with such an inoculum.
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$_2$.

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Web of Science (2015): 3.611 4.14 6.0 1.014 0.05542 0.929
Publication Forum (2015): 2
Scopus rating (2014): 1.667 2.331
Web of Science (2014): 3.52 4.091 6.4 0.815 0.04512 0.922
Publication Forum (2014): 3
Scopus rating (2013): 1.811 2.595
Publication Forum (2013): 3
Scopus rating (2012): 1.852 2.465
Publication Forum (2012): 3
Scopus rating (2011): 2.093 2.427
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Scopus rating (2009): 2.012 2.277
Scopus rating (2008): 1.635 2.184
Scopus rating (2007): 1.383 1.86
Scopus rating (2006): 1.278 1.64
Scopus rating (2005): 1.623 1.73
Scopus rating (2004): 1.273 1.883
Scopus rating (2003): 1.103 1.481
Scopus rating (2002): 1.13 1.301
Scopus rating (2001): 1.136 1.264
Scopus rating (2000): 1.047 1.272
Scopus rating (1999): 1.117 1.157
Original language: English
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).

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Authors: Virkki, K., Hakola, H., Urbaní, M., Tejerina, L., Ince, M., Martínez-Díaz, M. V., Torres, T., Golovanova, V., Golovanov, V., Tkachenko, N. V.
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Publication Forum (2015): 1
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Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
Publication Forum (2014): 3
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Scopus rating (2011): 2.32 1.457
Scopus rating (2010): 2.438 1.356
Scopus rating (2009): 2.128 1.417
Scopus rating (2008): 1.856 1.033
Alkyl thiophene vinylene electropolymerization in C8mimPF6, potential use in solar cells

We report the electrosynthesis of a novel semiconductor polymer based on alkyl vinylthiophene derivative in the presence of an ionic liquid (IL). The polymerization was performed under galvanostatic conditions and the polymer was studied as potential donor component of a multilayer heterojunction organic solar cell (OSC). The monomer used was (E)-1,2-di-(3-octyl-2-thienyl) vinylene (OTV) and the IL used for the electropolymerization was 1-octyl-3-methylimidazole hexafluorophosphate C8mimPF6. Optical properties, stability and morphology of the polymer were analyzed using FT-IR, UV-vis, Raman and XPS spectroscopy. Voltammetry analysis and scanning electron microscopy (SEM-EDX) were also performed on the polymer. The OSC assembled with the polymer of OTV was used as electro donor and C60 as acceptor. Molybdenum trioxide (MoO3) and bathocuproine (BCP) were used as buffer layer between anode and cathode respectively. I-V curves, in the dark and under AM 1.5 solar simulator were performed to measure its efficiency.

General information

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Synthesis, Structural Characterization, Hirshfeld Surface and Antioxidant Activity Analysis of a Novel Organic Cation Antimonate Complex

A new organic–inorganic hybrid material of formula (C10H15N2)7 Sb2Cl10 Sb2Cl9 (SbCl5)2 SbCl4 2Cl·7H2O was synthesized and characterized by an X-ray diffraction analysis. It crystallizes in the triclinic system with the P(space group and the following unit cell parameters a = 11.8127(3) Å, b = 15.7557(4) Å, c = 35.4511(8) Å, α = 89.409(1)°, β = 84.04(1)°, γ = 71.116(1)°, Z = 2 and V = 6207.3(3) Å3. 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.
Crystallisation-enhanced bulk hole mobility in phenothiazine-based organic semiconductors

A series of three novel donor-acceptor systems based on C(3)-malononitrile-substituted phenothiazines was synthesised in good overall yields and their thermal, spectroscopic, and electrochemical properties were characterised. The compounds were prepared through a sequence of Ullmann-coupling, Vilsmeier-Haack formylation and Knoevenagel-condensation, followed by Suzuki-coupling reactions for introduction of aryl substituents at C(7) position of the phenothiazine. The introduction of a donor unit at the C(7) position exhibited a weak impact on the optical and electrochemical characteristics of the compounds and led to amorphous films with bulk hole mobilities in the typical range reported for phenothiazines, despite the higher charge delocalisation as attested by computational studies. In contrast, highly ordered films were formed when using the C(7)-unsubstituted 3-malononitrile phenothiazine, exhibiting an outstanding mobility of 1 × 10−3 cm2 V−1 s−1, the highest reported for this class of compounds. Computational conformational analysis of the new phenothizanes suggested that free rotation of the substituents at the C(7) position...
suppresses the ordering of the system, thereby hampering suitable packing of the new materials needed for high charge carrier mobility.

**General information**

**State:** Published

**Ministry of Education publication type:** A1 Journal article-refereed

**Organisations:** Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Supramolecular photochemistry

**Authors:** Shinde, D. B., Salunke, J. K., Candeias, N. R., Francesca, T., Massimo, G., Wadgaonkar, P. P., Priimagi, A., Nadia, C., Vivo, P.

**Number of pages:** 10

**Publication date:** 12 Apr 2017

**Peer-reviewed:** Yes

**Publication information**

**Journal:** Scientific Reports

**Volume:** 7

**Article number:** 46268

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- **Scopus rating (2016):** 1.625 1.401
- **Publication Forum (2016):** 2
- **Scopus rating (2015):** 2.057 1.684
- **Web of Science (2015):** 5.228 5.525 2.1 0.559 0.20942 1.865
- **Publication Forum (2015):** 2
- **Scopus rating (2014):** 2.103 1.544
- **Web of Science (2014):** 5.578 5.597 1.7 0.722 0.11476 2.075
- **Publication Forum (2014):** 1
- **Scopus rating (2013):** 1.886 1.51
- **Publication Forum (2013):** 1
- **Scopus rating (2012):** 1.458 0.896
- **Publication Forum (2012):** 1

**Original language:** English

**Electronic versions:**

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**Links:**


**Research output:** Scientific - peer-review » Article

**Building up colors: multilayered arrays of peryleneimides on flat surfaces and on mesoporous layers**

Novel monoisomeric perylene imide derivatives with terpyridinyl and pyrrolidinyl substituents were synthesized and deposited onto solid substrates, such as a thin film of Al2O3 and mesoporous TiO2 nanoparticle layer, by using a simple dip-by-dip method. Arrays of up to 33 layers were built on Al2O3. In the case of mesoporous TiO2, the interstitial volume between the particles was filled up with dye assemblies. Deposition could produce either layers of microcrystals or molecular layers if an appropriate washing procedure was used. The resultant arrays were studied by means of scanning electron microscopy, X-ray photoelectron spectroscopy measurements, and UV/Vis absorption.

**General information**

**State:** Published

**Ministry of Education publication type:** A1 Journal article-refereed

**Organisations:** Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Industrial Bioengineering and Applied Organic Chemistry, Photonics, Research group: Surface Science

**Authors:** George, L., Efimova, E., Sariola-Leikas, E., Lahtonen, K., Valden, M., Vivo, P., Hakola, H., Hiltunen, A., Efimov, A.

**Publication date:** 7 Apr 2017

**Peer-reviewed:** Yes

**Publication information**

**Journal:** ChemPlusChem
Metallic engineered nanomaterials (ENMs) undergo various transformations in the environment which affect their fate, toxicity and bioavailability. Although constructed wetlands (CWs) are applied as treatment systems for waste streams potentially containing metallic ENMs, little is known about the fate and effects of ENMs in CWs. Hence, literature data from related fields such as activated sludge wastewater treatment and natural wetlands is used to predict the fate and effects of ENMs in CWs and to analyze the risk of nanomaterials being released from CWs into surface waters. The ENMs are likely to reach the CW (partly) transformed and the transformations will continue in the CW. The main transformation processes depend on the type of ENM and the ambient environmental conditions in the CW. In general, ENMs are expected to undergo sorption onto (suspended) organic matter and plant roots. Although the risk of ENMs being released at high concentrations from CWs is estimated low, caution is warranted because of the estimated rise in the production of these materials. As discharge of (transformed) ENMs from CWs during normal operation is predicted to be low, future research should rather focus on the effects of system malfunctions (e.g. short-circuiting). Efficient retention in the CW and increasing production volumes in the future entail increasing concentrations within the CW substrate and further research needs to address possible adverse effects caused.

General information
State: E-pub ahead of print
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Laboratory of Industrial Water and Ecotechnology, Universiteit Gent, Laboratory of Analytical Chemistry and Applied Ecochemistry, Laboratory of Chemistry and Bioengineering, Royal Military College of Canada
Authors: Auvinen, H., Gagnon, V., Rousseau, D. P. L., du Laing, G.
Keywords: (Discharge, Effluent, Nanoparticle, Transformation, TSS, Wastewater)
Number of pages: 16
Pages: 1-16
Publication date: 5 Apr 2017
Peer-reviewed: Yes
ASJC Scopus subject areas: Environmental Engineering, Applied Microbiology and Biotechnology, Waste Management and Disposal, Pollution

Publication information
Journal: Reviews in Environmental Science and Bio-Technology
ISSN (Print): 1569-1705
Ratings:
Publication Forum (2017): 1
Crystals of trans- and cis-isomers of a fluorinated azobenzene derivative have been prepared and characterized by single-crystal X-ray diffraction. The presence of F atoms on the aromatic core of the azobenzene increases the lifetime of the metastable cis-isomer, allowing single crystals of the cis-azobenzene to be grown. Structural analysis on the cis-azobenzene, complemented with density functional theory calculations, highlights the active role of the halogen-bond contact (N...I synthon) in promoting the stabilization of the cis-isomer. The presence of a long aliphatic chain on the azobenzene unit induces a phase segregation that stabilizes the molecular arrangement for both the trans- and cis-isomers. Due to the rarity of cis-azobenzene crystal structures in the literature, our paper makes a step towards understanding the role of non-covalent interactions in driving the packing of metastable azobenzene isomers. This is expected to be important in the future rational design of solid-state, photoresponsive materials based on halogen bonding. We show by single-crystal X-ray diffraction studies and computational analysis that halogen bonding can stabilize a metastable cis-azobenzene derivative in the solid state.
High-rate autotrophic denitrification in a fluidized-bed reactor at psychrophilic temperatures

In this study, high-rate autotrophic denitrification driven by thiosulfate (S2O32-) was maintained under psychrophilic conditions in a lab-scale fluidized-bed reactor (FBR) with a Thiobacillus-dominated biofilm. The temperature effects on the denitrifying performance of the FBR were monitored by gradually decreasing the temperature from 20 to 3°C. The potential of the FBR biofilm to maintain thiosulfate-driven denitrification at 3°C was further investigated at different HRTs (5.4, 3 and 1 h) and influent NO3- concentrations (200, 600 and 1078 mg/L), resulting in a gradual increase of the nitrogen loading rate (NLR) from 0.20 to 3.3 kg N-NO3-/m3 d. Complete thiosulfate-driven denitrification could be maintained at all temperatures, HRTs and influent NO3- concentrations tested. PCR-DGGE analysis revealed the dominance of the sulfur-oxidizing chemolithotrophs T. denitrificans and T. thioparus at all temperatures investigated. The FBR operation at a temperature as low as 3°C promoted bed expansion and increased the dissolved organic carbon (DOC) concentration in the effluent, but had no significant effects on the denitrification efficiency. The findings of this study are highly significant for the treatment of cold nitrogen-contaminated waters poor in organics and confirm the FBR as a robust and powerful bioreactor system for autotrophic denitrification.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry
Authors: Di Capua, F., Milone, I., Lakaniemi, A., N.L. Lens, P., Esposito, G.
Keywords: (Autotrophic denitrification, Fluidized-bed reactor, Psychrophilic temperatures, Thiobacillus, Thiosulfate)
Publication date: Apr 2017
Peer-reviewed: Yes
Early online date: 25 Dec 2016

Publication information

Journal: Chemical Engineering Journal
ISSN (Print): 1385-8947
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.745 1.933
Publication Forum (2016): 2
Scopus rating (2015): 1.695 1.919
Web of Science (2015): 5.31 5.439 3.9 1.579 0.09079 1.019
Publication Forum (2015): 2
Scopus rating (2014): 1.703 1.981
Web of Science (2014): 4.321 4.621 3.7 1.048 0.07967 0.945
Publication Forum (2014): 2
Scopus rating (2013): 1.602 1.914
Publication Forum (2013): 2
Scopus rating (2012): 1.517 1.85
Publication Forum (2012): 2
Hydrophobin-nanofibrillated cellulose stabilized emulsions for encapsulation and release of BCS class II drugs

The purpose of this study was to construct biopolymer-based oil-in-water emulsion formulations for encapsulation and release of poorly water soluble model compounds naproxen and ibuprofen. Class II hydrophobin protein HFBII from Trichoderma reesei was used as a surfactant to stabilize the oil/water interfaces of the emulsion droplets in the continuous aqueous phase. Nanofibrillated cellulose (NFC) was used as a viscosity modifier to further stabilize the emulsions and encapsulate protein coated oil droplets in NFC fiber network. The potential of both native and oxidized NFC were studied for this purpose. Various emulsion formulations were prepared and the abilities of different formulations to control the drug release rate of naproxen and ibuprofen, used as model compounds, were evaluated. The optimal formulation for sustained drug release consisted of 0.01% of drug, 0.1% HFBII, 0.15% oxidized NFC, 10% soybean oil and 90% water phase. By comparison, the use of native NFC in combination with HFBII resulted in an immediate drug release for both of the compounds. The results indicate that these NFC originated biopolymers are suitable for pharmaceutical emulsion formulations. The native and oxidized NFC grades can be used as emulsion stabilizers in sustained and immediate drug release applications. Furthermore, stabilization of the emulsions was achieved with low concentrations of both HFBII and NFC, which may be an advantage when compared to surfactant concentrations of conventional excipients traditionally used in pharmaceutical emulsion formulations.

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, University of Helsinki, VTT Technical Research Centre of Finland, Universita degli Studi di Padova, Italy, Division of Biopharmaceutical Sciences
Authors: Paukkonen, H., Ukkonen, A., Szilvay, G., Yliperttula, M., Laaksonen, T.
Keywords: (Drug release, Emulsions, Hydrophobin, Ibuprofen, Nanofibrillated cellulose, Naproxen)
Number of pages: 11
Pages: 238-248
Publication date: 30 Mar 2017
Peer-reviewed: Yes
ASJC Scopus subject areas: Pharmaceutical Science

Publication information
Journal: European Journal of Pharmaceutical Sciences
Volume: 100
ISSN (Print): 0928-0987
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.223 1.499
Publication Forum (2016): 2
Scopus rating (2015): 1.156 1.415
Web of Science (2015): 3.773 3.752 6.6 0.561 0.01365 0.802
Publication Forum (2015): 2
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.
Optimizing ammonium adsorption on natural zeolite for wastewaters with high loads of ammonium and solids

Ion exchange (IE) has been so far limited to treating waters and wastewaters low in solids (TS) and ammonium (NH$_4^+$). This study provides a new insight into the application of IE for NH$_4^+$ removal from wastewaters with high NH$_4^+$ and TS, using natural zeolite as adsorbent medium. Assays were carried out in continuously stirred batch reactors to study the effect of initial NH$_4^+$, pH, TS, contact time, and zeolite pore size (0.2–0.5 and 0.6–2.0 mm). Results confirmed the suitability of this zeolite to remove NH$_4^+$ from wastewater with high amounts of solids (up to 2% TS) and NH$_4^+$ (up to 2500 mg NH$_4^+$-N/L). Ammonium adsorption capacity ($q_t$) was faster with 0.2–0.5 mm size because of the greater specific surface area and shorter diffusion path than 0.6–2.0 mm zeolite. Both zeolites showed increasing $q_t$ with increasing initial NH$_4^+$ due to the higher driving force produced by higher concentrations. The process followed a pseudo-second order kinetic and was best described by the Freundlich isotherm. Varying the pH (6–8.5) of the wastewater had no effect on NH$_4^+$ removal capacity. In conclusion, this natural zeolite showed high affinity for NH$_4^+$ in wastewater with high loads of NH$_4^+$ and solids, returning a viable treatment method when other techniques are not applicable.

General information
State: E-pub ahead of print
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering
Authors: Taddeo, R., Prajapati, S., Lepistö, R.
Keywords: (Ammonium, Ion exchange, Kinetics, Solids, Zeolite)
Number of pages: 10
Pages: 1-10
Publication date: 3 Mar 2017
Peer-reviewed: Yes
ASJC Scopus subject areas: Materials Science(all), Mechanics of Materials, Mechanical Engineering

Publication information
Journal: Journal of Porous Materials
ISSN (Print): 1380-2224
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.483 0.679
Publication Forum (2016): 1
Scopus rating (2015): 0.404 0.615
Web of Science (2015): 1.385 1.428 5.7 0.35 0.00254 0.279
Publication Forum (2015): 1
Scopus rating (2014): 0.462 0.735
Web of Science (2014): 1.108 1.343 5.8 0.27 0.0025 0.274
Publication Forum (2014): 1
Scopus rating (2013): 0.497 0.884
Publication Forum (2013): 1
Scopus rating (2012): 0.522 0.977
Publication Forum (2012): 1
Scopus rating (2011): 0.538 0.85
Scopus rating (2010): 0.418 0.465
Scopus rating (2009): 0.455 0.527
Scopus rating (2008): 0.448 0.496
Scopus rating (2007): 0.481 0.634
Scopus rating (2006): 0.435 0.59
Scopus rating (2005): 0.383 0.621
Twin-layer biosensor for real-time monitoring of alkane metabolism

Intracellular metabolic sensors can be used for efficient screening and optimization of microbial cell factories. In particular, the sensors are useful in acquiring information about pathway dynamics and bottlenecks in a straightforward manner. Here, we developed a twin-layer biosensor that functions simultaneously at two levels: Through transcription factor mediated sensing and enzyme-metabolite interaction, providing insights into the dynamics of alkane metabolism. In addition, the sensor can be used for monitoring either alkane degradation or biosynthesis, depending on the used cellular context. Alkanes are monitored using a fluorescent reporter green fluorescent protein placed under a native alkane-inducible promoter, whereas a bacterial luciferase producing bioluminescence signal enzymatically detects a specific metabolic intermediate in the alkane production/degradation pathway. First, we employed the sensor to investigate the native alkane degradation route in Acinetobacter baylyi ADP1. The highest fluorescence and luminescence signals were obtained for dodecane. Second, we constructed a non-native alkane synthesis pathway in A. Baylyi ADP1, of which the functionality was confirmed with the sensor. The twin-layer approach provides convenient means to study and optimize the kinetics and performance of the heterologous pathway and will facilitate the development of an efficient cell factory.
Origin and fate of methane in the Eastern Tropical North Pacific oxygen minimum zone

Oxygen minimum zones (OMZs) contain the largest pools of oceanic methane but its origin and fate are poorly understood. High-resolution (<15 m) water column profiles revealed a 300 m thick layer of elevated methane (20–105 nM) in the anoxic core of the largest OMZ, the Eastern Tropical North Pacific. Sediment core incubations identified a clear benthic methane source where the OMZ meets the continental shelf, between 350 and 650 m, with the flux reflecting the concentration of methane in the overlying anoxic water. Further incubations characterised a methanogenic potential in the presence of both porewater sulphate and nitrate of up to 88 nmol g⁻¹ day⁻¹ in the sediment surface layer. In these methane-producing sediments, the majority (85%) of methyl coenzyme M reductase alpha subunit (mcrA) gene sequences clustered with Methanosarcinaceae (greater than 96% similarity to Methanococcoides sp.), a family capable of performing non-competitive methanogenesis. Incubations with 13C-CH4 showed potential for both aerobic and anaerobic methane oxidation in the waters within and above the OMZ. Both aerobic and anaerobic methane oxidation is corroborated by the presence of particulate methane monoxygenase (pmoA) gene sequences, related to type I methanotrophs and the lineage of Candidatus Methylomirabilis oxyfera, known to perform nitrite-dependent anaerobic methane oxidation (N-DAMO), respectively.
UV exposure in artificial and natural weathering: A comparative study

We report on a study focusing on UV exposure conditions in three different types of chambers used for accelerated ageing of materials. The first chamber is equipped with four 300-W UVA/UVB mercury vapour lamps (Ultra-Vitalux/Osram). The second chamber uses four 40-W UVA fluorescent lamps (QUV-340/Q-Lab). The third chamber is Weather-Ometer Ci3000+ from Atlas with a 4500-W xenon arc lamp. UV irradiance prevailing in each chamber was measured using Bentham DM150 double monochromator spectroradiometer. The results were compared to measurements of solar spectral UV irradiance at Jokioinen, Finland, with a Brewer MkIII double monochromator spectrophotometer. The spectral shapes of the exposing UV radiation in the different chambers were found to notably differ from each other and from the solar UV spectrum. Both spatial inhomogeneities and temporal variability caused by various factors, like the ageing of the lamps, were detected. The effects were found to strongly depend on wavelength of the exposing UV radiation. The findings of this study underline the necessity of careful characterization of the UV exposure conditions provided by the facilities used in accelerated testing of materials.

General information

State: Published
Organisations: Materials Science, Chemistry and Bioengineering, Research area: Design, Development and LCM, Finnish Meteorological Institute, World Radiation Cent, Aalto University, Paper Converting and Packaging Technology, Independent Researcher
Authors: Heikkilä, A., Kazadzis, S., Meinander, O., Vaskuri, A., Kärhä, P., Mylläri, V., Syrjälä, S., Koskela, T.
Publication date: 22 Feb 2017

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Article number: 110004
ISBN (Electronic): 9780735414785
ASJC Scopus subject areas: Physics and Astronomy(all)

Publication series

Name: AIP conference proceedings
Volume: 1810
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ISSN (Electronic): 1935-0465
DOIs: 10.1063/1.4975566

Source: Scopus
Research output: Scientific - peer-review › Conference contribution

Optimization of convectively cooled heat sinks

Many factors of heat sink, such as its size and mass, component locations, number of fins, and fan power affect heat transfer. Owing to the opposite effects of these factors on heat sink maximum temperature, we have now a multi-objective optimization problem. A typical optimization case consists of hundreds of heat sink temperature field evaluations, which would be impractical to do with CFD. Instead, we propose to combine analytical results of convection and numerical
solution of conduction to address these so-called conjugated heat transfer problems. We solve heat conduction in a solid numerically using the finite volume method and tackle convection with the analytical equation of forced convection in a parallel plate channel. This model is suitable for forced and natural convection heat sinks, and we have verified its validity by comparing its results to measured data and CFD calculations. We use the model to improve two industrial examples, using a multi-objective version of the particle swarm optimization (PSO) algorithm. The first example is a forced convection heat sink composed of nine heat generating components at the base plate, and the other is a natural convection case with two components. In both cases, mass is minimized; the other criterion is maximum temperature for the forced convection case and heat sink outer volume for the natural convection case. Our method is many orders of magnitude faster than CFD. Additionally, we provide some LES results of pin fins with natural convection for further use in similar optimizations.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Mechanical Engineering and Industrial Systems
Authors: Lampio, K., Karvinen, R.
Keywords: (Fin array, Forced convection, Heat sink, Multi-objective optimization, Natural convection, Pin fins)
Publication date: 20 Feb 2017
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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Safety, Risk, Reliability and Quality, Surfaces, Coatings and Films, Electrical and Electronic Engineering

Publication information
Journal: Microelectronics Reliability
ISSN (Print): 0026-2714
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.47 0.976
Publication Forum (2016): 1
Scopus rating (2015): 0.618 1.193
Web of Science (2015): 1.202 1.285 5.4 0.167 0.01019 0.352
Publication Forum (2015): 1
Scopus rating (2014): 0.601 1.432
Web of Science (2014): 1.433 1.336 5.8 0.154 0.00964 0.351
Publication Forum (2014): 1
Scopus rating (2013): 0.594 1.264
Publication Forum (2013): 1
Scopus rating (2012): 0.586 1.414
Publication Forum (2012): 1
Scopus rating (2011): 0.621 1.382
Scopus rating (2010): 0.602 1.114
Scopus rating (2009): 0.736 1.176
Scopus rating (2008): 0.932 1.235
Scopus rating (2007): 0.743 1.228
Scopus rating (2006): 0.716 1.153
Scopus rating (2005): 0.514 1.009
Scopus rating (2004): 0.537 0.823
Scopus rating (2003): 0.472 0.786
Scopus rating (2002): 0.592 0.756
Scopus rating (2001): 0.411 0.694
Scopus rating (2000): 0.349 0.382
Scopus rating (1999): 0.22 0.562
Original language: English
DOIs:
10.1016/j.microrel.2017.06.011
Source: Scopus
Source-ID: 85020690970
Research output: Scientific - peer-review › Article
Effect of hydraulic retention time on continuous electricity production from xylose in up-flow microbial fuel cell

Aerobic wastewater management is energy intensive and thus anaerobic processes are of interest. In this study, a microbial fuel cell was used to produce electricity from xylose which is an important constituent of lignocellulosic waste. Hydraulic retention time (HRT) was optimized for the maximum power density by gradually decreasing the HRT from 3.5 d to 0.17 d. The highest power density (430 mW/m²) was obtained at 1 d HRT. Coulombic efficiency decreased from 30% to 0.6% with HRTs of 3.5 d and 0.17 d, respectively. Microbial community analysis revealed that anode biofilm contained known exoelectrogens, including Geobacter sp. and fermentative organisms were present in both anolyte and the anode biofilm. The peak power densities were obtained at 1-1.7 d HRTs and xylose degraded almost completely even with the lowest HRT of 0.17 d, which demonstrates the efficiency of up-flow MFC for treating synthetic wastewater containing xylose.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Feng Chia University
Authors: Haavisto, J. M., Kokko, M. E., Lay, C., Puhakka, J. A.
Keywords: (Continuous operation, Hydraulic retention time, Microbial community, Microbial fuel cell, Up-flow, Xylose)
Publication date: 10 Feb 2017
Peer-reviewed: Yes

Publication information
ISSN (Print): 0360-3199
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.142 1.286
Publication Forum (2016): 1
Scopus rating (2015): 1.294 1.319
Web of Science (2015): 3.205 3.419 4.6 0.651 0.08996 0.619
Publication Forum (2015): 1
Scopus rating (2014): 1.212 1.494
Web of Science (2014): 3.313 3.659 4.3 0.539 0.08226 0.619
Publication Forum (2014): 3
Scopus rating (2013): 1.278 1.467
Publication Forum (2013): 3
Scopus rating (2012): 1.515 1.729
Publication Forum (2012): 3
Scopus rating (2011): 1.456 1.837
Scopus rating (2010): 1.589 1.871
Scopus rating (2009): 1.333 1.885
Scopus rating (2008): 1.401 2.096
Scopus rating (2007): 1.279 2.201
Scopus rating (2006): 1.073 2.161
Scopus rating (2005): 1.107 1.787
Scopus rating (2004): 1.225 1.626
Scopus rating (2003): 1.003 1.319
Scopus rating (2002): 0.763 1.157
Scopus rating (2001): 0.487 1.185
Scopus rating (2000): 0.518 0.866
Scopus rating (1999): 0.382 0.897
Original language: English
DOIs: 10.1016/j.ijhydene.2017.05.068

Bibliographical note
EXT="Lay, Chyi-How"
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

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Siiskonen, A., Priimägi, A.
Keywords: (Basis set, Benchmarking, Density functional theory, Halogen bonding)
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
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Publication Forum (2017): 1
Scopus rating (2016): 0.447 0.482
Publication Forum (2016): 1
Scopus rating (2015): 0.454 0.589
Web of Science (2015): 1.438 1.508 4.2 0.406 0.01025 0.345
Publication Forum (2015): 1
Scopus rating (2014): 0.51 0.727
Web of Science (2014): 1.736 1.711 3.8 0.189 0.00979 0.374
Publication Forum (2014): 1
Scopus rating (2013): 0.523 0.734
Publication Forum (2013): 1
Scopus rating (2012): 0.571 0.679
Publication Forum (2012): 1
Scopus rating (2011): 0.52 0.773
Scopus rating (2010): 0.919 1.148
Scopus rating (2009): 0.752 1.025
Scopus rating (2008): 0.75 0.719
Scopus rating (2007): 0.637 0.75
Scopus rating (2006): 0.466 0.532
Scopus rating (2005): 0.542 0.688
Scopus rating (2004): 0.977 1.158
Scopus rating (2003): 0.925 1.027
Scopus rating (2002): 0.561 0.676
Scopus rating (2001): 0.583 0.611
High-rate thiosulfate-driven denitrification at pH lower than 5 in fluidized-bed reactor

Abstract This study investigated the potential of a fluidized-bed biofilm dominated by Thiobacillus denitrificans to sustain thiosulfate-driven denitrification under increasingly acidic conditions. A fluidized-bed reactor (FBR) performing denitrification via thiosulfate (S2O3^2−) oxidation of a nitrate-contaminated synthetic wastewater was first operated under decreasing feed pH values from 7.00 to 5.25. Denitrification efficiency > 99% was observed even at feed and effluent pH of 5.75 and 5.30, respectively. At lower feed pH values, the denitrification efficiency decreased rapidly due to inorganic carbon deficiency. The addition of a carbonation unit continuously feeding anaerobic grade CO2 to the FBR biofilm allowed to investigate denitrification at pH values lower than 5.0. This new configuration, i.e. FBR with a carbonation unit, was able to sustain a complete and stable denitrification even at pH as low as 4.75. Denaturing gradient gel electrophoresis (DGGE) showed the evolution of the denitrifying biofilm during the FBR operation, resulting in a robust and high-performing mixotrophic consortium of chemolithotrophic and heterotrophic bacteria dominated by T. denitrificans. Batch activity tests performed at three different stages of the FBR operation (feed pH 7.0, 6.0 and 5.25) showed that low pH cultivation enhanced the denitrification activity (mg N/g VS d) of the FBR biofilm at acidic pH values.

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Authors: Di Capua, F., Lakaniemi, A., Puhakka, J. A., Lens, P. N. L., Esposito, G.
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Publication Forum (2015): 2
Scopus rating (2014): 1.703 1.981
Web of Science (2014): 4.321 4.621 3.7 1.048 0.07967 0.945
Publication Forum (2014): 2
Scopus rating (2013): 1.602 1.914
Publication Forum (2013): 2
Scopus rating (2012): 1.517 1.85
Publication Forum (2012): 2
Scopus rating (2011): 1.39 1.762
Scopus rating (2008): 1.056 1.513
Scopus rating (2007): 1.121 1.52
The Role of Inorganics in Biomass Gasification: Catalytic Effects on Char Reactions and Toxic Emissions

This thesis studied the role of inorganic elements in biomass gasification, focusing on catalytic effects in char gasification and removal of toxic metals from the product gas. A combination of experimental, including gasification using thermogravimetric analysis and fluidized beds, and modeling techniques were used.

Spruce and birch woods were leached of the naturally occurring ash forming elements and loaded with varying amounts of calcium or potassium. These woods were then gasified in either an isothermal thermogravimetric analysis device or a bubbling fluidized bed reactor. In the case of the spruce wood gasified using the thermogravimetric analysis device, char conversion models were evaluated against the measured data and an empirical model was developed which uses the concentration of calcium and potassium in wood to predict the conversion rate behavior of the char when gasified in CO2. The results from the fluidized bed gasification tests of birch wood showed that calcium was the primary active catalyst in the wood and the increased reactivity resulting from calcium doping was clear even in the much larger scale of a fluidized bed compared to the thermogravimetric analysis. The potassium doped samples did not exhibit increased reactivity in the fluidized bed due to a nonreactive layer of secondary char being deposited on the char surface.

The behavior of arsenic in the product gas of chromated-copper arsenate wood was modeled using equilibrium calculations and measured experimentally in a bubbling fluidized bed. The equilibrium model accurately predicted that the product gas could be cleaned by cooling the gas below 260°C and filtering to remove condensed arsenic.

While there are methods for modeling the effects of inorganics in catalyzing char gasification, further research into interconnected issues of surface area, pore sizes, pyrolysis conditions and inorganic concentrations is needed. Similarly, while equilibrium modeling has been shown to predict the behavior of arsenic during gasification in some cases, there are many gaps in understanding which arsenic compounds are most relevant.
Enhancing the activity of iron-oxidising bacteria: A case study with process liquors from heap bioleaching of a complex sulphide ore

In the present study, six process liquors (PL1 - PL6) originating from heap bioleaching of a complex sulphide ore were examined to reveal factors limiting microbial activity in the bioheaps. PL4 had the lowest iron oxidation activity even though its indigenous iron-oxidising community was diverse (Acidithiobacillus, Leptospirillum, Acidiferrobacter, and Sulfobacillus species). Shake flask experiments at 27 °C revealed that ferrous iron (Fe2+) and aluminium (Al3+) concentrations up to 16 and 12 g/L, respectively, were not inhibitory for the iron-oxidising microorganisms in PL4. In addition, Al3+ concentrations of ≤6 g/L were shown to enhance iron oxidation rates. High correlation between increased concentrations of cadmium (Cd), sulphate (SO42−), and vanadium (V) and decreased iron oxidation rates was detected when comparing process liquors 1–6. Moreover, possible nutrient limitation in PL4 was delineated by selectively supplementing it with macro- and micronutrients. Supplementation of 320 mg/L of nitrogen (as NH4+) to PL4 significantly increased iron oxidation rates from 20 mg/L/h (no nutrient supplementation) to 160 mg/L/h and would likely also enhance the heap bioleaching process. Additionally, microorganisms growing in high inhibitory ion concentrations (e.g., Cd2+) were shown to be more sensitive to nitrogen deficiency than microorganisms growing in more dilute liquors.

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Publication Forum (2016): 1
Scopus rating (2015): 1.173 1.888
Web of Science (2015): 2.29 2.947 8.1 0.419 0.00907 0.672
Publication Forum (2015): 1
Scopus rating (2014): 1.247 2.25
Web of Science (2014): 1.933 2.566 8.2 0.295 0.00887 0.595
Publication Forum (2014): 2
Scopus rating (2013): 1.626 2.967
Publication Forum (2013): 2
Scopus rating (2012): 1.523 2.4
Publication Forum (2012): 2
Scopus rating (2011): 1.521 1.796
Scopus rating (2010): 1.104 1.672
Scopus rating (2009): 1.185 2.458
Scopus rating (2008): 1.066 1.56
Scopus rating (2007): 1.027 1.45
Scopus rating (2006): 0.972 1.482
Scopus rating (2005): 1.076 1.605
Scopus rating (2004): 1.089 1.869
Scopus rating (2003): 0.843 1.565
Scopus rating (2002): 0.833 1.308
Scopus rating (2001): 0.481 1.317
Scopus rating (2000): 0.596 1.44
A light-driven artificial flytrap

The sophistication, complexity and intelligence of biological systems is a continuous source of inspiration for mankind. Mimicking the natural intelligence to devise tiny systems that are capable of self-regulated, autonomous action to, for example, distinguish different targets, remains among the grand challenges in biomimetic micro-robotics. Herein, we demonstrate an autonomous soft device, a light-driven flytrap, that uses optical feedback to trigger photomechanical actuation. The design is based on light-responsive liquid-crystal elastomer, fabricated onto the tip of an optical fibre, which acts as a power source and serves as a contactless probe that senses the environment. Mimicking natural flytraps, this artificial flytrap is capable of autonomous closure and object recognition. It enables self-regulated actuation within the fibre-sized architecture, thus opening up avenues towards soft, autonomous small-scale devices.

General information

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Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Wani, O. M., Zeng, H., Priimägi, A.
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Web of Science (2014): 11.47 11.904 1.9 1.706 0.26326 5.723
Publication Forum (2014): 2
Scopus rating (2013): 5.967 2.776
Publication Forum (2013): 2
Scopus rating (2012): 5.586 2.724
Publication Forum (2012): 2
Scopus rating (2011): 3.122 1.544
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Source: PubMed
Source-ID: 28534872
Research output: Scientific - peer-review › Article
Base catalysed N-functionalisation of boroxazolidones
A method for the condensation of boroxazolidones derived from L-valine with aromatic aldehydes, catalysed by 1,5,7-triazabicyclo[4.4.0]dec-5-ene was developed. The preparation and isolation of a series of highly functionalised stable ketimines derived from the reaction of 2,2-diaryl-1,3,2-oxazaborolidin-5-ones with aryl aldehydes is herein described. Several unreported boroxazolidones were prepared by condensation of triethylammonium tetra-arylborates with L-valine in up to 98% yield. The newly synthesised compounds were determined to be moderately cytotoxic against colorectal adenocarcinoma cells, with the best compound in this series having an IC50 of 76 μM. A brief inspection of the effect of the same compound against human brain astrocytoma cells showed an IC50 of 268 μM.

General information
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Authors: J., R., Mannoja, J., Nguyen, T., N., A., N. M., K., Franzén, R. G., Kandhavelu, M., Candeias, N. R.
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Publication Forum (2016): 1
Scopus rating (2015): 0.959 0.837
Web of Science (2015): 3.289 3.485 1.8 0.676 0.13014 0.628
Publication Forum (2015): 1
Scopus rating (2014): 1.114 0.965
Web of Science (2014): 3.84 3.907 1.7 0.597 0.0623 0.747
Publication Forum (2014): 1
Scopus rating (2013): 1.117 0.903
Publication Forum (2013): 1
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INT="Raunio, J."
INT="Nguyen, T."
INT="Ahmad, N."
INT="Kemppainen, N. M."
Research output: Scientific - peer-review > Article

Biological removal of selenate and ammonium by activated sludge in a sequencing batch reactor
Wastewaters contaminated by both selenium and ammonium need to be treated prior to discharge into natural water bodies, but there are no studies on the simultaneous removal of selenium and ammonium. A sequencing batch reactor (SBR) was inoculated with activated sludge and operated for 90 days. The highest ammonium removal efficiency achieved was 98%, while the total nitrogen removal was 75%. Nearly a complete chemical oxygen demand removal efficiency was attained after 16 days of operation, whereas complete selenate removal was achieved only after 66 days. The highest total Se removal efficiency was 97%. Batch experiments showed that the total Se in the aqueous phase decreased by
This study investigated the feasibility of combining bioremediation of selenium (Se) containing wastewater and biorecovery of Se as cadmium selenide nanoparticles (CdSe NPs). A microbial community of anaerobic granular sludge was enriched with increasing initial ammonium concentration from 50 to 100 mg L\(^{-1}\). This study showed that SBR can remove both selenate and ammonium via, respectively, bioreduction and partial nitrification-denitrification and thus offer possibilities for treating selenium and ammonium contaminated effluents.
for 300 days in the presence of Cd(ii) and selenite (Se(iv)). Complete Se(iv) (79 mg L\(^{-1}\)) reduction in the presence of Cd (30 mg L\(^{-1}\)) was observed after the 16th transfer (8 months) with the formation of both elemental selenium (Se(0)) and dissolved selenide (Se(-ii)). Cd either was associated with Se(0) or remained in the aqueous phase as free Cd(ii) ions and/or CdSe. The absorption and the fluorescence spectra of the aqueous phase showed formation of CdSe NPs. UV-vis and X-ray photoelectron spectroscopy (XPS) confirmed that the CdSe NPs were capped by extracellular polymeric substances (EPS) originating from the anaerobic granular sludge. Raman spectroscopy and XPS analysis further confirmed the presence of CdSe NPs in the aqueous phase, while Cd present in the Se(0) pellet after centrifugation was mainly precipitated as a Se(0)-Cd complex. A CdSe/CdS core/shell structure was found in the sludge, suggesting that Cd(ii) ions on the surface of the CdSe core interact with the sulfhydryl (-SH) groups present in the EPS of the UASB granules.

General information
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Authors: Mal, J., Nancharaiah, Y. V., Bera, S., Maheshwari, N., Van Hullebusch, E. D., Lens, P. N.
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ASJC Scopus subject areas: Materials Science (miscellaneous), Environmental Science(all)

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Research output: Scientific - peer-review » Article

Difference in the core-shell dynamics of polyethyleneimine and poly(l-lysine) DNA polyplexes
Electrostatic polymer-DNA complexes (polyplexes) have been widely investigated for DNA delivery, and remarkable differences in transfection efficacy have been seen among the materials. For example, polyethyleneimine (PEI) mediates DNA transfection more effectively than poly(l-lysine) (PLL). Biophysical properties of the polyplexes may explain their different properties in gene delivery. We investigated the structural dynamics in DNA polyplexes, especially the material exchange between the core and shell regions of the PEI and PLL polyplexes. Steady-state fluorescence spectroscopy and double labeling based fluorescence resonance energy transfer (FRET) techniques were used to study the DNA polyplexes. According to our results there is a clear difference between these two polymers: core exchange takes place in PEI but not in PLL polyplexes. Such differences in structural dynamics of polyplexes explain, at least partly, the differences in DNA release and transfection efficacy at cellular level.

General information
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Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, University of Helsinki, Ita-Suomen yliopisto, Universita degli Studi di Padova, Italy
Authors: Vuorimaa-Laukkanen, E., Lisitsyna, E. S., Ketola, T., Morin-Pickardat, E., Liang, H., Hanzliková, M., Yliperttula, M.
Keywords: (DNA complexation, Fluorescence spectroscopy, Non-viral gene delivery, Poly-l-lysine, Polyethylene imine, Polyplex)
Publication date: 2017
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ASJC Scopus subject areas: Pharmaceutical Science

Publication information
Journal: European Journal of Pharmaceutical Sciences
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°, 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

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Organisations: Physics, Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Research group: Electronic Structure Theory, Research area: Computational Physics, Center of Innovation Technologies
Authors: Golovanov, V. V., Nazarchuk, B. V., Golovanova, V. V., Tkachenko, N. V., Rantala, T. T.
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ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry

Publication information
Fluorescence spectroscopy "knife" for polyplex "cakes": taste the filling

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Authors: Vuorimaa-Laukkanen, E., Lisitsyna, E. S., Ketola, T., Morin-Pickardat, E., Liang, H., Hanzlikova, M., Urtti, A., Yliperttula, M. L.
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ASJC Scopus subject areas: Chemistry(all), Pharmaceutical Science
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Research output: Scientific › peer-review › Article

Influence of TiO₂ compact layer precursor on the performance of perovskite solar cells
The optimization of the hole-blocking layer in perovskite solar cells (PSC), typically based on TiO₂, is crucial, as it strongly affects the device performance. In this work, we thoroughly characterize the thickness, roughness, and crystal structure of a set of TiO₂ compact layers produced by spin coating of different precursor sols and correlate the choice of the TiO₂ precursor to the photovoltaic performance of the PSC. By replacing the commonly used titanium isopropoxide (TTIP) blocking layer precursor with titanium tetrachloride (TiCl₄), a clear enhancement in the PSC performance was observed, particularly in the hysteresis behavior and stability. The results from the morphological/structural analysis and transient
photoluminescence studies clarify the different behavior of the compact layers in PSCs.

**Light-Driven, Caterpillar-Inspired Miniature Inching Robot**

Liquid crystal elastomers are among the best candidates for artificial muscles, and the materials of choice when constructing microscale robotic systems. Recently, significant efforts are dedicated to designing stimuli-responsive actuators that can reproduce the shape-change of soft bodies of animals by means of proper external energy source. However, transferring material deformation efficiently into autonomous robotic locomotion remains a challenge. This paper reports on a miniature inching robot fabricated from a monolithic liquid crystal elastomer film, which upon visible-light excitation is capable of mimicking caterpillar locomotion on different substrates like a blazed grating and a paper surface. The motion is driven by spatially uniform visible light with relatively low intensity, rendering the robot "human-friendly," i.e., operational also on human skin. The design paves the way toward light-driven, soft, mobile microdevices capable of operating in various environments, including the close proximity of humans.
Microbial community response on wastewater discharge in boreal lake sediments

Despite high performance, municipal wastewater treatment plants (WWTPs) still discharge significant amounts of organic material and nitrogen and even microbes into the receiving water bodies, altering physico-chemical conditions and microbial functions. In this study, we examined how nitrified wastewater affects the microbiology of boreal lake sediments. Microbial community compositions were assessed with next generation sequencing of the 16S rRNA gene, and a more detailed view on nitrogen transformation processes was gained with qPCR targeting on functional genes (nirS, nirK, nosZI, nosZII, amoAarchaea, and amoAbacteria). In both of the two studied lake sites, the microbial community composition differed significantly between control point and wastewater discharge point, and a gradual shift toward natural community composition was seen downstream following the wastewater gradient. SourceTracker analysis predicted that ~2% of sediment microbes were of WWTP-origin on the study site where wastewater was freely mixed with the lake water, while when wastewater was specially discharged to the sediment surface, ~6% of microbes originated from WWTP, but the wastewater-influenced area was more limited. In nitrogen transformation processes, the ratio between nitrifying archaea (AOA) and bacteria (AOB) was affected by wastewater effluent, as the AOA abundance decreased from the control point...
(AOA:AOB 28:1 in Keuruu, 11:1 in Petäjävesi) to the wastewater-influenced sampling points, where AOB dominated (AOA:AOB 1:2–1:15 in Keuruu, 1:3–1:19 in Petäjävesi). The study showed that wastewater can affect sediment microbial community through importing nutrients and organic material and altering habitat characteristics, but also through bringing wastewater-originated microbes to the sediment, and may thus have significant impact on the freshwater biogeochemistry, especially in the nutrient-poor boreal ecosystems.

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Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, University of Jyväskylä
Authors: Saarenheimo, J., Aalto, S. L., Rissanen, A. J., Tiirola, M.
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Web of Science (2015): 4.165 4.36 2.5 0.564 0.03622 1.395
Publication Forum (2015): 1
Scopus rating (2014): 1.861 1.16
Web of Science (2014): 3.989 4.17 2.4 0.698 0.023 1.37
Publication Forum (2014): 1
Scopus rating (2013): 1.751 0.951
Publication Forum (2013): 1
Scopus rating (2012): 1.415 0.725
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Research output: Scientific - peer-review › Article

Occurrence of photoinduced charge separation by the modulation of the electronic coupling between pyrene dimers and chemically converted graphenes
The photoexcitation of the pyrene dimer on graphene resulted in the final formation of a charge-separated state following an exciplex formation, while that of the pyrene monomer on graphene generated the corresponding exciplex solely due to the difference in the electronic coupling between the pyrene and the graphene.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Umeyama, T., Baek, J., Mihara, J., Tkachenko, N. V., Imahori, H.
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Publication information
Journal: Chemical Communications
A series of 9-substituted 10-methylacridinium ions (Acr+-R) in which an electron-donor moiety (R) is directly linked with an electron-acceptor moiety (Acr+) at the 9-position was synthesized, and the photodynamics was fully investigated to determine the rate constants of photoinduced electron transfer (ET) and back electron transfer. The driving forces of photoinduced electron transfer and back electron transfer were determined by means of electrochemical and photophysical measurements. The dependence of the ET rate constants on driving force was well analyzed in the light of the Marcus theory of ET. The quantum yields of formation of the triplet ET states vary significantly, depending on the interaction between the donor (R) and acceptor (Acr+) moieties. Among the Acr+-R examined, the 9-mesityl-10-methylacridinium ion (Acr+-Mes) exhibits the best performance in terms of the lifetime of the triplet ET state and the quantum yield. Photoexcitation of Acr+-Mes results in formation of the triplet ET state [3(Acr.-Mes.+)], which has a long lifetime, a high energy (2.37 eV), and a high quantum yield (>75 %) in acetonitrile. The triplet ET state exhibits both the oxidizing and reducing activity of the Mes.+ and Acr. moieties, respectively.
Release of Potassium during Devolatilization of Spruce Bark

The spruce bark with different particle sizes were devolatilized under various final temperatures and heating rates. The char yield and potassium release from the spruce bark at studied conditions were quantified. Lower char yields realized from the smaller fuel particles at high temperature and heating rate. It is mainly attributed to shorter residence time of volatiles in the fuel/char particles and less intensive secondary reaction of volatiles consequently. The devolatilization temperature has the most significant effects on alkali release from the studied sprue bark. At 600°C, less than 5% of alkali released from the both small and large particles regardless of heating rate. However, at 850°C, release of potassium from the small sprue bark particles sharply increased from 2.63% to 12.87% and 17.89%, as they were heated under heating rate of 50 K/min and 500 K/min, respectively. Large fraction of alkali released from studied fuel particles as they were devolatilized under a high heating rate. Additionally, more potassium release from small particles (125 <d<180 μm) then the larger ones (500 <d<600 μm) and this tendency increased with devolatilization temperature. In brief, intensive devolatilization conditions may limit secondary reactions of potassium containing compounds in the volatiles and thereby formation of more stable phases. The results obtained in the present work are of importance for understanding of potassium release during thermal conversion of spruce bark and proposing measures for mitigating potassium related operational problems.
Structural and Photophysical Properties of Pentacene Alkanethiolate Monolayer-Protected Gold Nanoclusters and Nanorods: Supramolecular Intercalation and Photoinduced Electron Transfer with C60

6,13-Bis(trisopropylsilylethynyl)-pentacene (TIPS-pentacene: TP) alkanethiolate monolayer-protected gold nanoclusters (TP-Cn-X-MPCs: X stands for small (S) and large (L) nanocluster sizes) and nanorods (TP-Cn-MPRs) with different alkyl chain lengths (n = 7, 11) were synthesized to examine the structural and photophysical properties as well as intercalation trends with C60. The syntheses of TP-Cn-X-MPCs and TP-Cn-MPRs were successfully performed using two different precursors: TP disulfides and TP alkanethiols. The detailed structural properties were confirmed by 1H NMR, elemental analyses, and transmission electron micrograph (TEM). In the spectroscopic absorption and fluorescence excitation measurements, spectral shapes of TP units on the gold surface were clearly observed, whereas fluorescence intensities of TP units were strongly quenched as compared to the corresponding reference monomer (TP-Ref). Then, fluorescence quenching titration experiments to determine the association constants (Kapp) between C60 and TP assemblies (TP-Cn-X-MPC and TP-Cn-MPR) were performed by adding C60 in toluene. The Kapp values were largely dependent on the sizes of nanoclusters and alkyl chain lengths in TP-Cn-X-MPC. For example, the Kapp value of TP-C7-S-MPC (73 800 M⁻¹) was much larger than those of TP-C11-S-MPC (37 800 M⁻¹) and TP-C7-L-MPC (5350 M⁻¹). This trend is in sharp contrast with the similar Kapp values (~66 000 M⁻¹) in TP-Cn-MPR (n = 7, 11). These results suggest that the intercalation behaviors are dependent on the surface structures (nanocluster vs nanorod). Such fluorescence quenching processes by photoinduced electron transfer (PET) in the complex between TP-C7-S-MPC and C60 were directly observed by femtosecond transient absorption measurements, monitoring the TP radical cation and C60 radical anion.
Synthesis of phenol-derivatives and biological screening for anticancer activity
Phenolic compounds are known for their cytotoxic properties against cancer cells despite their still unclear general mechanism of action. Herein is reported the evaluation of the cytotoxic effects of on human osteosarcoma cells of nine phenol derivatives against osteosarcoma cells, and some insights on their mechanism. The cytotoxicity was characterized by cell viability, scratch assay, cellular DNA content measurement, Annexin V apoptosis, mitochondrial calcium and caspase 3/7 assays. The study shows that out of the nine compounds used in this study, a tetrahydroquinoline derivative, 2-((1,2,3,4-tetrahydroquinolin-1-yl)(4-methoxyphenyl)methyl)phenol, was found to exhibit strong inhibitory response with IC50 of 50.5 ± 3.8 μM, and therefore can be a potential chemotherapeutic agent. Further experiments revealed that this compound induces cell death by apoptosis and also act as a migration inhibitor. Analysis of the mitochondrial calcium following treatment with the compound on U2OS cells showed a significant reduction in the level of mitochondrial calcium concentration suggesting a mitochondrial calcium-independent mechanism in triggering apoptosis. Treatment of HEK293 cells with the compound confirmed the cytotoxic effects of the compound, however, an increase in the level of mitochondrial calcium was observed. Moreover, the caspase 3/7 mediated cell death was also observed in both cell types. Overall, the study suggests that the derivatives of this compound can be used for development of new therapeutics for osteosarcoma and other cancers.
The impact of long-term water level draw-down on microbial biomass: A comparative study from two peatland sites with different nutrient status

We examined the effects of long-term (51 years) drainage on peat microbial communities using phospholipid fatty acid (PLFA) analysis. We analysed the peat profiles of natural and adjacent drained fen and bog sites. Viable microbes (i.e. microbial PLFA) were present in relatively large amounts even in the deepest peat layers of both peatland sites, a finding that warrants further investigation. Microbial biomass was generally higher in the fen than in the bog. Microbial community structure (indexed from PLFA) differed between the fen and bog sites and among depths. Although we did not exclude other factors, the effect of drainage on the total microbial biomass and community structure was not limited to the surface layers, but extended to the deepest layers of the fen and bog. Long-term drainage increased the total microbial PLFA biomass in the surface, subsurface and bottom layers of the fen, but decreased it in the surface and bottom layers of the bog site. Drainage also increased the characteristic FAs of Gram-positive and Gram-negative bacteria in the surface and subsurface layers of the fen, and decreased them in the bottom layers of the bog site. The characteristic fungal FA was only reduced in the surface layers of the bog site by drainage. Thus, by affecting the microbial community beyond the surface layers, long-term peatland water-level draw-down can alter the microbial contribution to deeper peat organic matter stabilization. This suggests that long-term drainage may have a more significant climate change effect than revealed by the surface layer analyses alone.
Vapor Phase Fabrication of Nanoheterostructures Based on ZnO for Photoelectrochemical Water Splitting

Nanoheterostructures based on metal oxide semiconductors have emerged as promising materials for the conversion of sunlight into chemical energy. In the present study, ZnO-based nanocomposites have been developed by a hybrid vapor phase route, consisting in the chemical vapor deposition of ZnO systems on fluorine-doped tin oxide substrates, followed by the functionalization with Fe$_2$O$_3$ or WO$_3$ via radio frequency-sputtering. The target systems are subjected to thermal treatment in air both prior and after sputtering, and their properties, including structure, chemical composition, morphology, and optical absorption, are investigated by a variety of characterization methods. The obtained results evidence the formation of highly porous ZnO nanocrystal arrays, conformally covered by an ultrathin Fe$_2$O$_3$ or WO$_3$ overlayer. Photocurrent density measurements for solar-triggered water splitting reveal in both cases a performance improvement with respect to bare zinc oxide, that is mainly traced back to an enhanced separation of photogenerated charge carriers thanks to the intimate contact between the two oxides. This achievement can be regarded as a valuable result in view of future optimization of similar nanoheterostructured photoanodes.
A comparison of fate and toxicity of selenite, biogenically and chemically synthesized selenium nanoparticles to zebrafish (Danio rerio) embryogenesis

Microbial reduction of selenium (Se) oxyanions to elemental Se is a promising technology for bioremediation and treatment of Se wastewaters. But a fraction of biogenic nano-Selenium (nano-Se(b)) formed in bioreactors remains suspended in the treated waters, thus entering the aquatic environment. The present study investigated the toxicity of nano-Se(b) formed by anaerobic granular sludge biofilms on zebrafish embryos in comparison with selenite and chemogenic nano-Se (nano-Se(c)). The nano-Se(b) formed by granular sludge biofilms showed a LC50 value of 1.77 mg/L, which was 3.2-fold less toxic to zebrafish embryos than selenite (LC50 = 0.55 mg/L) and 10-fold less toxic than bovine serum albumin stabilized nano-Se(c) (LC50 = 0.16 mg/L). Smaller (nano-Se(cs); particle diameter range: 25-80 nm) and larger (nano-Se(cl); particle diameter range: 50-250 nm) sized chemically synthesized nano-Se(c) particles showed comparable toxicity on zebrafish embryos. The lower toxicity of nano-Se(b) in comparison to nano-Se(c) was analyzed in terms of the stabilizing organic layer. The results confirmed that the organic layer extracted from the nano-Se(b) consisted of components of the extracellular polymeric substances (EPS) matrix, which govern the physiochemical stability and surface properties like ζ-potential of nano-Se(b). Based on the data, it is contended that the presence of humic acid like substances of EPS on the surface of nano-Se(b) plays a major role in lowering the bioavailability (uptake) and toxicity of nano-Se(b) by decreasing the interactions between nanoparticles and embryos.

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Controlling the shape of Janus nanostructures through supramolecular modification of ABC terpolymer bulk morphologies

Abstract
Block copolymers microphase separate into a variety of bulk morphologies that serve as scaffolds, templates, masks and source for polymeric nano-particles. While supramolecular additives are common to complex within diblock copolymers to modify the morphology, the subtle effects of complexation on ABC triblock terpolymer morphologies are less explored. Here, we describe the manipulation of polystyrene-block-poly(4-vinylpyridine)-block-poly(tert-butyl methacrylate) (PS-b-P4VP-b-PT or S4VT) triblock terpolymer bulk morphologies through supramolecular complexation with rod-like 4-(4-pentylphenylazo)phenol (5PAP). The 5PAP molecule hydrogen bonds by phenolic groups to the 4VP repeating units and with increasing molar fraction of 5PAP, initially observed P4VP cylinders flatten into elliptic cylinders until a morphological transition occurs into a third (P4VP/5PAP) lamella. At sufficient 5PAP loadings, the cylinders can even merge into a perforated P4VP lamella located at the PS/PT interface. Quaternization of the P4VP phase and re-dispersion in organic solvent allows liberating S4VT Janus nanostructures from the bulk, including Janus cylinders, nanoporous Janus membranes and Janus sheets. The manipulation of “sandwiched” microphases through supramolecular binding motifs could allow the preparation of previously inaccessible terpolymer bulk morphologies and, in case of cross-linkable phases, lead to a larger library of Janus nano-objects.

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Scopus rating (2016): 1.191 1.252
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Scopus rating (2015): 1.157 1.286
Web of Science (2015): 3.586 3.775 10.0 0.8 0.04557 0.796
Publication Forum (2015): 2
Web of Science (2014): 3.562 3.91 9.4 0.726 0.0502 0.842
Publication Forum (2014): 2
Scopus rating (2013): 1.415 1.666
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Publication Forum (2012): 2
Scopus rating (2011): 1.623 1.82
Scopus rating (2010): 1.851 1.8
Scopus rating (2009): 1.999 1.72
Influence of torrefaction pretreatment on the pyrolysis of Eucalyptus clone: A study on kinetics, reaction mechanism and heat flow

The adverse nature of biomass requires specific pretreatment processes to better utilize it in bioenergy applications, and torrefaction is one of the most recognized thermal pretreatment methods. In this regard, we studied the effect of torrefaction pretreatment on kinetics, reaction mechanism and heat flow during the pyrolysis of biomass by making a comparative analysis between the pyrolysis of dried and torrefied Eucalyptus wood. Torrefied biomass was produced at three temperatures, namely 250, 275 and 300 °C. Pyrolysis was performed at 700 °C. The char yield during pyrolysis increased from 22.39 percent to 36.34 percent when the torrefaction temperature was increased from 250 to 300 °C. Kinetic analysis showed that torrefied biomass has higher activation energy values than dried biomass. The reported activation energy values for dried biomass were within the range of 165–185 kJ/mol, and for the biomass torrefied at 300 °C they were within the range of 180–245 kJ/mol. We used two different approaches, namely master plots and kinetic compensation parameters, to identify the reaction mechanism. The results showed that torrefaction treatment had an effect on the reaction mechanism of the biomass pyrolysis. The reason could be the degradation of hemicellulose during torrefaction, and thereby the formation of smaller molecules during the pyrolysis of torrefied biomass. The heat flow data from differential scanning calorimetry (DSC) showed that pyrolysis started with exothermic reactions for dried samples, and endothermic reactions for torrefied samples. The results presented provide valuable insights into increasing the understanding of the pyrolysis of torrefied biomass.
Remarkable Dependence of Exciplex Decay Rate on Through-Space Separation Distance Between Porphyrin and Chemically Converted Graphene

A series of chemically converted graphenes (CCGs) covalently functionalized with multiple zincporphyrins (ZnPs) through tuned lengths of linear oligo-p-phenylene bridges (ZnP-phn-CCG, n = 1–5) were prepared to address the bridge length effect on their photodynamics. Irrespective of the bridge length, photoexcitation of ZnP-phn-CCG led to exclusive formation of an exciplex state, which rapidly decayed to the ground state without yielding the completely charge-separated state. The notable dependence of the exciplex lifetime as a function of separation distance between the porphyrin and CCG has been observed for the first time, supporting the hypothesis that the decay to the ground state is dominated by the through-space interaction rather than the through-bond one. The basic information on the interaction between ZnP and CCG in the excited state will provide us with deeper insight on the intrinsic nature of the exciplex state as a function of donor–acceptor interaction.

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Publication Forum (2016): 1
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Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
The effect of low-temperature pretreatment on the solubilization and biomethane potential of microalgae biomass grown in synthetic and wastewater media

Microalgae have been suggested as a sustainable raw material for biofuel production in the form of methane via anaerobic digestion. Here, pretreatments at 60–80 °C were investigated, aiming to study the impact of algae culture media on biomethane potential and pretreatment efficiency. Chlorella vulgaris and mixed culture of native algae species (dominating by Scenedesmus sp.) were grown in synthetic medium, wastewater (sterilized and non-sterilized) and digestate from anaerobic digestion of pulp and paper biosludge (sterilized and non-sterilized). The biomethane potential for native microalgal biomass varied between 154 and 252 L CH₄ kg⁻¹ VS depending on culture media. The efficiency of the low-temperature pretreatment (80 °C, 3 h) for solubilization (9–12%) of C. vulgaris and native algae biomass was similar for algae grown in sterilized and non-sterilized wastewater media. The pretreatment increased the biomethane potential of native algae biomass by 11–24%.

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Web of Science (2015): 4.917 5.744 5.0 1.012 0.13375 1.089
Publication Forum (2015): 2
Scopus rating (2014): 2.41 2.104
Web of Science (2014): 4.494 5.33 4.6 0.822 0.12645 1.042
Publication Forum (2014): 2
Scopus rating (2013): 2.412 2.503
Publication Forum (2013): 2
Scopus rating (2012): 2.389 2.465
Publication Forum (2012): 2
Anaerobic digestion of microalgae and pulp and paper biosludge

In recent decades, microalgae have attracted attention as a promising biomass source for a variety of different biofuels, including methane via anaerobic digestion (AD). However, the energy intensity and cost (e.g., for the nutrient supply) of the process chain mean that breakthroughs in algal biofuels have yet to be realized. The objective of this study was to improve the AD of wastewater-grown microalgal biomass, marine algal residues following lipid extraction for renewable diesel production and to improve the AD of pulp and paper industry biosludge. The digestate from the latter substrate could provide nutrients for algae cultivation and lipid extraction followed by AD offers the possibility of obtaining multiple products from algal biomass, as envisaged by the algal biorefinery concept.

Based on the results of this experimental work, pretreatments and novel reactor designs can be used to improve the AD of microalgae. In this study, BMPs for wastewater- and digestate-grown mixed populations of microalgae varied between 154 and 273 L CH₄ kg⁻¹ volatile solids (VS). Low-temperature (3 h, 80°C) pretreatments enhanced the BMPs by 11–27%. However, to ensure positive energy balances, the availability of waste heat was necessary. Due to longer solid retention times, the AD of microalgae in unmixed, accumulating-volume reactors (AVRs) at 16–21°C was more feasible than AD in conventional completely stirred tank reactors (CSTRs) at 35°C when the solid concentration of the algal biomass was low (< 4% total solids [TSs]). Biological (at ~60°C) and freeze-thaw pretreatments enhanced the methane yield (32–50% increase) and the mineralization of nitrogen and phosphorus (41–84% increase) in the low-temperature AVRs.

In the present study, the AD of marine algae residue after lipids were extracted for renewable diesel production was demonstrated and the salt concentration of the marine algal biomass did not affect AD. Thermophilic AD in the CSTR resulted in a 48% higher methane yield (220 L CH₄ kg⁻¹ VSs) of algal residues compared with mesophilic AD. However, unlike mesophilic AD, ammonia, which originated from the high nitrogen content of the algal biomass, inhibited the thermophilic process.

AD of pulp and paper industry biosludge mineralized nutrients to a soluble form, making effluent a potential media for algal cultivation. The methane yield from the biosludge was low (78 L CH₄ kg⁻¹ VS) but increased by 77% with thermal pretreatment (20 min, 121°C). The pretreatment also resulted in AD with a retention time of 10 d, as compared to 14 d for untreated biosludge. However, the energy balance of the pretreatment was dependent on the solid concentration and temperature of the biosludge from the industrial process.

To conclude, this work demonstrated AD of microalgae under psychrophilic, mesophilic, and thermophilic conditions. The low energy balances emphasize that improvements in algae cultivation are required and/or other benefits (e.g., nutrient recovery, value-added products, and waste treatment) obtained for algal AD to become a full-scale application.

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Organisations: Department of Chemistry and Bioengineering
Authors: Kinnunen, V.
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The Orange Side of Disperse Red 1: Humidity-Driven Color Switching in Supramolecular Azo-Polymer Materials Based on Reversible Dye Aggregation

Humidity detection, and the quest for low-cost facile humidity-sensitive indicator materials is of great interest for many fields, including semi-conductor processing, food transport and storage, and pharmaceuticals. Ideal humidity-detection materials for these applications might be based on simple clear optical readout with no power supply, i.e.: a clear color change observed by the naked eye of any untrained observer, since it doesn't require any extra instrumentation or interpretation. Here, the introduction of a synthesis-free one-step procedure, based on physical mixing of easily available commercial materials, for producing a humidity memory material which can be easily painted onto a wide variety of surfaces and undergoes a remarkable color change (approximately 100 nm blue-shift of λMAX) upon exposure to various thresholds of levels of ambient humidity is reported. This strong color change, easily visible to as a red-to-orange color switch, is locked in until inspection, but can then be restored reversibly if desired, after moderate heating. By taking advantage of spontaneously-forming reversible 'soft' supramolecular bonds between a red-colored azo dye and a host polymer matrix, a reversible dye 'migration' aggregation appearing orange, and dis-aggregation back to red can be achieved, to function as the sensor.

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Authors: Schoelch, S., Vapaavuori, J., Rollet, F., Barrett, C. J.
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Anaerobic batch conversion of pine wood torrefaction condensate

Organic compound rich torrefaction condensate, owing to their high water content and acidic nature, have yet to be exploited for practical application. In this study, microbial conversion of torrefaction condensate from pine wood through anaerobic batch digestion (AD) to produce methane was evaluated. Torrefaction condensate exhibited high methane potentials in the range of 430-492mL/g volatile solids (VS) and 430-460mL/gVS under mesophilic and thermophilic conditions, respectively. Owing to the changes in the composition, the methane yields differed with the torrefaction condensates produced at different temperatures (225, 275 and 300°C), with a maximum of 492±18mL/gVS with the condensate produced at 300°C under mesophilic condition. The cyclic batch AD experiments showed that 0.1VSsubstrate:VSinoculum is optimum, whereas the higher substrate loading (0.2-0.5) resulted in a reversible inhibition of the methane production. The results suggest that torrefaction condensate could be practically valorized through AD.

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Publication Forum (2015): 2
Scopus rating (2014): 2.41 2.104
Web of Science (2014): 4.494 5.33 4.6 0.822 0.12645 1.042
Publication Forum (2014): 2
Scopus rating (2013): 2.412 2.503
Publication Forum (2013): 2
Scopus rating (2012): 2.389 2.465
Publication Forum (2012): 2
Scopus rating (2011): 2.314 2.508
Scopus rating (2010): 2.086 2.355
Scopus rating (2009): 1.912 2.231
Efficient Light-Induced Phase Transitions in Halogen-Bonded Liquid Crystals

Here, we present a new family of light-responsive, fluorinated supramolecular liquid crystals (LCs) showing efficient and reversible light-induced LC-to-isotropic phase transitions. Our materials design is based on fluorinated azobenzenes, where the fluorination serves to strengthen the noncovalent interaction with bond-accepting stilbazole molecules, and increase the lifetime of the cis-form of the azobenzene units. The halogen-bonded LCs were characterized by means of X-ray diffraction, hot-stage polarized optical microscopy, and differential scanning calorimetry. Simultaneous analysis of light-induced changes in birefringence, absorption, and optical scattering allowed us to estimate that <4% of the mesogenic units in the cis-form suffices to trigger the full LC-to-isotropic phase transition. We also report a light-induced and reversible crystal-to-isotropic phase transition, which has not been previously observed in supramolecular complexes. In addition to fundamental understanding of light-responsive supramolecular complexes, we foresee this study to be important in the development of bistable photonic devices and supramolecular actuators.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Fernandez-Palacio, F., Poutanen, M., Saccone, M., Siiskonen, A., Terraneo, G., Resnati, G., Ikkala, O., Metrangolo, P., Priimägi, A.
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Scopus rating (2016): 4.114 1.905
Publication Forum (2016): 3
Scopus rating (2015): 4.038 2.102
Web of Science (2015): 9.407 9.363 7.5 1.737 0.12692 2.376
Scopus rating (2014): 3.603 2.253
Web of Science (2014): 8.354 9.21 7.3 2.078 0.12128 2.2
Publication Forum (2014): 3
Scopus rating (2013): 3.658 2.277
Publication Forum (2013): 3
Scopus rating (2012): 4.169 2.264
Publication Forum (2012): 3
High Water-Splitting Efficiency through Intentional In and Sn Codoping in Hematite Photoanodes

The effects of intermittent thin ITO layers on the water-splitting efficiency of α-Fe2O3 films grown by PECVD on FTO substrates are reported. The α-Fe2O3 was codoped with indium and tin by temperature-driven ionic transport and diffusion from the ultrathin ITO layer sputtered between the α-Fe2O3 layer and FTO substrate. The α-Fe2O3/ITO/FTO photoanodes showed a remarkable interdependence between the thickness of the ITO layer and PEC efficiency. Hematite photoanodes with a 32 nm thick ITO underlayer showed the highest photocurrent density of 2.5 mA cm−2, corresponding to an approximate 3-fold enhancement over pristine α-Fe2O3 at 1.23 V vs RHE, whereas the thinner (8 nm) ITO underlayer yielded the lowest onset potential at 0.6 V vs RHE. Although the electrode with a thicker 72 nm ITO underlayer showed a higher onset potential of 0.9 V vs RHE, it still showed an enhancement in the photocurrent density at higher bias voltages. α-Fe2O3 was also deposited on metallic titanium substrates with intermittent sputtered tin and ITO layers. The codoping with indium and tin from ITO was observed to yield greatly enhanced performance when compared with both α-Fe2O3 alone and tin-doped α-Fe2O3. Transient absorption decays in the sub-nanosecond time scale were not affected by the doping, indicating that the doping had little effect on the primary charge carrier generation and recombination. On the other hand, fewer trapped electrons on the microsecond to millisecond time scale and a greatly increased amount of long-lived surface photoholes were observed for the ITO-doped samples. The transient absorption results imply that the large increases in photoelectrochemical efficiency were obtained due to higher electron mobility, which reduces recombination and leads to more efficient electron extraction from the electrodes.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Kaouk, A., Ruoko, T., Pyeon, M., Gönüllü, Y., Kaunisto, K., Lemmetyinen, H., Mathur, S.
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Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Periodic Surface Structures Induced by a Single Laser Beam Irradiation

Methods for inscribing periodic surface patterns by light, especially those characterized by the ability to control the pattern dimensions, are continuously sought for. In this paper, a periodic pattern, which is called the willow structure, is written to a supramolecular polymer-azobenzene complex using a single coherent laser beam of linear polarization. The willow structure can be an alternative to the commonly used surface relief grating written with an interference pattern once it is known how to manipulate its period. It is shown that the periodicity of the structure obtained with the one-beam approach can be controlled by changing the thickness of the polymer layer and the inscription temperature, in addition to the wavelength of the inscribing light. This information is useful for the utilization of the single-beam method as a way for obtaining periodic structures with desired dimensions.

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Authors: Noga, J., Sobolewska, A., Bartkiewicz, S., Virkki, M., Priimägi, A.
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Scopus rating (2016): 0.894 0.971
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Scopus rating (2015): 0.852 1.097
Web of Science (2015): 2.834 2.779 6.5 0.692 0.00571 0.616
Publication Forum (2015): 1
Scopus rating (2014): 1.005 1.309
Web of Science (2014): 2.661 2.779 6.8 0.551 0.00578 0.638
Publication Forum (2014): 1
Scopus rating (2013): 0.952 1.244
Publication Forum (2013): 1
Scopus rating (2012): 0.949 1.145
Publication Forum (2012): 1
Scopus rating (2011): 0.962 1.055
Scopus rating (2010): 0.923 0.917
Magnesium aminoclay enhances lipid production of mixotrophic Chlorella sp. KR-1 while reducing bacterial populations

Improving lipid productivity and preventing overgrowth of contaminating bacteria are critical issues relevant to the commercialization of the mixotrophic microalgae cultivation process. In this paper, we report the use of magnesium aminoclay (MgAC) nanoparticles for enhanced lipid production from oleaginous Chlorella sp. KR-1 with simultaneous control of KR-1-associated bacterial growth in mixotrophic cultures with glucose as the model substrate. Addition of 0.01–0.1 g/L MgAC promoted microalgal biomass production better than the MgAC-less control, via differential biocidal effects on microalgal and bacterial cells (the latter being more sensitive to MgAC’s bio-toxicity than the former). The inhibition effect of MgAC on co-existing bacteria was, as based on density-gradient-gel-electrophoresis (DGGE) analysis, largely dosage-dependent and species-specific. MgAC also, by inducing an oxidative stress environment, increased both the cell size and lipid content of KR-1, resulting in a considerable, ~25% improvement of mixotrophic algal lipid productivity (to ~410 mg FAME/L/d) compared with the untreated control.

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Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Chungnam National University, Korea Institute of Energy Research, Gachon University
Authors: Kim, B., Praveenkumar, R., Lee, J., Nam, B., Kim, D. M., Lee, K., Lee, Y. C., Oh, Y. K.
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Publication Forum (2015): 2
Scopus rating (2014): 2.41 2.104
Web of Science (2014): 4.494 5.33 4.6 0.822 0.12645 1.042
Publication Forum (2014): 2
Scopus rating (2013): 2.412 2.503
Publication Forum (2013): 2
Mild pressure induces rapid accumulation of neutral lipid (triacylglycerol) in Chlorella spp.

Effective enhancement of neutral lipid (especially triacylglycerol, TAG) content in microalgae is an important issue for commercialization of microalgal biorefineries. Pressure is a key physical factor affecting the morphological, physiological, and biochemical behaviors of organisms. In this paper, we report a new stress-based method for induction of TAG accumulation in microalgae (specifically, Chlorella sp. KR-1 and Ch. sp. AG20150) by very-short-duration application of mild pressure. Pressure treatments of 10–15 bar for 2 h resulted in a considerable, ∼55% improvement of the 10–100 g/L cells' TAG contents compared with the untreated control. The post-pressure-treatment increase of cytoplasmic TAG granules was further confirmed by transmission electron microscopy (TEM). Notwithstanding the increased TAG content, the total lipid content was not changed by pressurization, implying that pressure stress possibly induces rapid remodeling/transformation of algal lipids rather than de novo biosynthesis of TAG.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Chungnam National University, Korea Institute of Energy Research
Keywords: (Induction, Microalgae, Neutral lipid, Pressure stress, Triacylglycerol)
Number of pages: 5
Pages: 661-665
Publication date: 1 Nov 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

Publication information
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ISSN (Print): 0960-8524
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.191 1.91
Publication Forum (2016): 2
Scopus rating (2015): 2.255 1.908
Web of Science (2015): 4.917 5.744 5.0 1.012 0.13375 1.089
Publication Forum (2015): 2
Scopus rating (2014): 2.41 2.104
Web of Science (2014): 4.494 5.33 4.6 0.822 0.12645 1.042
Two-step bioleaching of copper and gold from discarded printed circuit boards (PCB)

An effective strategy for environmentally sound biological recovery of copper and gold from discarded printed circuit boards (PCB) in a two-step bioleaching process was experimented. In the first step, chemolithotrophic acidophilic Acidithiobacillus ferrivorans and Acidithiobacillus thiooxidans were used. In the second step, cyanide-producing heterotrophic Pseudomonas fluorescens and Pseudomonas putida were used. Results showed that at a 1% pulp density (10. g/L PCB concentration), 98.4% of the copper was bioleached by a mixture of A. ferrivorans and A. thiooxidans at pH 1.0-1.6 and ambient temperature (23. ±. 2. °C) in 7. days. A pure culture of P. putida (strain WCS361) produced 21.5 (±1.5). mg/L cyanide with 10. g/L glycine as the substrate. This gold complexing agent was used in the subsequent bioleaching step using the Cu-leached (by A. ferrivorans and A. thiooxidans) PCB material, 44.0% of the gold was mobilized in alkaline conditions at pH 7.3-8.6, and 30. °C in 2. days. This study provided a proof-of-concept of a two-step approach in metal bioleaching from PCB, by bacterially produced lixiviants.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: İşildar, A., van de Vossenberg, J., Rene, E. R., van Hullebusch, E. D., Lens, P. N. L.
Keywords: (Bioleaching, Copper, Gold, PCB, Secondary resource, Two-step, WEEE)
Pages: 149–157
Publication date: Nov 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Waste Management and Disposal

Publication information

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ISSN (Print): 0956-053X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.354 2.044
Publication Forum (2016): 1
Scopus rating (2015): 1.739 2.256
Web of Science (2015): 3.829 4.297 6.1 0.7 0.01909 0.871
Recombinant antibodies for specific detection of clostridial [Fe-Fe] hydrogenases

Biological hydrogen production is based on activity of specific enzymes called hydrogenases. Hydrogenases are oxygen sensitive metalloenzymes containing Ni and/or Fe atoms at the active site, catalyzing reversible reduction of protons. Generally, [Fe-Fe] hydrogenases prefer proton reduction to molecular hydrogen, a potential energy carrier molecule that can be produced by bioprocesses in sustainable manner. Thus, monitoring tools have been developed to study the relationship between [Fe-Fe] hydrogenases and biohydrogen production in bioreactors at DNA and RNA levels. In the present study, novel molecular tools are introduced for quantitative monitoring of clostridial [Fe-Fe] hydrogenases at the protein level. Aerobic and anaerobic biopanning (for inactive and active [Fe-Fe] hydrogenase, respectively) of phage displayed single-chain variable fragment (scFv) antibody libraries aided in isolating nine potential scFvs. The enriched antibodies demonstrated high specificity towards Clostridium spp. [Fe-Fe] hydrogenases allowing detection from pure and mixed cultures. Additionally, the antibodies showed different binding characteristics towards hydrogenase catalytic states, providing a possible means for functional detection of clostridial [Fe-Fe] hydrogenases. From hydrogenase-antibody interaction studies we observed that though antibody binding reduced the enzyme catalytic activity, it facilitated to retain hydrogen evolution from oxygen exposed hydrogenases.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Univ Turku, University of Turku, Dept Biotechnol
Authors: Mangayil, R., Karp, M., Lamminmäki, U., Santala, V.
Number of pages: 9
Publication date: 27 Oct 2016
Peer-reviewed: Yes

Publication information
Journal: Scientific Reports
Volume: 6
Article number: 36034
ISSN (Print): 2045-2322
Ratings:
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.

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State: E-pub ahead of print
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, University of Helsinki, Division of Biopharmaceutical Sciences, Biomedicum Imaging Unit, FIN-00014 University of Helsinki
Number of pages: 14
Pages: 1-14
Publication date: 13 Oct 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Biotechnology, Molecular Medicine, Pharmacology, Pharmaceutical Science, Organic Chemistry, Pharmacology (medical)

Publication information
Journal: Pharmaceutical Research
ISSN (Print): 0724-8741
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.105 1.042
Publication Forum (2016): 2
Scopus rating (2015): 1.154 1.188
Web of Science (2015): 3.26 3.99 9.7 0.745 0.01854 0.93
Publication Forum (2015): 2
Scopus rating (2014): 1.332 1.306
Web of Science (2014): 3.42 4.29 9.5 0.551 0.02113 1.037
Publication Forum (2014): 3
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
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: Kramb, J., Konttinen, J., Backman, R., Salo, K., Roberts, M.
Keywords: (Arsenic, CCA wood, Equilibrium modeling, Gasification)
Number of pages: 6
Pages: 319-324
Publication date: 1 Oct 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

Publication information
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Ratings:
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Scopus rating (2016): 1.744 2.179
Publication Forum (2016): 2
Scopus rating (2015): 1.809 2.125
Web of Science (2015): 3.611 4.14 6.0 1.014 0.05542 0.929
Publication Forum (2015): 2
Scopus rating (2014): 1.667 2.331
Web of Science (2014): 3.52 4.091 6.4 0.815 0.04512 0.922
Publication Forum (2014): 3
Impacts of sulfur source and temperature on sulfur-driven denitrification by pure and mixed cultures of Thiobacillus

This study investigated the impacts of thiosulfate (S\textsubscript{2}O\textsubscript{3}\textsuperscript{2−}) as well as chemically synthesized and biogenic elemental sulfur (S\textsubscript{0}) on the rates of sulfur-based denitrification in batch bioassays. The use of S\textsubscript{2}O\textsubscript{3}\textsuperscript{2−} resulted in the highest denitrification rate (52.5 mg N-NO\textsubscript{3}−/L d), whereas up to 10 times slower nitrate (NO\textsubscript{3}−) removal was observed with S\textsubscript{0}. Biogenic S\textsubscript{0} was tested for the first time as electron donor for chemolithotrophic denitrification, resulting in 1.7-fold faster NO\textsubscript{3}− removal than that achieved with chemically synthesized S\textsubscript{0}. The effects of increasing concentrations of S\textsubscript{2}O\textsubscript{3}\textsuperscript{2−} and chemically synthesized S\textsubscript{0} on denitrification were evaluated testing three different sulfur-to-nitrogen (S/N) molar ratios (1.8, 3.5 and 5.1) on a pure culture of Thiobacillus denitrificans and a mixotrophic enrichment dominated by Thiobacillus thioparus. S\textsubscript{2}O\textsubscript{3}\textsuperscript{2−} concentrations exceeding 2.2 g/L inhibited the activity of T. denitrificans, whereas a stimulatory effect was observed on mixotrophic denitrification. The increase in S\textsubscript{0} concentration slightly enhanced denitrification by both microbial cultures due to the low solubility of chemically synthesized S\textsubscript{0}. The temperature dependence of the thiosulfate-driven denitrification by T. denitrificans was investigated to further optimize the process and modeled by the Arrhenius equation with an apparent activation energy Ea of 76.6 kJ/mol and a temperature coefficient Q\textsubscript{10} of 3.0.

**General information**

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, University of Cassino and Southern Lazio
Authors: Di Capua, F., Ahoranta, S. H., Papirio, S., Lens, P. N., Esposito, G.
Pages: 1576-1584
Publication date: 1 Oct 2016
Peer-reviewed: Yes

**Publication information**

Journal: Process Biochemistry
Volume: 51
Issue number: 10
ISSN (Print): 1359-5113
Ratings:

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<td>2.529 3.067 9.3 0.322 0.01515 0.651</td>
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Fossil Feedstock-free Preparation of Hydroquinone

General information
State: Published
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry
Authors: Rafael Candeias, N., Assoah, B.
Publication date: 23 Sep 2016
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Research output: Scientific › Paper, poster or abstract

Utilization of Food Waste via Anaerobic Digestion: From Feedstock to Biogas and Fertilizers

Food waste is a renewable resource that can be utilized as both energy and nutrients through anaerobic digestion to increase nutrient recycling and fertilizer self-sufficiency and promote the mitigation of greenhouse gas emissions. Anaerobic digestion of food wastes has, however, faced challenges due to the waste’s characteristics, e.g., high protein content, which is why the organic loading rates with food waste digestion are usually kept low to achieve a stable process. The digestate produced during digestion contains all of the nutrients from the food waste feedstock and can be used as a fertilizer in agriculture, where the availability of nutrients, the stability of organic matter, and biosecurity define its agronomic value. In this thesis, the aim was to analyze the potential of using anaerobic digestion for food waste utilization. The anaerobic digestion of food waste, feedstock pretreatment, and processing and utilization of the digestate for fertilizer use were studied.

This study shows the potential of food waste as feedstock for anaerobic digestion without dilution, with a total solids content of 20–25%. A high organic loading rate of 6 kgVS/m3d (VS, volatile solids) was achieved with methane yields 400–430 m3/kgVS in continuous food waste digestion while the optimum loading rate was 3 kgVS/m3d, yielding around 480 m3/kgVS of methane. Trace element supplementation enabled a stable long-term operation and gradual increase of loading rates without the accumulation of acids. The autoclave pretreatment (160°C and 6.2 bars) of the food waste affected the characteristics – and subsequently, the anaerobic digestion performance, where the formation of protein-based hardly biodegradable compounds led to a 10% lower methane yield during digestion, decreased hydrogen sulfide content in the biogas, and 50% decreased ammonium nitrogen concentration within the digestate. The decreased
availability of proteins and hydrogen sulfide formation due to the pretreatment reduce the risk of ammonia inhibition during anaerobic digestion and enable easier biogas cleaning and security.

The food waste digestates shows potential as a nutrient source in crop fertilization independently and after post-treatment. The studied digestates were considered suitable for fertilizer use, as they showed good agronomic value in terms of nutrient content and usability, as well as biosecurity. Food waste digestates produced around 5 to 30% higher ryegrass yield compared with a mineral fertilizer in pot experiments, and the majority (50–70%) of the nitrogen and phosphorus were in the soluble and plant-available forms. The integration of anaerobic digestion and digestate post-treatment technologies enabled the processing of the digestate liquid into concentrated nutrient products rich in nitrogen and potassium. With the combination of different processing technologies such as evaporation, stripping, and reverse osmosis, nutrient products with optimal composition can be produced to correspond with the fertilizer demand. Overall, due to the high energy potential of the food waste, the integration of the anaerobic digestion with heat-demanding digestate liquid post-treatment processes (e.g., stripping and/or evaporation) was possible.

In conclusion, anaerobic digestion has high potential for the utilization of food waste, as food waste produces high methane yields in optimized conditions. The food waste digestate was also shown to be a suitable nutrient (especially nitrogen) source in crop fertilization independently and after post-treatment.

**Photoinduced hole transfer in QD–phthalocyanine hybrids**

A series of CdSe quantum dot (QD)–phthalocyanine (Pc) hybrids were synthesized and their photophysics was studied using steady state and time-resolved spectroscopic methods. Emission of QDs was progressively quenched upon increasing the concentration of Pc in the hybrids. A detailed transient absorption study of the hybrids revealed that the mechanism of quenching is charge separation, resulting in the formation of hybrids with negatively charged QDs and the Pc cation. Direct photo-excitation of Pc did not show any detectable interaction between the excited state of Pc and the QD to which it is attached. An explanation is proposed, based on the suggestion that the energy of the lowest unoccupied molecular orbital (LUMO) of Pc is lower than the lower edge of the QD conduction band, while the energy of the highest occupied molecular orbital (HOMO) of Pc is sufficiently higher than the high energy edge of the QD valence band (VB), thus permitting hole transfer from the QD VB to the Pc HOMO after photo-excitation of QDs.

**General information**

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Electronics and Communications Engineering, Research group: Laboratory for Future Electronics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications
Authors: Arvani, M., Virkki, K., Abou-Chahine, F., Efimov, A., Schramm, A., Tkachenko, N. V., Lupo, D.
Pages: 27414-27421
Publication date: 5 Sep 2016
Peer-reviewed: Yes

Publication Information
Long-term stability of bioelectricity generation coupled with tetrathionate disproportionation

To prevent uncontrolled acidification of the environment, reduced inorganic sulfur compounds (RISCs) can be bioelectrochemically removed from water streams. The long-term stability of bioelectricity production from tetrathionate (S\textsubscript{4}O\textsubscript{6}\textsuperscript{2-}) was studied in highly acidic conditions (pH <2.5) in two-chamber fed-batch microbial fuel cells (MFCs). The maximum current density was improved from previously reported 80 mA m\textsuperscript{-2} to 225 mA m\textsuperscript{-2} by optimizing the external resistance. The observed reaction products of tetrathionate disproportionation were sulfate and elemental sulfur. In long-term run, stable electricity production was obtained for over 700 days with the average current density of 150 mA m\textsuperscript{-2}. The internal resistance of the MFC decreased over time and no biofouling was observed. This study shows that tetrathionate is an efficient substrate also for long-term bioelectricity production.

General information

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Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry
Authors: Sulonen, M. L. K., Lakaniemi, A. M., Kokko, M. E., Puhakka, J. A.
Keywords: (Acidophile, Disproportionation, Long-term stability, Microbial fuel cell, Tetrathionate)
Number of pages: 7
Pages: 876-882
Publication date: 1 Sep 2016
Peer-reviewed: Yes
Selenium: environmental significance, pollution, and biological treatment technologies

Selenium is an essential trace element needed for all living organisms. Despite its essentiality, selenium is a potential toxic element to natural ecosystems due to its bioaccumulation potential. Though selenium is found naturally in the earth's crust, especially in carbonate rocks and volcanic and sedimentary soils, about 40% of the selenium emissions to atmospheric and aquatic environments are caused by various industrial activities such as mining-related operations. In recent years, advances in water quality and pollution monitoring have shown that selenium is a contaminant of potential environmental concern. This has practical implications on industry to achieve the stringent selenium regulatory discharge limit of 5 μg Se L⁻¹ for selenium containing wastewaters set by the United States Environmental Protection Agency. Over the last few decades, various technologies have been developed for the treatment of selenium-containing wastewaters. Biological selenium reduction has emerged as the leading technology for removing selenium from wastewaters since it offers a cheaper alternative compared to physico-chemical treatments and is suitable for treating dilute and variable selenium-laden wastewaters. Moreover, biological treatment has the advantage of forming elemental selenium nanospheres which exhibit unique optical and spectral properties for various industrial applications, i.e. medical, electrical, and manufacturing processes. However, despite the advances in biotechnology employing selenium reduction, there are still several challenges, particularly in achieving stringent discharge limits, the long-term stability of biogenic selenium and predicting the fate of bioreduced selenium in the environment. This review highlights the significance of selenium in the environment, health, and industry and biotechnological advances made in the treatment of selenium contaminated wastewaters. The challenges and future perspectives are overviewed considering recent biotechnological advances in the management of these selenium-laden wastewaters.
Cadmium (Cd) is a carcinogenic metal contaminating the environment and ending up in wastewaters. There is therefore a need for improved methods to remove Cd by adsorption. Biogenic elemental selenium nanoparticles have been shown to adsorb Zn, Cu and Hg, but these nanoparticles have not been tested for Cd removal. Here we studied the time-dependency and adsorption isotherm of Cd onto biogenic elemental selenium nanoparticles using batch adsorption experiments. We measured ζ-potential values to assess the stability of nanoparticles loaded with Cd. Results show that the maximum Cd adsorption capacity amounts to 176.8 mg of Cd adsorbed per g of biogenic elemental selenium nanoparticles. The ζ-potential of Cd-loaded nanoparticles became less negative from −32.7 to −11.7 mV when exposing nanoparticles to an initial Cd concentration of 92.7 mg L−1. This is the first study that demonstrates the high Cd uptake capacity of biogenic elemental selenium nanoparticles, of 176.8 mg g−1, when compared to that of traditional adsorbents such as carboxyl-functionalized activated carbon, of 13.5 mg g−1. An additional benefit is the easy solid–liquid separation by gravity settling due to coagulation of Cd-loaded biogenic elemental selenium nanoparticles.
Methodological approaches for fractionation and speciation to estimate trace element bioavailability in engineered anaerobic digestion ecosystems: An overview

Optimal supply of trace elements (TE) is a prerequisite for microbial growth and activity in anaerobic digestion (AD) bioprocesses. However, the required concentrations and ratios of essential TE for AD biotechnologies strongly depend on prevailing operating conditions as well as feedstock composition. Furthermore, TE in AD bioreactors undergo complex physicochemical reactions and may be present as free ions, complex bound or as precipitates depending on pH, or on the presence of sulfur compounds or organic macromolecules. To overcome TE deficiency, various commercial mineral products are typically applied to AD processes. The addition of heavy metals poses the risk of overdosing operating systems, which may be toxic to microbial consortia and ultimately the environment. Adequate supplementation, therefore, requires appropriate knowledge not only about the composition, but also on the speciation and bioavailability of TE. However, very little is yet fully understood on this specific issue. Evaluations of TE typically only include the measurement of total TE concentrations but do not consider the chemical forms in which TE exist. Thus detailed information on bioavailability and potential toxicity cannot be provided. This review provides an overview of the state of the art in approaches to determine bioavailable TE in anaerobic bioprocesses, including sequential fractionation and speciation techniques. Critical aspects and considerations, including with respect to sampling and analytical procedures, as well as mathematical modeling, are examined. The approaches discussed in this review are based on our experiences and on previously published studies in the context of the “COST Action 1302: European Network on Ecological Roles of Trace Metals in Anaerobic Biotechnologies.”
Structural photoactivation of a full-length bacterial phytochrome

Phytochromes are light sensor proteins found in plants, bacteria, and fungi. They function by converting a photon absorption event into a conformational signal that propagates from the chromophore through the entire protein. However, the structure of the photoactivated state and the conformational changes that lead to it are not known. We report time-resolved x-ray scattering of the full-length phytochrome from Deinococcus radiodurans on micro- and millisecond time scales. We identify a twist of the histidine kinase output domains with respect to the chromophore-binding domains as the dominant change between the photoactivated and resting states. The time-resolved data further show that the structural changes up to the microsecond time scales are small and localized in the chromophore-binding domains. The global structural change occurs within a few milliseconds, coinciding with the formation of the spectroscopic meta-Rc state. Our findings establish key elements of the signaling mechanism of full-length bacterial phytochromes.

General information
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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, University of Jyväskylä
Number of pages: 9
Publication date: 12 Aug 2016
Peer-reviewed: Yes

Publication information
Journal: Science Advances
Volume: 2
Issue number: 8
Article number: e160092
ISSN (Print): 2375-2548
Ratings:
Publication Forum (2017): 1
The red, purple and blue modifications of polymeric unsymmetrical hydroxyalkadiynyl-N-arylcarbamate derivatives in Langmuir-Schaefer films

Solid topochemical photopolymerization (STP) of Langmuir-Schaefer films of a new class of unsymmetrical diynes, containing N-arylcarbamate groups in the hydrophobic part and hydroxymethylene groups in the hydrophilic part of the molecules was examined. In addition, the monomeric Langmuir monolayer formation was studied by Brewster angle microscopy and the surface morphology of monomer and polymer films on solid substrates were studied by scanning electron microscopy and atomic force microscopy. Three phases of polydiacetylene (PDA) (red, purple and blue) were observed after UV-light polymerization of above-mentioned films of alcohol diacetylene (DA) derivatives. The substitution of MeO group in the aryl ring substituent by hydrogen atom and the variation of the methylene group number in the hydrophobic part from 5 to 6 changed significantly the result of STP: instead of blue phase PDA observed for diynes with MeO group, the red phase PDA was observed for DA with H-atom from the very beginning of diyne film UV irradiation. For two other diynilic N-arylcarnamates of identical chemical structures except of the substituents in the aryl ring of hydrophobic parts of the molecules, no changes in the efficiency of polymerization or the position and shape of absorption bands were observed. This indicated the formation of the purple phase PDA. For these molecules, the number of methylene groups in hydrophobic and hydrophilic parts of the molecules was 9 and 2, respectively.

General information
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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, Åbo Akademi University, St. Petersburg State University, NRC Kurchatov Institute, Russian Acad Sci, Russian Academy of Sciences, Kotel'nikov Inst Radio Engn & Elect
Keywords: (Langmuir monolayer, Langmuir-Schaefer film, Polydiacetylenes with urethane group, Solid topochemical photopolymerization)
Number of pages: 9
Pages: 463-471
Publication date: 1 Aug 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Materials Chemistry, Metals and Alloys, Surfaces, Coatings and Films, Surfaces and Interfaces

Publication information
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Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.64 0.897
Publication Forum (2016): 1
Scopus rating (2015): 0.705 0.98
Web of Science (2015): 1.761 1.79 0.356 0.04617 0.426
Publication Forum (2015): 1
Scopus rating (2014): 0.73 1.115
Web of Science (2014): 1.759 1.922 8.5 0.383 0.05315 0.456
Publication Forum (2014): 2
Scopus rating (2013): 0.818 1.215
Publication Forum (2013): 2
Scopus rating (2012): 0.899 1.162
Publication Forum (2012): 2
Characterization and Potential Use of Source-Separated Urine

Human urine is an abundant source of the main nutrients (N, P, and K), while in the modern age it may contain traces of pharmaceutical and hormonal compounds. In many parts of the world, urine is collected into sewers, mixed with other wastewaters and treated at centralized wastewater treatment plants. Recently, the source separation of urine has been considered as a way to promote nutrient recovery from households as concentrated streams which could promote its use as fertilizer. The presence of pharmaceuticals and estrogens in urine has raised questions regarding its safe agricultural use, thus leading to a need to monitor the presence of pharmaceutically active compounds in urine. As a minimum, six-month storage before agricultural use is recommended for urine for hygienic reasons. The objective of this thesis was to develop and facilitate the use of source-separated urine by making the characterization of urine easier and faster, to gain more understanding regarding pharmaceutical and estrogenic behavior during urine storage, and to evaluate the suitability of human urine in microalgal cultivations as a nutrient source.

An analytical liquid chromatographic method, which had the advantage of simultaneous analysis of eight pharmaceuticals in a short six-minute analysis time, was developed as no such method previously existed (Paper I). The method was validated, proven repeatable, and the obtained pharmaceutical recoveries were acceptable (81.6–109.2%). The limit of detection for the pharmaceuticals in urine was 39–1,610 µg/L. In addition, a previously developed bioluminescent yeast cell biosensor Saccharomyces cerevisiae (BMAEREluc/ERα) was applied on urine samples, as prior to this thesis no information was available on the use of yeast biosensor in estrogenic activity assessment from source-separated human urine (Paper II). The biosensor produced repeatable results in the estrogenic activity testing of fresh and stored human urine with the limit of detection corresponding to 0.28–35 µg/L of estrogens. To enhance the signal, incubation with β-glucuronidase enzyme was used. The biosensor gave a cumulative signal for estrogenic activity (estrogens and estrogen-like compounds), thus enabling the assessment of overall estrogenic activity during urine storage.

The method presented in Paper I was subsequently used in monitoring spiked pharmaceutical concentrations in urine during six-month storage (Paper III). Each pharmaceutical (three antivirals and four antibiotic compounds) was tested in laboratory storage both individually and in therapeutic groups, as well as in therapeutic groups either with feces or urease inhibitor amendment. During storage, the overall concentration reductions of <1% to >99% were detected, and in assays with amendments, concentrations reductions remained <50%, except for rifampicin (>99%). Four of the pharmaceuticals had reduced concentrations after a six-month storage, suggesting biological or chemical degradation and/or precipitation of the compounds.

Human urine was tested as nutrient source for biomass production from microalga Chlorella vulgaris (Paper IV). Biomass yield in diluted urine was comparable with growth in artificial growth medium and urine could be utilized up to 1:25-dilutions without inhibition to algal growth. The highest biomass production (0.6 g/L) was achieved in 1:100-diluted urine. C. vulgaris used 32.5–78.7% of N and 35.1–99.0% of P available in urine. At the beginning of cultivation, the majority of the biomass consisted of algal cells, while towards the end the share of living algal cells decreased, indicating accumulation of bacteria and algal cell debris.

In conclusion, the results obtained in this thesis indicated that the pharmaceutical concentrations did not reduce enough in order to safely use urine. The yeast biosensor demonstrated that during storage, the estrogenic activity changes most
likely due to bacterial enzyme activity, but some activity is still present after five months. The urine is a viable nutrient source for microalgal biomass production, thus having potential for sustainable use and recycling of nutrients.

**General information**

State: Published

Ministry of Education publication type: G5 Doctoral dissertation (article)

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry

Authors: Jaatinen, S.

Number of pages: 95

Publication date: 1 Jul 2016

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Jaatinen 1391

Links:


Research output: Collection of articles › Doctoral Thesis

**Structural characterization, spectroscopic, thermal, AC conductivity and dielectric properties and antimicrobial studies of (C₈H₁₂N)₂[SnCl₆]**

A new inorganic-organic hybrid material produced from 2,6-dimethylanilinium cations and tin halide (SnCl₆)²⁻ has been synthesized and structurally determined by X-ray diffraction method. The title compound crystallizes in the monoclinic system, space group C2/m with a = 19.8772(4), b = 6.9879(1), c = 8.3001(2) Å, β = 98.487(2)° and V = 1140.26(4) Å³. The crystal structure is built up of sheets of (SnCl₆)²⁻ octahedral anions and 2,6-xylidinium cations. The optical band gap was calculated and found to be 4.11 eV. At high temperature this compound exhibits a structural phase transition at 338 K. This has been characterized by differential scanning calorimetric and dielectric studies. Measurements of AC conductivity as a function of frequency at different temperatures indicated the hopping conduction mechanism. The bioassay results showed that the structure exhibits significant antibacterial activity.

**General information**

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Organisations: Department of Chemistry and Bioengineering, Carthage University

Authors: Mathlouthi, M., Valkonen, A., Rzaigui, M., Smirani, W.

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Publication Forum (2015): 1

Scopus rating (2014): 0.375 0.799

Web of Science (2014): 0.954 0.953 8.4 0.091 0.00208 0.266
Liquid fertilizer products from anaerobic digestion of food waste: Mass, nutrient and energy balance of four digestate liquid treatment systems

This study compared four different digestate liquid treatment systems of a theoretical anaerobic digestion plant in order to facilitate the utilization of municipal food waste nutrients in agriculture. The mass, nutrient and energy balances of a theoretical plant digesting 60 kt/y of food waste were used to evaluate the feasibility of the treatments to concentrate nutrients into liquid fertilizer products. The studied technologies for digestate liquid treatment were ammonia stripping, ammonia stripping combined with reverse osmosis (RO), evaporation combined with RO, and stripping combined with both evaporation and RO. As a result, processing of digestate into concentrated fertilizer products consumed less than 10% of the produced energy from food wastes and was also sufficient for the heat-demanding digestate liquid treatments, evaporation and stripping. The digestate liquid treatment systems were considered as nitrogen and potassium concentration methods which were able to concentrate up to 67% of the feedstock nitrogen into transportable fertilizer products with low mass. Of the studied digestate systems evaporation combined with RO was evaluated as the most efficient nutrient recovery technology for the production of transportable fertilizer products due to the high concentration of nutrients and nutrient availability as well as low product mass and energy consumption. Overall, the selection of the treatment technology is dependent on the location of the anaerobic digestion plant relative to the agricultural land and the type of fertilizer products needed.

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Authors: Tampio, E., Marttinen, S., Rintala, J.
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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-alkyphenylazo)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.

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Authors: Poutanen, M., Ikkala, O., Priimägi, A.
Number of pages: 7
Pages: 4095-4101
Publication date: 14 Jun 2016
Peer-reviewed: Yes
Indocyanine Green-Loaded Liposomes for Light-Triggered Drug Release

Light-triggered drug delivery systems enable site-specific and time-controlled drug release. In previous work, we have achieved this with liposomes containing gold nanoparticles in the aqueous core. Gold nanoparticles absorb near-infrared light and release the energy as heat that increases the permeability of the liposomal bilayer, thus releasing the contents of the liposome. In this work, we replaced the gold nanoparticles with the clinically approved imaging agent indocyanine green (ICG). The ICG liposomes were stable at storage conditions (4-22 °C) and at body temperature, and fast near-infrared (IR) light-triggered drug release was achieved with optimized phospholipid composition and a 1:50 ICG-to-lipid molar ratio. Encapsulated small molecular calcein and FITC-dextran (up to 20 kDa) were completely released from the liposomes after light exposure for 15 s. Location of ICG in the PEG layer of the liposomes was simulated with molecular dynamics. ICG has important benefits as a light-triggering agent in liposomes: fast content release, improved stability, improved possibility of liposomal size control, regulatory approval to use in humans, and the possibility of imaging the in vivo location of the liposomes based on the fluorescence of ICG. Near-infrared light used as a triggering mechanism has good tissue penetration and safety. Thus, ICG liposomes are an attractive option for light-controlled and efficient delivery of small and large drug molecules.

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Organisations: Department of Physics, Department of Chemistry and Bioengineering
Authors: Lajunen, T., Kontturi, L., Viitala, L., Manna, M., Cramariuc, O., Rög, T., Bunker, A., Laaksonen, T., Viitala, T., Murtomäki, L., Urtti, A.
Photoactive ZnO-Organic Nanostructures: Development and Characterization

Photoinduced processes in hybrid semiconductor-organic nanostructures were studied in this thesis. The work was divided into three tasks: (1) preparation of ZnO thin films and nanorod arrays in a controlled and cost-effective way, (2) functionalization of the ZnO surfaces with organic, photoactive layers and (3) study of photoinduced reactions on the surfaces by both steady state and time-resolved methods. Aluminum doped zinc oxide (AZO) electrodes were tested as an alternative for the traditionally used indium tin oxide semitransparent electrodes in organic solar cell devices. The electrodes were prepared by atomic layer deposition method. Devices with AZO electrodes showed performance comparable to that of the reference device but were more stable in open air showing no degradation during 40 days time interval. ZnO nanorod arrays were prepared and used as model substrates to study electronic interactions at semiconductor-organic interface. The growth was optimized to achieve well-aligned nanorods with high specific surface area. To control the semiconductor electronic properties, while keeping the morphology unchanged, the nanorods were further modified with thin layers of Al2O3 or TiO2 prepared by atomic layer deposition. Self-assembly monolayers (SAM) of three different porphyrin derivatives and one phthalocyanine derivative were formed on the ZnO nanorods using carboxylic acid or siloxane as anchor groups. The fastest electron transfer from zinc porphyrin (ZnP) to the semiconductor was observed for the ZnO nanorods modified with a 5 nm layer of TiO2 (<0.2 ps). On the contrary, the charge recombination was not any faster compared to that of ZnP on the unmodified nanorods. This indicates that the charge recombination depends mainly on the semiconductor bulk properties, whereas the charge separation is determined by the surface properties of the semiconductor. The charge generation mechanisms in the hybrid systems consisting of zinc phthalocyanine (ZnPc) SAM on ZnO nanorods covered by a spin coated layer of hole transporting materials, P3HT or Spiro-OMeTAD, were studied with time-resolved absorption spectroscopy. After selective excitation of ZnPc the primary electron transfer step was controlled by the hole transporting material. In the system with P3HT the first reaction step is a...
fast (1.8 ps) electron transfer to ZnO, whereas in the Spiro-OMeTAD system a fast (0.5 ps) hole transfer from the excited ZnPc to Spiro-OMeTAD is the dominant primary electron transfer step. However, in both cases long-lived (> 5 ns) charge-separated states are formed. In these states electrons are localized in ZnO and the holes in the organic donor layer, while ZnPc is in the ground state.

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Authors: Hakola, H.
Keywords: (Digital hydraulics, Power management, Energy efficiency)
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Publisher: Tampere University of Technology
Original language: English

Electronic structure of p-type perylene monoimide-based donor–acceptor dyes on the nickel oxide (100) surface: a DFT approach
A p-type dye-sensitized solar cell, where the dye injects a hole to the semiconductor, could be combined with typical Grätzel cell to create an efficient tandem device. However, the current p-type devices suffer from low efficiency. Here, geometries and electronic structures of four perylenemonoimide-based dyes (1–4) both as free and adsorbed on the NiO (100) semiconductor surface have been investigated to gain better understanding of the p-type devices. In particular, the electronic transitions relevant to charge transfer between the dye and the surface have been identified. Excitations have been evaluated by using the time dependent DFT calculations and the roles of frontier orbitals and band edges in transitions have been assessed. The adsorbed dyes can take either upright or slightly tilted geometries depending on the structure of the anchoring group and the binding mode of the dye. The adsorption slightly lowers the NiO band gap, from 4.06 eV to 3.90–3.96 eV depending on the surface–adsorbate system, and the band gaps of the dye molecules by 0.1–0.2 eV. Additionally, the adsorption mode of dye 1 moves the LUMO+1 level down by 0.5 eV. The effective mass of the charge carrier holes is significantly smaller at the NiO surface than in the bulk indicating the importance of the surface conductivity. We also found that the potential drop, i.e. the driving force for charge transfer from NiO to dye molecule depends on the adsorption mode of 1.

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Authors: Kontkanen, O., Niskanen, M., Hukka, T., Rantala, T.
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Photoexcitation and electron transfer at inorganic–organic interface — a DFT approach

General information
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Authors: Niskanen, M. O., Kontkanen, O. V., Hukka, T. I., Rantala, T. T.
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Research output: Scientific › Paper, poster or abstract

Synthesis and biological screening for cytotoxic activity of N-substituted indolines and morpholines
Development of novel anticancer drugs is inevitable to improve treatment of cancers. In this study, novel derivatives of indoline and morpholine were synthesized and tested for their cytotoxic effects on osteosarcoma and Human Embryonic Kidney cells. To characterize cytotoxicity and the mechanism of cell death, were used cytotoxicity, migration, apoptosis markers and mitochondrial calcium assays. Among the compounds tested, the indoline derivatives, generally, produced a higher cytotoxic effect compared to the morpholine derivatives, in osteosarcoma cells. Specifically, new indoline derivative N-(2-hydroxy-5-nitrophenyl(4′-methylphenyl)methyl)indoline exhibited effective cytotoxic activity, with an IC50 of ~74 μM. The same molecule induced cell death by apoptosis and inhibited migration of the cells. Further, analysis of mitochondrial calcium levels revealed the existence of calcium dependent cell death mechanisms in different cell types. Therefore, N-(2-hydroxy-5-nitrophenyl(4′-methylphenyl)methyl)indoline can be considered as a potential drug-lead compound towards the discovery of new anti-cancer agents.

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Organisations: Department of Signal Processing, Research group: Laboratory of Biosystem Dynamics-LBD, Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Molecular Signaling Lab
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.
Syntheses, Charge Separation, and Inverted Bulk Heterojunction Solar Cell Application of Phenothiazine-Fullerene Dyads

A series of phenothiazine-fulleropyrrolidine (PTZ-C$_{60}$) dyads having fullerene either at the C-3 aromatic ring position or at the N-position of phenothiazine macrocycle were newly synthesized and characterized. Photoinduced electron transfer leading to PTZ$^{+*}$-C$_{60}$$^{-*}$ charge-separated species was established from studies involving femtosecond transient absorption spectroscopy. Because of the close proximity of the donor and acceptor entities, the C-3 ring substituted PTZ-C$_{60}$ dyads revealed faster charge separation and charge recombination processes than that observed in the dyad functionalized through the N-position. Next, inverted organic bulk heterojunction (BHJ) solar cells were constructed using the dyads in place of traditionally used [6,6]-phenyl-C$_{61}$-butyric acid methyl ester (PCBM) and an additional electron donor material poly(3-hexylthiophene) (P3HT). The performance of the C-3 ring substituted PTZ-C$_{60}$ dyad having a polyethylene glycol substituent produced a power conversion efficiency of 3.5% under inverted bulk heterojunction (BHJ) configuration. This was attributed to optimal BHJ morphology between the polymer and the dyad, which was further promoted by the efficient intramolecular charge separation and relatively slow charge recombination promoted by the dyad within the BHJ structure. The present finding demonstrate PTZ-C$_{60}$ dyads as being good prospective materials for building organic photovoltaic devices.
Effect of temperature and concentration of precursors on morphology and photocatalytic activity of zinc oxide thin films prepared by hydrothermal route

Zinc oxide (ZnO) is an important semiconductive material due to its potential applications, such as conductive gas sensors, transparent conductive electrodes, solar cells, and photocatalysts. Photocatalytic activity can be exploited in the decomposition of hazardous pollutants from environment. In this study, we produced zinc oxide thin films on stainless steel plates by hydrothermal method varying the precursor concentration (from 0.029 M to 0.16 M) and the synthesis temperature (from 70 °C to 90 °C). Morphology of the synthesized films was examined using field-emission scanning electron microscopy (FESEM) and photocatalytic activity of the films was characterized using methylene blue decomposition tests. It was found that the morphology of the nanostructures was strongly affected by the precursor concentration and the temperature of the synthesis. At lower concentrations zinc oxide grew as thin needlelike nanorods of uniform length and shape and aligned perpendicular to the stainless steel substrate surface. At higher concentrations the shape of the rods transformed towards hexagon shaped units and further on towards flaky platelets. Temperature changes caused variations in the coating thickness and the orientation of the crystal units. It was also observed, that the photocatalytic activity of the prepared films was clearly dependent on the morphology of the surfaces.
Coordination networks incorporating halogen-bond donor sites and azobenzene groups

Two Zn coordination networks, [{Zn(1)(Py)2}(2-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⋯O contacts, thus increasing the stability of the solvated systems.
Arsenic removal from acidic solutions with biogenic ferric precipitates

Treatment of acidic solution containing 5 g/L of Fe(II) and 10 mg/L of As(III) was studied in a system consisting of a biological fluidized-bed reactor (FBR) for iron oxidation, and a gravity settler for iron precipitation and separation of the ferric precipitates. At pH 3.0 and FBR retention time of 5.7 h, 96–98% of the added Fe(II) precipitated (99.1% of which was jarosite). The highest iron oxidation and precipitation rates were 1070 and 28 mg/L/h, respectively, and were achieved at pH 3.0. Subsequently, the effect of pH on arsenic removal through sorption and/or co-precipitation was examined by gradually decreasing solution pH from 3.0 to 1.6 (feed pH). At pH 3.0, 2.4 and 1.6, the highest arsenic removal efficiencies obtained were 99.5%, 80.1% and 7.1%, respectively. As the system had ferric precipitates in excess, decreased arsenic removal was likely due to reduced co-precipitation at pH < 2.4. As(III) was partially oxidized to As(V) in the system. In shake flask experiments, As(V) sorbed onto jarosite better than As(III). Moreover, the sorption capacity of biogenic jarosite was significantly higher than that of synthetic jarosite. The developed bioprocess simultaneously and efficiently removes iron and arsenic from acidic solutions, indicating potential for mining wastewater treatment.
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 (Φₜ) 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 μs) 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.

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Quenching nematicon fluctuations via photo-stabilization

Light localization into optical spatial solitons can be achieved by launching optical beams in nonlocal nonlinear nematic liquid crystals. Such solitons often undergo undesired fluctuations of their trajectories. We demonstrate that partial polymerization in monoacrylate-doped nematic liquid crystals is effective in quenching such fluctuations in transverse space.

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Authors: Karimi, N., Alberucci, A., Virkki, M., Priimägi, A., Kauranen, M., Assanto, G.
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Publication Forum (2016): 0
Scopus rating (2015): 0.288 0.499
Agronomic characteristics of five different urban waste digestates

The use of digestate in agriculture is an efficient way to recycle materials and to decrease the use of mineral fertilizers. The agronomic characteristics of the digestates can promote plant growth and soil properties after digestate fertilization but also harmful effects can arise due to digestate quality, e.g. pH, organic matter and heavy metal content. The objective of this study was to evaluate the differences and similarities in agronomic characteristics and the value of five urban waste digestates from different biogas plants treating either food waste, organic fraction of organic solid waste or a mixture of waste-activated sludge and vegetable waste. The digestate agronomic characteristics were studied with chemical analyses and the availability of nutrients was also assessed with growth experiments and soil mineralization tests. All studied urban digestates produced 5-30% higher ryegrass yields compared to a control mineral fertilizer with a similar inorganic nitrogen concentration, while the feedstock source affected the agronomic value. Food waste and organic fraction of municipal solid waste digestates were characterized by high agronomic value due to the availability of nutrients and low heavy metal load. Waste-activated sludge as part of the feedstock mixture, however, increased the heavy metal content and reduced nitrogen availability to the plant, thus reducing the fertilizer value of the digestate.
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 cd m\(^{-2}\) and the power efficiency of 1.5 lm W\(^{-1}\) while that of PY-PH exhibited 2116 cd m\(^{-2}\) and 0.45 lm W\(^{-1}\) respectively.
Intrinsic Properties of Two Benzodithiophene-Based Donor–Acceptor Copolymers Used in Organic Solar Cells: A Quantum-Chemical Approach

Conjugated donor–acceptor (D–A) copolymers show tremendous promise as active components in thin-film organic bulk heterojunction solar cells and transistors, as appropriate combinations of D–A units enable regulation of the intrinsic electronic and optical properties of the polymer. Here, the structural, electronic, and optical properties of two D–A copolymers that make use of thieno[3,4-c]pyrrole-4,6-dione as the acceptor and differ by their donor unit—benzo[1,2-b:4,5-b′]dithiophene (BDT) vs the ladder-type heptacyclic benzodi(cyclopentadithiophene)—are compared using density functional theory methods. Our calculations predict some general similarities, although the differences in the donor structures lead also to clear differences. The extended conjugation of the stiff ladder-type donor destabilizes both the highest occupied and lowest unoccupied molecular orbital energies of the ladder copolymer and results in smaller gap energies compared to its smaller counterpart. However, more significant charge transfer nature is predicted for the smaller BDT-based copolymer by natural transition orbitals than for the ladder copolymer. That is, the influence of the acceptor on the copolymer properties is "diluted" to some extent by the already extended conjugation of the ladder-type donor. Thus, the use of stronger acceptor units with the ladder-type donors would benefit the future design of new D–A copolymers.
Cell-based bioreporter assay coupled to HPLC micro-fractionation in the evaluation of antimicrobial properties of the basidiomycete fungus Pycnoporus cinnabarinus

Context: Identification of bioactive components from complex natural product extracts can be a tedious process that aggravates the use of natural products in drug discovery campaigns. Objective: This study presents a new approach for screening antimicrobial potential of natural product extracts by employing a bioreporter assay amenable to HPLC-based activity profiling. Materials and methods: A library of 116 crude extracts was prepared from fungal culture filtrates by liquid–liquid extraction with ethyl acetate, lyophilised, and screened against Escherichia coli using TLC bioautography. Active extracts were studied further with a broth microdilution assay, which was, however, too insensitive for identifying the active microfractions after HPLC separation. Therefore, an assay based on bioluminescent E. coli K-12 (pTetLux1) strain was coupled with HPLC micro-fractionation. Results: Preliminary screening yielded six fungal extracts with potential antimicrobial activity. A crude extract from a culture filtrate of the wood-rotting fungus, Pycnoporus cinnabarinus (Jacq.) P. Karst. (Polyporaceae), was selected for evaluating the functionality of the bioreporter assay in HPLC-based activity profiling. In the bioreporter assay, the IC50 value for the crude extract was 0.10 mg/mL. By integrating the bioreporter assay with HPLC micro-fractionation, the antimicrobial activity was linked to LC-UV peak of a compound in the chromatogram of the extract. This compound was isolated and identified as a fungal pigment phlebiarubrone. Discussion and conclusion: HPLC-based activity profiling using the bioreporter-based approach is a valuable tool for identifying antimicrobial compound(s) from complex crude extracts, and offers improved sensitivity and speed compared with traditional antimicrobial assays, such as the turbidimetric measurement.
Advanced Solid Fuel Characterization for Reactivity and Physical Property Comparison

The main objective of this thesis was to formulate a method with which solid fuel combustion characteristics and physical properties could be accurately compared between different samples. The main study instrument used and further developed in the fuel reactivity tests during this work was a laminar drop-tube reactor (DTR). Five different solid fuel sample types were tested with the DTR. The samples were selected to represent a wide range of possible solid fuel types relevant to energy production in Finland. Fossil coal was selected as a reference fuel. Peat was chosen as it is commonly co-fired with biomass in Finland. The three other samples, raw, torrefied, and steam-exploded woody biomasses, were chosen to find out how thermochemical pretreatment of biomass feedstock affects the fuel combustion characteristics.

In addition to the DTR tests, the fine grinding energy requirement of the biomass samples was also examined. Moreover, collaboration work with other researchers was conducted to examine the effect of torrefaction on the fine grinding energy requirement, chlorine content, and heating value. Various domestic and foreign wood species were used in these studies. The torrefaction process was noted to reduce the energy required to fine grind the tested sample. It was also noted that during torrefaction the chlorine content of the solid matter was reduced and the specific heating value was slightly increased. Fine grinding the steam-exploded biomass produced more spherical particles compared to the raw and torrefied pellet samples.

The combustion behavior of the five main samples was tested in the DTR. The samples were preground and the particles sieved with vibration sieves with an opening of 100-125 μm. The pyrolysis process was examined separately at a temperature range of 973-1173 K in pure N2. The combined pyrolysis and combustion tests were conducted at a reactor temperature of 1123 K. The O2 concentrations used in the combustion measurements were 3–21 vol-% in either N2 or CO2 atmospheres. The surface temperature of the combusting sample particles was measured with a two-color pyrometer. The initial size distribution of the sample particles as well as their size and geometry evolution as a function of conversion was studied by using optical techniques. The density, specific surface area, and mean pore diameter were measured from the samples with a mercury porosimeter. The reactivity parameters, which describe the pyrolysis and char oxidation rates of the samples, were determined by using the data from the measurements. Using discretized size distribution in the model calculations explained better the measured particle surface temperatures than using a monosized single particle model. Moreover, combining the optical techniques with the DTR setup provided valuable data on the geometry evolution of the particles.

Based on the reactivity parameters, the sample combustion characteristics could be compared with one another. The reactivity comparison method presented in this thesis relies on consistent DTR measurements, determining accurately the size distribution and porosity of the sample particles, and using multiobjective optimization in fitting the model parameters.
Synthesis of Benzothiadiazole Derivatives by Applying C–C Cross-Couplings

The benzothiadiazole moiety has been extensively exploited as a building block in the syntheses of efficient organic semiconducting materials during the past decade. In this paper, parallel synthetic routes to benzothiadiazole derivatives, inspired by previous computational findings, are reported. The results presented here show that various C–C cross-couplings of benzothiadiazole, thiophene, and thiazole derivatives can be efficiently performed by applying Xantphos as a ligand of the catalyst system. Moreover, improved and convenient methods to synthesize important chemical building blocks, e.g., 4,7-dibromo-2,1,3-benzothiadiazole, in good to quantitative yields are presented. Additionally, the feasibility of Suzuki–Miyaura and direct coupling methods are compared in the synthesis of target benzothiadiazole derivatives. The computational characterization of the prepared benzothiadiazole derivatives shows that these compounds have planar molecular backbones and the possibility of intramolecular charge transfer upon excitation. The experimental electrochemical and spectroscopic studies reveal that although the compounds have similar electronic and optical properties in solution, they behave differently in solid state due to the different alkyl side-group substitutions in the molecular backbone. These benzothiadiazole derivatives can be potentially used as building blocks in the construction of more advanced small molecule organic semiconductors with acceptor–donor–acceptor motifs.

General information
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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
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Publication date: 15 Jan 2016
Peer-reviewed: Yes

Publication information
Journal: Journal of Organic Chemistry
Volume: 81
Issue number: 4
ISSN (Print): 0022-3263
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.976 1.03
Publication Forum (2016): 2
Scopus rating (2015): 2.018 1.174
Plasma-Assisted Fabrication of Fe2O3 - Co3O4 Nanomaterials as Anodes for Photoelectrochemical Water Splitting

Nanocomposite Fe2O3?Co3O4 photoanodes for photoelectrochemical H2O splitting were prepared by a plasma-assisted route. Specifically, Fe2O3 nanostructures were grown by plasma enhanced-chemical vapor deposition, followed by cobalt sputtering for different process durations. The systems were annealed in air after, or both prior and after, sputtering of Co, to analyze the treatment influence on functional performances. The interplay between processing conditions and chemico-physical features was investigated by a multi-technique characterization. Photocurrent density measurements in sunlight-assisted H2O splitting revealed a performance improvement upon Co3O4 loading. A cathodic shift of the onset potential was also observed, highlighting Co3O4 activity as catalyst for the oxygen evolution reaction.
Charge separation and charge recombination photophysical studies in a series of perylene–C₆₀ linear and cyclic dyads

A new donor–acceptor doubly bridged perylenediimide–fullerene dyad (PDI–C₆₀, DB-3), where the perylenediimide (PDI) acts as a donor, has been synthesized and studied by time-resolved absorption spectroscopy. The DB-3 undergoes an electron transfer (ET) in both polar and non-polar media under photo-excitation. Structurally the DB-3 dyad resembles four other recently studied dyads (R. K. Dubey et al., Chem. Eur. J., 2013, 19, 6791–6806). Analysis of the ET reactions in this series of dyads was suggests that the electronic coupling for the ET reaction is roughly 0.005 eV, internal reorganization carried out in frame of both classic and semi-quantum ET theories. The result of the analysis for DB-3 energy is 0.16 eV, and outer sphere or solvent reorganization energy is 0.5 and 0.3 eV in benzonitrile and toluene, respectively.
Color Bricks: Building Highly Organized and Strongly Absorbing Multicomponent Arrays of Terpyridyl Perylenes on Metal Oxide Surfaces

Terpyridine-substituted perylenes containing cyclic anhydrides in the peri position were synthesized. The anhydride group served as an anchor for assembly of the terpyridyl-crowned chromophores as monomolecular layers on metal oxide surfaces. Further coordination with Zn2+ ions allowed for layer-by-layer formation of supramolecular assemblies of perylene imides on the solid substrates. With properly selected anchor and linker molecules it was possible to build high quality structures of greater than ten successive layers by a simple and straightforward procedure. The prepared films were stable and had a broad spectral coverage and high absorbance. To demonstrate their potential use, the synthesized dyes were employed in solid-state dye-sensitized solar cells, and electron injection from the perylene antennas to titanium dioxide was observed.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Optoelectronics Research Centre, Research group: Surface Science, Optoelectronics Research Centre, Tampere University of Technology
Pages: 1501-1510
Publication date: Jan 2016
Peer-reviewed: Yes
Early online date: 3 Dec 2015

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Journal: Chemistry: A European Journal
Volume: 22
Issue number: 4
ISSN (Print): 0947-6539
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.247 1.046
Publication Forum (2016): 2
Scopus rating (2015): 2.416 1.184
Web of Science (2015): 5.771 5.572 4.6 1.338 0.19837 1.407
Publication Forum (2015): 2
Scopus rating (2014): 2.487 1.219
Web of Science (2014): 5.731 5.635 4.4 1.255 0.19743 1.433
Toward the prediction of porous membrane permeability from morphological data

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Universitat Rovira i Virgili
Authors: Nurra, C., Pitol, L., Carraud, R., Pertuz, S., Puig, D., Garcia, M. A., Salvado, J., Torras, C.
Pages: 118–124
Publication date: Jan 2016
Peer-reviewed: Yes

Publication information
Journal: Polymer Engineering and Science
Volume: 56
Issue number: 1
ISSN (Print): 0032-3888
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.579 0.835
Publication Forum (2016): 1
Scopus rating (2015): 0.563 0.913
Web of Science (2015): 1.719 1.61 >10.0 0.291 0.00731 0.328
Publication Forum (2015): 1
Scopus rating (2014): 0.555 1.092
Web of Science (2014): 1.52 1.608 >10.0 0.305 0.00795 0.346
Publication Forum (2014): 1
Scopus rating (2013): 0.569 1.037
Publication Forum (2013): 1
Scopus rating (2012): 0.691 1.298
Publication Forum (2012): 1
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
State: Published
Ministry of Education 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
Authors: 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
ASJC Scopus subject areas: Biomedical Engineering, Medicine(all), Chemistry(all), Materials Science(all)

Publication information
Journal: Journal of Materials Chemistry B
Volume: 4
Issue number: 19
ISSN (Print): 2050-7518
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.46 1.014
Publication Forum (2016): 2
Scopus rating (2015): 1.566 1.163
Web of Science (2015): 4.872 4.879 1.9 0.985 0.02307 0.971
Publication Forum (2015): 2
Scopus rating (2014): 1.331 1.007
Web of Science (2014): 4.726 4.729 1.4 0.98 0.00974 0.871
Publication Forum (2014): 3
Publication Forum (2013): 3
Original language: English
DOIs: 10.1039/c6tb00580b
Anaerobes in bioelectrochemical systems

In bioelectrochemical systems (BES), the catalytic activity of anaerobic microorganisms generates electrons at the anode which can be used, for example, for the production of electricity or chemical compounds. BES can be used for various purposes, including wastewater treatment, production of electricity, fuels and chemicals, biosensors, bioremediation, and desalination. Electrochemically active microorganisms are widely present in the environment and they can be found, in sediment, soil, compost, wastewaters and their treatment plants. Exoelectrogens are microorganisms capable of donating electrons to anode electrode or accepting electrons from cathode electrode and are mainly responsible for current generation or use in BES. However, current generation from fermentable substrates often requires the presence of electrochemically inactive microorganisms that break down complex substrates into metabolites which can be further utilized by exoelectrogens. The growth and electron transfer efficiency of anaerobes depend on several parameters, such as system architecture, electrode material and porosity, electrode potential and external resistance, pH, temperature, substrate concentration, organic loading rate, and ionic strength. In this chapter, the principles and microbiology of bioelectrochemical systems as well as selective factors for exoelectrogens are reviewed. The anaerobic microorganisms and their electron transfer mechanisms at the anode and cathode are described and future aspects are briefly discussed.

Are Sphagnum-species potential antagonistics for pathogens?

General information
State: Published
Ministry of Education publication type: D3 Professional conference proceedings
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry
Authors: Kuovi, A., Karp, M., Franzén, R., Sarjala, T., Muilu-Mäkelä, R., Aro, T., Tienaho, J., Silvan, N.
Publication date: 2016

Host publication information
Title of host publication: XIV Meeting of the IOBC-WPRS Working Group Biological Control of Fungal and Bacterial Plant Pathogens Biocontrol and Microbial Ecology
Article number: 067
Links: http://www.iobc-wprserlin2016.de/ (Conference website)
Research output: Professional › Conference contribution
A study on raw, torrefied, and steam-exploded wood: Fine grinding, drop-tube reactor combustion tests in N₂/O₂ and CO₂/O₂ atmospheres, particle geometry analysis, and numerical kinetics modeling

The purpose of this study was to compare the fine grinding properties and combustion behavior of three wood pellet products: raw, torrefied, and steam-exploded wood. The energy required to fine grind the pellets was tested, and so was the geometry and size distribution of the resulting ground products. Out of all the samples the steam-exploded wood pellet required the most energy for grinding. However, it also produced more sphere-like particles compared to the other two types of samples. The combustion behavior of the samples was tested in a laminar drop-tube reactor (DTR). The samples were preground and the particles were sieved with vibration sieves with an opening of 112–125 μm. The pyrolysis process was examined separately at a temperature range of 973–1173 K. The combined pyrolysis and combustion tests were carried out at a reactor temperature of 1123 K. The O₂ concentrations used in the measurements were 3–21 vol-% in either N₂ or CO₂ atmospheres. The initial size distribution of the sample particles as well as their diameter evolution during pyrolysis and combustion was studied by using optical techniques. The surface temperature of the combusting particles was measured with a two-color pyrometer from within the DTR. The density, specific surface area, and pore diameter were measured from the ground samples with a mercury porosimeter. The chemical kinetic parameters, which describe the pyrolysis and char oxidation rates of the samples, were determined by using the data from the measurements.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology
Authors: Tolvanen, H., Keipi, T., Raiko, R.
Keywords: (Combustion, Biomass, Chemical kinetics, Carbon dioxide, Drop-tube reactor)
Pages: 153-164
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Fuel
Volume: 176
ISSN (Print): 0016-2361
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.744 2.179
Publication Forum (2016): 2
Scopus rating (2015): 1.809 2.125
Web of Science (2015): 3.611 4.14 6.0 1.014 0.05542 0.929
Publication Forum (2015): 2
Scopus rating (2014): 1.667 2.331
Web of Science (2014): 3.52 4.091 6.4 0.815 0.04512 0.922
Publication Forum (2014): 3
Scopus rating (2013): 1.811 2.595
Publication Forum (2013): 3
Scopus rating (2012): 1.852 2.465
Publication Forum (2012): 3
Scopus rating (2011): 2.093 2.427
Scopus rating (2010): 1.984 2.319
Scopus rating (2009): 2.012 2.277
Scopus rating (2008): 1.635 2.184
Scopus rating (2007): 1.383 1.86
Scopus rating (2006): 1.278 1.64
Scopus rating (2005): 1.623 1.73
Scopus rating (2004): 1.273 1.883
Scopus rating (2003): 1.103 1.481
Scopus rating (2002): 1.13 1.301
Scopus rating (2001): 1.136 1.264
Scopus rating (2000): 1.047 1.272
Scopus rating (1999): 1.117 1.157
Original language: English
DOIs:
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
State: Published
Ministry of Education 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
Authors: 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
ASJC Scopus subject areas: Chemistry(all)

Publication information
Journal: Chemistry: A European Journal
Volume: 22
Issue number: 5
ISSN (Print): 0947-6539
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.247 1.046
Publication Forum (2016): 2
Scopus rating (2015): 2.416 1.184
Web of Science (2015): 5.771 5.572 4.6 1.338 0.19837 1.407
Publication Forum (2015): 2
Scopus rating (2014): 2.487 1.219
Web of Science (2014): 5.731 5.635 4.4 1.255 0.19743 1.433
Publication Forum (2014): 3
Scopus rating (2013): 2.604 1.239
Publication Forum (2013): 3
Scopus rating (2012): 2.884 1.294
Publication Forum (2012): 3
Scopus rating (2011): 2.726 1.336
Scopus rating (2010): 2.527 1.292
Scopus rating (2009): 2.499 1.365
Scopus rating (2007): 3.233 1.532
Scopus rating (2006): 2.911 1.505
Scopus rating (2005): 2.62 1.454
Scopus rating (2004): 2.32 1.472
Scopus rating (2003): 2.156 1.45
Scopus rating (2001): 2.834 1.612
Scopus rating (2000): 2.956 1.652
Scopus rating (1999): 3.013 1.73
Original language: English
DOIs:
10.1002/chem.201503943
Biological and Bioelectrochemical Recovery of Critical and Scarce Metals

Metal-bearing solid and liquid wastes are increasingly considered as secondary sources of critical and scarce metals. Undoubtedly, microorganisms are a cost-effective resource for extracting and concentrating diffuse elements from secondary sources. Microbial biotechnology for extracting base metals from ores and treatment of metal-laden wastewaters has already been applied at full scale. By contrast, microbe-metal interactions in the recovery of scarce metals and a few critical metals have received attention, whereas the recovery of many others has been barely explored. Therefore, this article explores and details the potential application of microbial biotechnologies in the recovery of critical and scarce metals. In the past decade bioelectrochemical systems have emerged as a new technology platform for metal recovery coupled to the removal of organic matter. Overview of potential applications of microorganisms in critical metal recovery. Engineering of microbe-metal interactions for recovering rare earth elements and platinum group metals. Reductive mineral dissolution is a new dimension to biomining. Bioelectrochemical systems offer a new technology platform in metal recovery.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Biofouling and Biofilm Processes Section, Bhabha Atomic Research Centre, Council of Scientific and Industrial Research India, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education
Authors: Nancharaiah, Y. V., Mohan, S. V., Lens, P. N. L.
Keywords: (Bioelectrochemical systems, Biomining, Bioprecipitation, Biorecovery, Critical metals, Microbial fuel cells, Platinum group metals, Rare earth elements)
Number of pages: 19
Pages: 137-155
Publication date: 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Biotechnology, Bioengineering

Publication information
Journal: Trends in Biotechnology
Volume: 34
Issue number: 2
ISSN (Print): 0167-7799
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 4.037 3.143
Publication Forum (2016): 2
Web of Science (2015): 12.065 12.052 7.7 2.288 0.01926 3.513
Publication Forum (2015): 2
Scopus rating (2014): 4.344 3.35
Web of Science (2014): 11.958 11.681 7.4 1.8 0.02109 3.56
Publication Forum (2014): 2
Scopus rating (2013): 3.763 3.151
Publication Forum (2013): 2
Publication Forum (2012): 2
Scopus rating (2011): 3.321 3.05
Scopus rating (2010): 3.062 2.734
Scopus rating (2009): 2.751 2.682
Scopus rating (2008): 2.509 2.185
Scopus rating (2007): 2.361 2.393
Scopus rating (2006): 2.149 2.196
Scopus rating (2005): 1.911 2.109
Scopus rating (2004): 1.797 1.762
Scopus rating (2003): 1.552 2.063
Biomass-Based and Oxidant-Free Preparation of Hydroquinone from Quinic Acid

A biomass-based route to the preparation of hydroquinone starting from the renewable starting material quinic acid is described. Amberlyst-15 in the dry form promoted the one-step formation of hydroquinone from quinic acid in toluene without any oxidants or metal catalysts in 72% yield. Several acidic polymer-based resins and organic acids as promoters as well as a variety of reaction conditions were screened including temperature, concentration and low- and high-boiling-point solvents. A 1:4 (w/w) ratio of quinic acid/Amberlyst-15 was determined to be optimal to promote hydroquinone formation with only traces of a dimeric side-product. A mechanism has been proposed based on the decarbonylation of protonated quino-1,5-lactone that is supported by experimental and computational calculation data.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Supramolecular photochemistry
Authors: Assoah, B., Veiros, L. F., Afonso, C. A. M., R. Candeias, N.
Number of pages: 6
Pages: 3856-3861
Publication date: 2016
Peer-reviewed: Yes

Publication information
Volume: 2016
Issue number: 22
ISSN (Print): 1434-193X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.133 0.653
Publication Forum (2016): 1
Scopus rating (2015): 1.198 0.758
Web of Science (2015): 3.068 2.971 5.5 0.777 0.04165 0.677
Publication Forum (2015): 1
Scopus rating (2014): 1.181 0.767
Web of Science (2014): 3.065 3.034 5.3 0.744 0.04326 0.703
Publication Forum (2014): 3
Scopus rating (2013): 1.292 0.796
Publication Forum (2013): 3
Scopus rating (2012): 1.471 0.811
Publication Forum (2012): 3
Scopus rating (2011): 1.536 0.857
Scopus rating (2010): 1.572 0.785
Scopus rating (2009): 1.497 0.778
Scopus rating (2008): 1.652 0.759
Scopus rating (2007): 1.711 0.84
Scopus rating (2006): 1.505 0.849
Scopus rating (2005): 1.246 0.763
Scopus rating (2004): 1.2 0.81
Scopus rating (2003): 1.19 0.802
Chemical and bacterial leaching of metals from a smelter slag in acid solutions

The purpose of this study was to assess the dissolution of Si, Fe, Cu and Zn from a smelter slag sample under acidic chemical and bacterial leaching conditions. The Cu-containing solid phases were Cu-sulfides (57% distribution), fayalite (18%) and metallic Cu (16%). Zn was mostly associated with fayalite, magnetite and Na-silicate phases (Σ94%). Two mixed cultures (HB1 and HB2) were enriched from samples taken from the slag lagoon site at the smelter location. Comparable results of metal dissolution were obtained with the two mixed cultures. The enrichment culture HB1 was characterized further by denaturing gradient gel electrophoresis (DGGE) of polymerase chain reaction amplified 16S rRNA genes. Based on the 16S rRNA gene sequences, culture HB1 contained at least Acidithiobacillus ferrivorans and Alicyclobacillus cycloheptanicus, with sequences of three DGGE bands matching distantly with Alicyclobacillus tolerans and Alicyclobacillus herbarium in the database. Alicyclobacillus spp. have not been previously associated with slag lagoons or slag bioleaching. Approximately 80% Cu and 25% Zn were dissolved from the slag (10% pulp) in shake flasks when $S_0$ was provided for the bacteria to produce $H_2SO_4$. Bioleaching in stirred tanks was conducted at controlled pH values and was practiced at pH levels promoting metal dissolution and suppressing iron and silicate solubilization from fayalite and Na-silicate. Chemical leaching at pH 2.3-4.0 did not yield substantial dissolution of valuable metals.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, CSIRO Land and Water Flagship, Boliden Harjavalta Oy, Department of Microbiology, Ohio State University
Authors: Kaksonen, A. H., Särkijärvi, S., Puhakka, J. A., Peuraniemi, E., Junnikkala, S., Tuovinen, O. H.
Keywords: (Acidithiobacillus, Alicyclobacillus, Bacterial leaching, Bioleaching, Chemical leaching, Smelter slag)
Pages: 46-53
Publication date: 2016
Peer-reviewed: Yes
Early online date: 1 Jan 2015
ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Materials Chemistry, Metals and Alloys

Publication information
Journal: Hydrometallurgy
Volume: 159
ISSN (Print): 0304-386X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.148 1.737
Publication Forum (2016): 1
Scopus rating (2015): 1.173 1.888
Web of Science (2015): 2.29 2.947 8.1 0.00907 0.672
Publication Forum (2015): 1
Scopus rating (2014): 1.247 2.25
Web of Science (2014): 1.933 2.566 8.2 0.295 0.00887 0.595
Publication Forum (2014): 2
Scopus rating (2013): 1.626 2.967
Publication Forum (2013): 2
Scopus rating (2012): 1.523 2.4
Publication Forum (2012): 2
Scopus rating (2011): 1.521 1.796
Scopus rating (2010): 1.104 1.672
Compact hematite buffer layer as a promoter of nanorod photoanode performances

The effect of a thin α-Fe2O3 compact buffer layer (BL) on the photoelectrochemical performances of a bare α-Fe2O3 nanorods photoanode is investigated. The BL is prepared through a simple spray deposition onto a fluorine-doped tin oxide (FTO) conducting glass substrate before the growth of a α-Fe2O3 nanorods via a hydrothermal process. Insertion of the hematite BL between the FTO and the nanorods markedly enhances the generated photocurrent, by limiting undesired losses of photogenerated charges at the FTO||electrolyte interface. The proposed approach warrants a marked improvement of material performances, with no additional thermal treatment and no use/dispersion of rare or toxic species, in agreement with the principles of green chemistry.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Milan, R., Cattarin, S., Comisso, N., Baratto, C., Kaunisto, K., Tkachenko, N. V., Concina, I.
Number of pages: 10
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Scientific Reports
Volume: 6
Article number: 35049
ISSN (Print): 2045-2322
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.625 1.401
Publication Forum (2016): 2
Scopus rating (2015): 2.057 1.684
Web of Science (2015): 5.228 5.525 2.1 0.559 0.20942 1.865
Publication Forum (2015): 2
Scopus rating (2014): 2.103 1.544
Web of Science (2014): 5.578 5.597 1.7 0.722 0.11476 2.075
Publication Forum (2014): 1
Scopus rating (2013): 1.886 1.51
Publication Forum (2013): 1
Scopus rating (2012): 1.458 0.896
Publication Forum (2012): 1
Original language: English
Electronic versions:
srep35049
DOIs:
Controllable Electronic Structures and Photoinduced Processes of Bay-Linked Perylenediimide 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 \((\text{PDI})_2\) is much larger than those of para- and meta-phenylene-bridged PDI dimers \(p-(\text{PDI})_2\) and \(m-(\text{PDI})_2\). 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 \(p-(\text{PDI})_2\) 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.
Downstream integration of microalga harvesting and cell disruption by means of cationic surfactant-decorated Fe$_3$O$_4$ nanoparticles

Microalgal biofuel, albeit an exciting potential fossil-fuel-replacement candidate, still requires the development of more advanced downstream processing technology for its price competitiveness. The major challenge in a microalgae-based biorefinery is the efficient separation of microalgae from low-concentration culture broth. The post-harvesting cell-disruption step necessary to render microalgae suitable for lipid extraction, moreover, further raises energy consumption and cost. For the mitigation of biorefinery complexity and costs, we suggest herein a new scheme that integrates the critical downstream processes (harvesting and cell disruption) by means of cationic surfactant-decorated Fe$_3$O$_4$ nanoparticles. The cationic surfactants’ quaternary ammonium heads play an important role in not only flocculating negatively charged microalgae but also weakening thick cell walls. In the present study, the harvesting efficiency and cell-damaging effects of three cationic surfactants - cetrimonium bromide (CTAB), cetylpyridinium chloride (CPC), and cetylpyridinium bromide (CPB) - were evaluated. The CTAB-decorated Fe$_3$O$_4$ nanoparticles, which were found to be the most effective, achieved a 96.6% microalgae harvesting efficiency at a dosage of 0.46 g particle per g cell. Next, for the purposes of magnetic nanoparticle recycling and high-purity microalgal biomass obtainment, microalgae detachment from microalgae-Fe$_3$O$_4$ flocs was performed by addition of an anionic surfactant, sodium dodecyl sulfate (SDS). The detached CTAB-decorated Fe$_3$O$_4$ nanoparticles showed a steady reuse efficiency of about 80%. Furthermore, microalgae harvesting by CTAB-decorated Fe$_3$O$_4$ nanoparticles could contribute to a great improvement in the total extracted lipid content and greener wet extraction without the additional energy-intensive cell-disruption step, thus demonstrating the cell-disruption ability of CTAB-decorated Fe$_3$O$_4$ nanoparticles.
Effect of source-separated urine storage on estrogenic activity detected using bioluminescent yeast *Saccharomyces cerevisiae*

The objective was to demonstrate that a microbial whole cell biosensor, bioluminescent yeast, *Saccharomyces cerevisiae* (BMAERE1uc/ER alpha) can be applied to detect overall estrogenic activity from fresh and stored human urine. The use of source-separated urine in agriculture removes a human originated estrogen source from wastewater influents, subsequently enabling nutrient recycling. Estrogenic activity in urine should be diminished prior to urine usage in agriculture in order to prevent its migration to soil. A storage period of 6 months is required for hygienic reasons; therefore, estrogenic activity monitoring is of interest. The method measured cumulative female hormone-like activity. Calibration curves were prepared for estrone, 17 beta-estradiol, 17 alpha- ethinylestradiol and estriol. Estrogen concentrations of 0.29-29,640 μg L⁻¹ were detectable while limit of detection corresponded to 0.28-35 μg L⁻¹ of estrogens. The yeast sensor responded well to fresh and stored urine and gave high signals corresponding to 0.38-3,804 μg L⁻¹ of estrogens in different urine samples. Estrogenic activity decreased during storage, but was still higher than in fresh urine implying insufficient storage length. The biosensor was suitable for monitoring hormonal activity in urine and can be used in screening anthropogenic estrogen-like compounds interacting with the receptor.
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 $Q_e$ of EHC was 14.3 mg orthophosphate adsorbed per g of EHC when the initial orthophosphate concentration was increased to 150 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 g L$^{-1}$ and an initial orthophosphate concentration of 13.1 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

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Ministry of Education publication type: A1 Journal article-refereed
Authors: 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
ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)

Publication information

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Scopus rating (2016): 0.875 0.743
Publication Forum (2016): 1
Scopus rating (2015): 0.959 0.837
Web of Science (2015): 3.289 3.485 1.8 0.676 0.13014 0.628
Publication Forum (2015): 1
Formation and stability of porphyrin and phthalocyanine self-assembled monolayers on ZnO surfaces

Formation of self-assembled monolayers (SAMs) of three porphyrin and one phthalocyanine derivatives on thin ZnO film was studied by monitoring absorption spectra of the samples. The compounds were equipped with carboxylic or phosphate groups to bind to the surface. The SAM formation was found to be fast. The layer was formed in less than 15 min for all studied porphyrins, and 30 min was sufficient to form phthalocyanine layer. For porphyrins with different anchor groups the SAM formation was too fast to see any difference between the anchoring groups. The stability of SAMs was tested then by immersing the samples into neat solvents. Upon immersion the SAMs were gradually losing the absorbance for all the compounds with degradation trends being in line with pKa values of the binding groups of the same type. However, even for the weakest binding group the SAM was relatively stable after a few tens of minutes of washing, which was sufficient to remove physisorbed compounds but the SAM was essentially not destroyed. Comparison of SAMs on thin films with SAMs on ZnO nanorods and TiO2 nanoparticle films indicated the same fast layer formation but relatively weaker SAMs stability, showing 20–40% faster absorption losses during the washing.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Department of Chemistry and Bioengineering, Tampere University of Technology
Authors: Hakola, H., Sariola-Leikas, E., Jäntti, P., Mokus, T., Stranius, K., Efimov, A., Tkachenko, N. V.
Keywords: (self-assembled monolayer; porphyrin; phthalocyanine; TiO2; nanorods)
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Publication information
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ISSN (Print): 1088-4246
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.354 0.379
Publication Forum (2016): 1
Scopus rating (2015): 0.419 0.467
Web of Science (2015): 1.087 1.387 7.0 0.323 0.00257 0.267
Publication Forum (2015): 1
Scopus rating (2014): 0.486 0.545
Web of Science (2014): 1.397 1.603 6.7 0.179 0.00338 0.326
Publication Forum (2014): 1
Scopus rating (2013): 0.537 0.602
Publication Forum (2013): 1
Scopus rating (2012): 0.62 0.537
Publication Forum (2012): 1
Scopus rating (2011): 0.553 0.612
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

State: Published  
Ministry of Education publication type: A1 Journal article-refereed  
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Keio University  
Authors: Kato, D., Sakai, H., Tkachenko, N. V., Hasobe, T.  
Keywords: (Gold, Nanoparticles, Pentacene, Self-assembled monolayers, Singlet fission)  
Pages: 5230-5234  
Publication date: 2016  
Peer-reviewed: Yes  
ASJC Scopus subject areas: Chemistry(all), Catalysis

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- Scopus rating (2016): 5.8 2.104  
- Publication Forum (2016): 3  
- Scopus rating (2015): 5.958 2.235  
- Web of Science (2015): 11.709 12.111 5.8 2.937 0.55213 3.432  
- Scopus rating (2014): 5.805 2.309  
- Web of Science (2014): 11.261 12.06 5.8 2.61 0.53069 3.39  
- Publication Forum (2014): 3  
- Scopus rating (2013): 5.681 2.204  
- Publication Forum (2013): 3
Homologation Reaction of Ketones with Diazo Compounds
This review covers the addition of diazo compounds to ketones to afford homologated ketones, either in the presence or in the absence of promoters or catalysts. Reactions with diazoalkanes, aryl diazomethanes, trimethylsilyldiazomethane, \( \alpha \)-diazo esters, and disubstituted diazo compounds are covered, commenting on the complex regiochemistry of the reaction and the nature of the catalysts and promoters. The recent reports on the enantioselective version of ketone homologation reactions are gathered in one section, followed by reports on the use of cyclic ketones ring expansion in total synthesis. Although the first reports of this reaction appeared in the literature almost one century ago, the recent achievements, in particular, for the asymmetric version, forecast the development of new breakthroughs in the synthetically valuable field of diazo chemistry.
Metathesis Reactions on Solid-Phase: Towards New Synthesis Challenges

Today there are many types of transition-metal-catalyzed carbon–carbon bond-forming reactions. Of these, the olefin metathesis has made possible a wide range of transformations with commercially available and easily handled catalysts. Olefin metathesis is widely considered as one of the most powerful synthetic tool in organic chemistry. During the last 20 years many new catalysts with excellent selectivity and efficiency have been developed, also to be used in solid phase organic chemistry protocols. The understanding of the mechanisms and interactions between the catalyst and substrate has resulted that an increasing number of research groups have employed these reactions in multistep procedures and in the synthesis of active pharmaceutical ingredients and natural products. Although the olefin metathesis reaction still proceeds better in homogeneous phase, some structural modifications of the catalyst and new approaches for immobilization have provided interesting possibilities towards more efficient use also in heterogeneous phase. To celebrate 10 years since the Nobel Prize in Chemistry given to Yves Chauvin, Richard Schrock and Robert Grubbs for the “development of the metathesis method in organic synthesis” and to summarize recent results obtained in the field of solid phase metathesis chemistry this short review was written.
Multicomponent Petasis-borono Mannich Preparation of Alkylaminophenols and Antimicrobial Activity Studies

In this work we report the antibacterial activity of alkylaminophenols. A series of such compounds was prepared by a multicomponent Petasis-borono Mannich reaction starting from salicylaldehyde and its derivatives. The obtained compounds were tested against a large panel of microorganisms, Gram-positive and Gram-negative bacteria, and a yeast. Among the several tertiary amine derivatives tested, indoline-derived aminophenols containing a nitro group at the para-phenol position showed considerable activity against bacteria tested with minimal inhibitory concentrations as low as 1.36 μm against Staphylococcus aureus and Mycobacterium smegmatis. Cytotoxicity of the new para-nitrophenol derivatives was observed only at concentrations much higher than those required for antibacterial activity.

General information

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Industrial Bioengineering and Applied Organic Chemistry
Authors: Neto, Í., Andrade, J., Pinto Reis, C., Salunke, J. K., Priimagi, A., R. Candeias, N., Rijo, P.
Publication date: 2016
Peer-reviewed: Yes

Publication information

Journal: CHEMMEDCHEM
ISSN (Print): 1860-7179
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.13 0.906
Publication Forum (2016): 1
Scopus rating (2015): 1.148 0.905
Web of Science (2015): 2.98 2.89 4.6 0.781 0.01314 0.786
Publication Forum (2015): 1
Scopus rating (2014): 1.11 0.907
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 PC71BM, we compare the performance of global hybrid functionals (B3LYP and B3LYP-D) alongside two LRC functionals (ωB97X and ωB97X-D) and their optimally tuned (OT) analogs (OT-ωB97X and OT-ωB97X-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, PC71BM 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

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Department of Physics, University of Kentucky
Authors: Kastinen, T., Niskanen, M., Risko, C., Cramariuc, O., Hukka, T. I.
Number of pages: 17
Pages: 27654-27670
Publication date: 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry
Photoinduced nonlinear optical response in azobenzene-functionalized molecular glass

We show that methylaminotriazine molecular glass functionalized with the azobenzene derivative Disperse Red 1 shows equally strong second-order nonlinear optical response as well-known polymers with the same photoactive component. Furthermore, even high chromophore loading does not adversely affect the nonlinear response. This suggests that chromophore-chromophore intermolecular interactions do not greatly limit the response of such molecular glasses, which therefore provide an excellent materials platform for nonlinear optical applications.
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
State: Published
Ministry of Education 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
Authors: Akamatsu, N., Aizawa, M., Tatsumi, R., Hisano, K., Priimägi, A., Shishido, A.
Keywords: (Bragg diffraction, Inverse opal structure, Photoresponsive film)
Number of pages: 4
Pages: 145-148
Publication date: 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Organic Chemistry, Polymers and Plastics, Materials Chemistry

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Journal: JOURNAL OF PHOTOPOLYMER SCIENCE AND TECHNOLOGY
Volume: 29
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Porphyrrin-Based Donor-Acceptor Dyads: Engineering the Linker and Tuning the Photoinduced Electron Transfer

General information
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Ministry of Education publication type: A3 Part of a book or another research book
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Tkachenko, N. V., Efimov, A., Lemmetyinen, H.
Number of pages: 51
Pages: 121-171
Publication date: 2016

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Title of host publication: Handbook of Porphyrin Science: With Applications to Chemistry, Physics, Materials Science, Engineering, Biology and Medicine — Volume 42: Towards Tuned Properties of Porphyrinoids
Volume: 42
Publisher: World Scientific Publishing
Editors: Kadish, K. M., Smith, K. M., Guilard, R.
ISBN (Print): 9789813143524
DOIs: 10.1142/9789813149625_0002
Research output: Scientific - peer-review › Chapter

Sorption of zinc onto elemental selenium nanoparticles immobilized in Phanerochaete chrysosporium pellets
The use of a novel hybrid biosorbent, elemental selenium nanoparticles (nSe0) immobilized in pellets of Phanerochaete chrysosporium, to remove Zn from aqueous solutions was investigated. Fungal pellets containing nSe0 (nSe0-pellets)
showed to be better biosorbents as they removed more Zn (88.1 ± 5.3 %) compared to Se-free fungal pellets (56.2 ± 2.8 %) at pH 4.5 and an initial Zn concentration of 10 mg L⁻¹. The enhanced sorption capacity of nSe⁰-pellets was attributed to a higher concentration of sorption sites resulting in a more negative surface charge density, as determined by analysis of the potentiometric titration data. Fourier transform infrared spectroscopy (FT-IR) analysis of fungal pellets prior to and after being loaded with Zn showed the functional groups, including hydroxyl and carboxyl groups, involved in the sorption process. The experimental data indicated that the sorption rate of the nSe⁰-pellets fitted well to the pseudo-second order kinetic model (R² = 0.99), and the sorption isotherm was best represented by the Sips model (Langmuir-Freundlich) with heterogeneous factor n = 1 (R² = 0.99), which is equivalent to the Langmuir model. Operational advantages of fungal pelleted reactors and the Zn removal efficiencies achieved by nSe⁰-pellets under mild acidic conditions make nSe⁰-pellet based bioreactors an efficient biosorption process.

General information
State: Published
Ministry of Education 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, Environmental Engineering and Water Technology Department, Université Paris-Est
Authors: Espinosa-Ortiz, E. J., Shakya, M., Jain, R., Rene, E. R., van Hullebusch, E. D., Lens, P. N. L.
Keywords: (Fungal pellets, Hybrid biosorbent, Phanerochaete chrysosporium, Selenium nanoparticles, Zinc biosorption)
Number of pages: 12
Pages: 21619–21630
Publication date: 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Environmental Chemistry, Medicine(all), Pollution, Health, Toxicology and Mutagenesis

Publication information
Journal: Environmental Science and Pollution Research
Volume: 23
Issue number: 21
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Publication Forum (2017): 1
Scopus rating (2016): 0.813 1.048
Publication Forum (2016): 1
Scopus rating (2015): 0.879 1.02
Web of Science (2015): 2.76 2.876 2.5 0.468 0.02623 0.608
Publication Forum (2015): 1
Scopus rating (2014): 0.949 1.178
Web of Science (2014): 2.828 2.92 2.5 0.367 0.01716 0.653
Publication Forum (2014): 1
Scopus rating (2013): 0.879 1.163
Publication Forum (2013): 1
Scopus rating (2012): 1.017 1.232
Publication Forum (2012): 1
Scopus rating (2011): 1.13 1.1
Scopus rating (2010): 1.084 1.045
Scopus rating (2009): 1.022 1.014
Scopus rating (2008): 0.925 1.019
Scopus rating (2007): 0.809 0.993
Scopus rating (2006): 0.446 0.598
Scopus rating (2005): 0.576 0.952
Scopus rating (2004): 0.781 1.001
Scopus rating (2003): 0.556 0.75
Scopus rating (2002): 0.606 0.936
Scopus rating (2001): 0.56 0.633
Scopus rating (2000): 0.692 0.855
Scopus rating (1999): 0.849 0.953
Original language: English
DOIs: 10.1007/s11356-016-7333-6
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 \([\text{C}_n\text{F}_{2n+1}-\text{I}\cdots\text{I}\cdots\text{I}-\text{C}_n\text{F}_{2n+1}]^{-}\) 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
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Cavallo, G., Terraneo, G., Monfredini, A., Saccone, M., Priimägi, A., Pilati, T., Resnati, G., Metrangolo, P., Bruce, D. W.
Keywords: (Fluorophobic effect, Halogen bonding, Ionic liquid crystals, Self-assembly, Supramolecular chemistry)
Pages: 6300-6304
Publication date: 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Chemistry(all), Catalysis

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ISSN (Print): 1433-7851
Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 5.8 2.104
Publication Forum (2016): 3
Scopus rating (2015): 5.958 2.235
Web of Science (2015): 11.709 12.111 5.8 2.937 0.55213 3.432
Scopus rating (2014): 5.805 2.309
Web of Science (2014): 11.261 12.06 5.8 2.61 0.53069 3.39
Publication Forum (2014): 3
Scopus rating (2013): 5.681 2.204
Publication Forum (2013): 3
Scopus rating (2012): 6.362 2.338
Publication Forum (2012): 3
Scopus rating (2011): 6.062 2.387
Scopus rating (2010): 5.858 2.31
Scopus rating (2009): 5.52 2.218
Scopus rating (2008): 5.438 2.115
Scopus rating (2007): 4.406 1.87
Scopus rating (2006): 4.71 2.119
Scopus rating (2005): 4.7 2.295
Scopus rating (2004): 4.165 2.166
Scopus rating (2003): 3.41 2.126
Scopus rating (2002): 3.659 2.146
Scopus rating (2001): 3.695 2.07
Scopus rating (2000): 3.793 2.217
Scopus rating (1999): 3.59 2.156
Original language: English
Electronic versions:
Superfluorinated Ionic Liquid Crystals Based on Supramolecular, Halogen-Bonded Anions
DOIs:
10.1002/anie.201601278
The effect of urine storage on antiviral and antibiotic compounds in the liquid phase of source-separated urine

The behaviour of pharmaceuticals related to the human immunodeficiency virus treatment was studied in the liquid phase of source-separated urine during six-month storage at 20°C. Six months is the recommended time for hygienization and use of urine as fertilizer. Compounds were spiked in urine as concentrations calculated to appear in urine. Assays were performed with separate compounds and as therapeutic groups of antivirals, antibiotics and anti-tuberculotics. In addition, urine was amended either with faeces or urease inhibitor. The pharmaceutical concentrations were monitored from filtered samples with solid phase extraction and liquid chromatography. The concentration reductions of the studied compounds as such or with amendments ranged from less than 1% to more than 99% after six-month storage. The reductions without amendments were 41.9–99% for anti-tuberculotics; <52% for antivirals (except with 3TC 75.6%) and <50% for antibiotics. In assays with amendments, the reductions were all <50%. Faeces amendment resulted in similar or lower reduction than without it even though bacterial activity should have increased. The urease inhibitor prevented ureolysis and pH rise but did not affect pharmaceutical removal. In conclusion, removal during storage might not be enough to reduce risks associated with the studied pharmaceuticals, in which case other feasible treatment practises or urine utilization means should be considered.
Use of laboratory anaerobic digesters to simulate the increase of treatment rate in full-scale high nitrogen content sewage sludge and co-digestion biogas plants

The aim of this study was to assess the effect of increasing feedstock treatment rate on the performance of full-scale anaerobic digestion using laboratory-scale reactors with digestate and feedstock from full-scale digesters. The studied nitrogen-containing feedstocks were i) a mixture of industrial by-products and pig slurry, and ii) municipal sewage sludge, which digestion was studied at 41 and 52 degrees C, respectively. This study showed the successful reduction of hydraulic retention times from 25 and 20 days to around 15 days, which increased organic loading rates from 2 to 3.5 kg volatile solids (VS)/m(3) d and 4 to 6 kg VS/m(3) d. As a result, the optimum retention time in terms of methane production and VS removal was 10-15% lower than the initial in the full-scale digesters. Accumulation of acids during start-up of the co-digestion reactor was suggested to be connected to the high ammonium nitrogen concentration and intermediate temperature of 41 degrees C. (C) 2016 Elsevier Ltd. All rights reserved.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Gasum Biovakka Ltd, Natural Resources Institute Finland (Luke)
Authors: Tampio, E., Ervasti, S., Paavola, T., Rintala, J.
Keywords: (Anaerobic digestion, Nitrogen, Co-digestion, Sewage sludge, Hydraulic retention time, MICROBIAL COMMUNITY STRUCTURE, FOOD WASTE, SUBSTRATE RATIO, AMMONIA, INOCULUM, TEMPERATURE, PERFORMANCE, MANURE)
Number of pages: 8
Pages: 47-54
Publication date: 2016
Peer-reviewed: Yes

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Scopus rating (2016): 2.191 1.91
Publication Forum (2016): 2
Scopus rating (2015): 2.255 1.908
Web of Science (2015): 4.917 5.744 5.0 1.012 0.13375 1.089
Publication Forum (2015): 2
Scopus rating (2014): 2.41 2.104
Web of Science (2014): 4.494 5.33 4.6 0.822 0.12645 1.042
Publication Forum (2014): 2
Scopus rating (2013): 2.412 2.503
Publication Forum (2013): 2
Scopus rating (2012): 2.389 2.465
Publication Forum (2012): 2
Scopus rating (2011): 2.314 2.508
Scopus rating (2010): 2.086 2.355
Scopus rating (2009): 1.912 2.231
Scopus rating (2008): 1.734 2.732
Scopus rating (2007): 1.529 2.423
Scopus rating (2006): 1.315 1.98
Scopus rating (2005): 1.269 2.006
Scopus rating (2004): 1.197 1.659
Scopus rating (2003): 0.948 1.639
Scopus rating (2002): 0.882 1.3
Scopus rating (2001): 0.541 1.208
Scopus rating (2000): 0.464 1.049
Scopus rating (1999): 0.869 1.061
Original language: English
DOIs:
10.1016/j.biortech.2016.08.058
Preparation and antimicrobial characterization of silver-containing packaging materials for meat
In food technology, antimicrobial packaging materials could inhibit or limit the growth of spoilage bacteria and thus improve the shelf life of packaged products. The present study provides new insights into the preparation and antimicrobial characterization of silver-containing packaging materials and their efficacy against typical meat spoilage bacteria. Antimicrobial efficacy of packaging films produced by coextrusion or liquid flame spray process was determined by bioluminescence imaging and conventional antimicrobial assay. Fresh pork sirloin was packaged in selected films and composition of meat microbiota was analyzed by 16S rRNA amplicon sequencing. Shelf life of meat was not affected by any of the silver-containing packaging films, even though meat microbiota mostly consisted of bacteria that were inhibited or retarded in vitro by nanoscale silver coating. This may be due to different release dynamics of silver ions on meat surfaces compared to the circumstances in the antimicrobial assay or interactions between silver and amino acids.

Graphene-intercalated Fe₃O₄/TiO₂ heterojunctions for efficient photoelectrolysis of water
Interfacial modification of α-Fe₂O₃/TiO₂ 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 α-Fe₂O₃ films (1 V vs. RHE), the α-Fe₂O₃/TiO₂ bilayer structure yielded a better onset potential (0.3 V vs. RHE). Heterojunctioned bilayers exhibited a higher photocurrent
density (0.32 mA cm⁻² at 1.23 V vs. RHE) than the single α-Fe₂O₃ layer (0.22 mA cm⁻² 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 α-Fe₂O₃/TiO₂ interface, which substantially increased the photocurrent density to 0.85 mA cm⁻² (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 α-Fe₂O₃ and TiO₂ layers resulted in reduced recombination in the α-Fe₂O₃ layer. The results showed that graphene intercalation improved the charge separation and the photocurrent density of the FTO/α-Fe₂O₃/FLG/TiO₂ system.

Organic Molecular Films as Light-Emitting and Light-Confining Material in Rolled-Up AlnP Semiconductor Microtube Resonators

A hybrid inorganic/organic microcavity system is presented in which an AlnP-based rolled-up microtube resonator is combined with a thin film of naphthyl end-capped bithiophene molecules. The film is laterally structured into stripes on top of the AlnP layer system before the roll-up process. During the process, the strained bilayer together with the organic molecular stripes rolls up, and a hybrid microtube is formed. The stripes act as visible-light emitters inside the otherwise passive microtube. Furthermore, they induce a light confinement in the axial direction of the microtube, additional to the radial and azimuthal confinement that is intrinsic to a microtube. As the organic material defines the cavity and represents the emitter at the same time, an efficient light coupling into the three-dimensionally confined optical modes of the microtube resonator is ensured. The hybrid microtubes open up the opportunity for novel experiments on the light–molecule interaction as well as their application in optical components.
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.
Changes in global gene expression of *Vibrio parahaemolyticus* induced by cold- and heat-stress

**Background:** *Vibrio (V.) parahaemolyticus* causes seafood-borne gastro-intestinal bacterial infections in humans worldwide. It is widely found in marine environments and is isolated frequently from seawater, estuarine waters, sediments and raw or insufficiently cooked seafood. Throughout the food chain, *V. parahaemolyticus* encounters different temperature conditions that might alter metabolism and pathogenicity of the bacterium. In this study, we performed gene expression profiling of *V. parahaemolyticus* RIMD 2210633 after exposure to 4, 15, 20, 37 and 42°C to describe the cold and heat shock response. 

**Methods:** Gene expression profiles of *V. parahaemolyticus* RIMD 2210633 after exposure to 4, 15, 20, 37 and 42°C were investigated via microarray. Gene expression values and RT-qPCR experiments were compared by plotting the log2 values. Moreover, volcano plots of microarray data were calculated to visualize the distribution of differentially expressed genes at individual temperatures and to assess hybridization qualities and comparability of data. Finally, enriched terms were searched in annotations as well as functional-related gene categories using the Database for Annotation, Visualization and Integrated Discovery. 

**Results:** Analysis of 37°C normalised transcriptomics data resulted in differential expression of 19 genes at 20°C, 193 genes at 4°C, 625 genes at 42°C and 638 genes at 15°C. Thus, the largest number of significantly expressed genes was observed at 15 and 42°C with 13.3 and 13%, respectively. Genes of many functional categories were highly regulated even at lower temperatures. Virulence associated genes (tdh1, tdh2, toxR, toxS, vopC, T6SS-1, T6SS-2) remained mostly unaffected by heat or cold stress.

**Conclusion:** Along with folding and temperature shock depending systems, an overall temperature-dependent regulation of expression could be shown. Particularly the energy metabolism was affected by changed temperatures. Whole-genome gene expression studies of food related pathogens such as *V. parahaemolyticus* reveal how these pathogens react to stress impacts to predict its behaviour under conditions like storage and transport.
Regenerative Astaxanthin Extraction from a Single Microalgal (Haematococcus pluvialis) Cell Using a Gold Nano-Scalpel

Milking of microalgae, the process of reusing the biomass for continuous production of target compounds, can strikingly overcome the time and cost constraints associated with biorefinery. This process can significantly improve production efficiency of highly valuable chemicals, for example, astaxanthin (AXT) from Haematococcus pluvialis. Detailed understanding of the biological process of cell survival and AXT reaccumulation after extraction would be of great help for successful milking. Here we report extraction of AXT from a single cell of H. pluvialis through incision of the cell wall by a...
gold nanoscalpel (Au-NS), which allows single-cell analysis of wound healing and reaccumulation of AXT. Interestingly, upon the Au-NS incision, the cell could reaccumulate AXT at a rate two times faster than the control cells. Efficient extraction as well as minimal cellular damage, keeping cells alive, could be achieved with the optimized shape and dimensions of Au-NS: a well-defined sharp tip, thickness under 300 nm, and 1-3 μm of width. The demonstration of regenerative extraction of AXT at a single cell level hints toward the potential of a milking process for continuous recovery of target compounds from microalgae while keeping the cells alive.

Characterization of thermally aged polyetheretherketone fibres: Mechanical, thermal, rheological and chemical property changes

This paper investigates the effects of thermal degradation on polyetheretherketone (PEEK) fibres. PEEK samples were aged at a constant temperature of 250 °C for 1-128 days and characterized with mechanical tests, FTIR (Fourier Transform Infrared Spectroscopy), DSC (Differential Scanning Calorimetry), rheology, TGA (Thermogravimetric Analysis), SEM (Scanning Electron Microscopy), and UV-Vis diffuse reflectance spectroscopy. The short-term thermal annealing had a positive effect on the mechanical properties, due to the formation and growth of secondary crystals. Crosslinking in the material was verified by rheological inspections. The crosslinking increased the mechanical strength and modulus but reduced the elongation at break of the fibres. FTIR tests showed that carbonyl and hydroxyl groups were slowly formed on the surface of the fibres while ring opening reactions took place. The thermal ageing reduced the thermal stability of PEEK. The decreased stability was observed in the decomposition onset temperature after 8 d and in the melting point and the glass transition temperature after 32 d. The first signs of degradation, crosslinking, embrittlement, and reduced
thermal stability, were visible roughly after 8 d of ageing, whereas the deterioration in general usability occurred after 64 d.

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Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Engineering materials science and solutions (EMASS)
Authors: Mylläri, V., Ruoko, T., Vuorinen, J., Lemmetyinen, H.
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Scopus rating (2013): 1.341 2.12
Publication Forum (2013): 2
Scopus rating (2012): 1.423 2.105
Publication Forum (2012): 2
Scopus rating (2011): 1.347 2.099
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Scopus rating (2006): 1.367 1.787
Scopus rating (2005): 1.197 1.461
Scopus rating (2004): 1.062 1.43
Scopus rating (2003): 0.922 1.24
Scopus rating (2002): 0.821 1.058
Scopus rating (2001): 0.93 1.151
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http://www.scopus.com/inward/record.url?scp=84942433318&partnerID=8YFLogxK (Link to publication in Scopus)
Cultivation of Nannochloropsis for eicosapentaenoic acid production in wastewaters of pulp and paper industry

The eicosapentaenoic acid (EPA) containing marine microalga Nannochloropsis oculata was grown in an effluent from anaerobic digestion of excess activated sludge from a wastewater treatment plant serving a combination of a pulp and a paper mill and a municipality (digester effluent, DE), mixed with the effluent of the same wastewater treatment plant. The maximum specific growth rate and photosynthesis of N. oculata were similar in the DE medium and in artificial sea water medium (ASW) but after 7 days, algae grown in the DE medium contained seven times more triacylglycerols (TAGs) per cell than cells grown in ASW, indicating mild stress in the DE medium. However, the volumetric rate of EPA production was similar in the ASW and DE media. The results suggest that N. oculata could be used to produce EPA, utilizing the nutrients available after anaerobic digestion of excess activated sludge of a pulp and paper mill.

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Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Urban circular bioeconomy (UrCirBio), University of Turku, Department of Biochemistry/Molecular Plant Biology, Department of Biochemistry/Food Chemistry and Food Development
Authors: Polishchuk, A., Valev, D., Tarvainen, M., Mishra, S., Kinnunen, V., Antal, T., Yang, B., Rintala, J., Tyystjärvi, E.
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ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

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Scopus rating (2015): 2.255 1.908
Web of Science (2015): 4.917 5.744 5.0 1.012 0.13375 1.089
Publication Forum (2015): 2
Scopus rating (2014): 2.41 2.104
Web of Science (2014): 4.494 5.33 4.6 0.822 0.12645 1.042
Publication Forum (2014): 2
Scopus rating (2013): 2.412 2.503
Publication Forum (2013): 2
Scopus rating (2012): 2.389 2.465
Publication Forum (2012): 2
Scopus rating (2011): 2.314 2.508
Scopus rating (2010): 2.086 2.355
Scopus rating (2009): 1.912 2.231
Scopus rating (2008): 1.734 2.732
Scopus rating (2007): 1.529 2.423
Scopus rating (2006): 1.315 1.98
Scopus rating (2005): 1.269 2.006
Scopus rating (2004): 1.197 1.659
Scopus rating (2003): 0.948 1.639
Measuring the green color of vegetables from digital images using image analysis
When analyzing the color of foods, a measurement device consisting of a digital camera and image analysis software is an attractive alternative to traditional instruments such as spectrophotometers, colorimeters and sensory evaluations. The device enables the measuring of the surface of a sample pixel-by-pixel and offers versatile possibilities for new imaging-based analysis strategies for food research. Our objective was to evaluate if this apparatus could detect differences in colors existing in green vegetables. We showed that the device separated batches of green vegetables and detected color differences that existed in vegetables with different degrees of green color. We demonstrated that this device could measure the color change of green vegetables during heat treatments. We conclude that this experimental setup has the potential to evaluate the healthiness of a diet by analyzing the proportion and quality of green vegetables for use in a serving at a buffet table or dinner plate.

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Authors: Manninen, H., Paakki, M., Hopia, A., Franzén, R.
Keywords: (a, b, Digital camera, Green vegetables, L, Thermal degradation)
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Publication Forum (2016): 1
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Publication Forum (2015): 1
Scopus rating (2014): 1.348 1.8
Web of Science (2014): 2.416 3.095 6.4 0.385 0.01769 0.746
Publication Forum (2014): 2
Scopus rating (2013): 1.365 1.824
Publication Forum (2013): 2
Scopus rating (2012): 1.574 2.013
Publication Forum (2012): 2
Scopus rating (2011): 1.442 1.877
Scopus rating (2010): 1.347 1.508
Effects of anode potentials on bioelectrogenic conversion of xylose and microbial community compositions

The results on the effects of different anode potentials on current densities, coulombic efficiencies and microbial communities are contradictory and have not been studied with xylose, an important constituent of lignocellulosic materials. In this study, the effects of different anode potentials (+0.2, 0 and -0.2V vs. Ag/AgCl) on current generation, xylose degradation and microbial communities were examined with an exoelectrogenic enrichment culture originating from anaerobic sludge. Anode potential of +0.2V (vs. Ag/AgCl) resulted in the highest current density and coulombic efficiency of 1.5±0.2A/m<sup>2</sup> and 62±11%, respectively, and there was no accumulation of soluble metabolites. With anode potentials of 0 and -0.2V the current densities remained low and acetate, butyrate and propionate were detected in the end of batch runs. Different anode potentials resulted in substantial differences in the anodic bacterial species. At more positive anode potentials, Ochrobactrum intermedium reported to be capable of direct electron transfer dominated. At more negative anode potentials, a known mediator-producer, Alcaligenes faecalis, and Desulfotobacterium hafniense, that has been reported to use mediated electron transfer, were detected. This study shows that the anode potential has a substantial effect on microbial communities and on xylose metabolism.
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$^{-1}$. In addition, changes proposed to the graphene oxide exfoliation process can improve the synthesis yield by up to 70%.
Gene expression profiles of *Vibrio parahaemolyticus* in the early stationary phase

*Vibrio (V.) parahaemolyticus* is an aquatic bacterium capable of causing foodborne gastroenteritis. In the environment or the food chain, *V. parahaemolyticus* cells are usually forced into the stationary phase, the common phase for bacterial survival in the environment. So far, little is known about whole genomic expression of *V. parahaemolyticus* in the early stationary phase compared with the exponential growth phase. We performed whole transcriptomic profiling of *V. parahaemolyticus* cells in both phases (exponential and early stationary phase). Our data showed in total that 172 genes were induced in early stationary phase, while 61 genes were repressed in early stationary phase compared with the exponential phase. Three functional categories showed stable gene expression in the early stationary phase. Eleven functional categories showed that up-regulation of genes was dominant over down-regulation in the early stationary phase. Although genes related to endogenous metabolism were repressed in the early stationary phase, massive regulation of gene expression occurred in the early stationary phase, indicating the expressed gene set of *V. parahaemolyticus* in the early stationary phase impacts environmental survival.

**General information**

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Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Institute of Food Hygiene, Freie Universitaet Berlin

Authors: Meng, L., Alter, T., Aho, T., Huehn, S.

Keywords: (Vibrio parahaemolyticus, Early stationary phase, Exponential phase, Microarray, Whole genome gene expression)
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**

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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

Authors: Bajamundi, C. J. E., Vainikka, P., Hedman, M., Silvennoinen, J., Heinanen, T., Taipale, R., Konttinen, J.

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Web of Science (2015): 3.611 4.14 6.0 1.014 0.05542 0.929

Publication Forum (2015): 2

Scopus rating (2014): 1.667 2.331

Web of Science (2014): 3.52 4.091 6.4 0.815 0.04512 0.922

Publication Forum (2014): 3

Scopus rating (2013): 1.811 2.595

Publication Forum (2013): 3

Scopus rating (2012): 1.852 2.465

Publication Forum (2012): 3

Scopus rating (2011): 2.093 2.427

Scopus rating (2010): 1.984 2.319

Scopus rating (2009): 2.012 2.277

Scopus rating (2008): 1.635 2.184

Scopus rating (2007): 1.383 1.86

Scopus rating (2006): 1.278 1.64

Scopus rating (2005): 1.623 1.73

Scopus rating (2004): 1.273 1.883

Scopus rating (2003): 1.103 1.481

Scopus rating (2002): 1.13 1.301

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Scopus rating (2000): 1.047 1.272

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Research output: Scientific - peer-review › Article
Fe₂O₃-TiO₂ nanosystems by a hybrid PE-CVD/ALD approach: controllable synthesis, growth mechanism, and photocatalytic properties

Supported Fe₂O₃-TiO₂ nanocomposites are fabricated by an original vapor phase synthetic strategy, consisting of the initial growth of Fe₂O₃ nanosystems on fluorine-doped tin oxide substrates by plasma enhanced-chemical vapor deposition, followed by atomic layer deposition of TiO₂ 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 Fe₂O₃ (hematite) and TiO₂ (anatase), with an intimate Fe₂O₃-TiO₂ 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 TiO₂ overlayer thickness. This finding opens attractive perspectives for eventual applications in wastewater treatment.

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Number of pages: 8
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Scopus rating (2016): 1.043 0.904
Publication Forum (2016): 1
Scopus rating (2015): 1.063 0.999
Web of Science (2015): 3.849 3.801 3.4 0.928 0.05518 0.67
Publication Forum (2015): 1
Scopus rating (2014): 1.131 1.11
Web of Science (2014): 4.034 4.022 3.0 0.988 0.05187 0.717
Publication Forum (2014): 2
Scopus rating (2013): 1.079 1.11
Publication Forum (2013): 2
Scopus rating (2012): 1.253 1.142
Publication Forum (2012): 2
Scopus rating (2011): 1.174 1.191
Scopus rating (2010): 1.233 1.229
Scopus rating (2009): 1.227 1.257
Scopus rating (2008): 1.297 1.183
Scopus rating (2007): 1.42 1.704
Scopus rating (2005): 1.419 1.051
Scopus rating (2004): 1.0 0.951
Scopus rating (2003): 0.73 0.751
Scopus rating (2002): 0.228 0.509
Fluorescent Protein Based FRET Pairs with Improved Dynamic Range for Fluorescence Lifetime Measurements

Fluorescence Resonance Energy Transfer (FRET) using fluorescent protein variants is widely used to study biochemical processes in living cells. FRET detection by fluorescence lifetime measurements is the most direct and robust method to measure FRET. The traditional cyan-yellow fluorescent protein based FRET pairs are getting replaced by green-red fluorescent protein variants. The green-red pair enables excitation at a longer wavelength which reduces cellular autofluorescence and phototoxicity while monitoring FRET. Despite the advances in FRET based sensors, the low FRET efficiency and dynamic range still complicates their use in cell biology and high throughput screening. In this paper, we utilized the higher lifetime of NowGFP and screened red fluorescent protein variants to develop FRET pairs with high dynamic range and FRET efficiency. The FRET variations were analyzed by proteolytic activity and detected by steady-state and time-resolved measurements. Based on the results, NowGFP-tdTomato and NowGFP-mRuby2 have shown high potentials as FRET pairs with large fluorescence lifetime dynamic range. The in vitro measurements revealed that the NowGFP-tdTomato has the highest Forster radius for any fluorescent protein based FRET pairs yet used in biological studies. The developed FRET pairs will be useful for designing FRET based sensors and studies employing Fluorescence Lifetime Imaging Microscopy (FLIM).

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Authors: George Abraham, B., Sarkisyan, K. S., Mishin, A. S., Santala, V., Tkachenko, N. V., Karp, M.
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Publication Forum (2015): 1
Scopus rating (2014): 1.545 1.141
Web of Science (2014): 3.234 3.702 2.7 0.489 1.53341 1.209
Publication Forum (2014): 2
Scopus rating (2013): 1.74 1.147
Publication Forum (2013): 2
Scopus rating (2012): 1.945 1.142
Publication Forum (2012): 2
Scopus rating (2011): 2.369 1.23
Scopus rating (2010): 2.631 1.161
Photoinduced Electron Transfer in CdSe/ZnS Quantum Dot-Fullerene Hybrids

Photoinduced electron transfer (ET) in CdSe/ZnS core-shell quantum dot (QD) - fullerene (COOH-C60) 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.

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Authors: Virikki, K., Demir, S., Lemmetyinen, H., Tkachenko, N. V.
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Peer-reviewed: Yes
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Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Scopus rating (2014): 2.027 1.448
Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
Publication Forum (2014): 3
Scopus rating (2013): 2.134 1.439
Publication Forum (2013): 3
Scopus rating (2012): 2.514 1.46
Publication Forum (2012): 3
Scopus rating (2011): 2.32 1.457
Scopus rating (2010): 2.438 1.356
Scopus rating (2009): 2.128 1.417
Scopus rating (2008): 1.856 1.033
Subpicosecond to Second Time-Scale Charge Carrier Kinetics in Hematite-Titania Nanocomposite Photoanodes

Water splitting with hematite is negatively affected by poor intrinsic charge transport properties. However, they can be modified by forming heterojunctions to improve charge separation. For this purpose, charge dynamics of TiO2:alpha-Fe2O3 nanocomposite photoanodes are studied using transient absorption spectroscopy to monitor the evolution of photogenerated charge carriers as a function of applied bias voltage. The bias affects the charge carrier dynamics, leading to trapped electrons in the submillisecond time scale and an accumulation of holes with a lifetime of 0.4 +/- 0.1 s. By contrast, slower electron trapping and only few long-lived holes are observed in a bare hematite photoanode. The decay of the long-lived holes is 1 order of magnitude faster for the composite photoanodes than previously published for doped hematite, indicative of higher catalytic efficiency. These results illustrate the advantages of using composite materials to overcome poor charge carrier dynamics, leading to a 30-fold enhancement in photocurrent.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology, Department of Materials Engineering, Frontier Photonics, ETH Zürich, Laboratory for Multifunctional Materials
Authors: Ruoko, T. P., Kaunisto, K., Bärtsch, M., Pohjola, J., Hiltunen, A., Niederberger, M., Tkachenko, N. V., Lemmetynen, H.
Keywords: (FILM ELECTRODES, IRON-OXIDE, SEMICONDUCTOR ELECTRODES, WATER OXIDATION, VISIBLE-LIGHT, ALPHA-FE2O3, PHOTOELECTRODES, TIO2, RECOMBINATION, ELECTROLYSIS)
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Scopus rating (2016): 4.583 1.68
Publication Forum (2016): 3
Scopus rating (2015): 4.233 1.829
Web of Science (2015): 8.539 7.803 3.0 1.971 0.11885 2.482
Publication Forum (2015): 2
Web of Science (2014): 7.458 7.536 2.8 2.017 0.09524 2.425
Publication Forum (2014): 2
Scopus rating (2013): 3.515 1.61
Publication Forum (2013): 2
Scopus rating (2012): 3.943 1.751
Publication Forum (2012): 2
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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$_2$ 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.

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**

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Authors: Mylläri, V., Ruoko, T., Syrjälä, S.

Keywords: (aging, degradation, rheology, thermoplastics, PHOTOOXIDATION, FILMS, PHOTOLYSIS)

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

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Scopus rating (2015): 0.574 0.827

Web of Science (2015): 1.866 1.647 8.9 0.485 0.0441 0.315

Publication Forum (2015): 1

Scopus rating (2014): 0.658 0.964

Web of Science (2014): 1.768 1.662 8.5 0.378 0.04912 0.323

Publication Forum (2014): 2

Scopus rating (2013): 0.628 1.085

Publication Forum (2013): 2

Scopus rating (2012): 0.658 1.081

Publication Forum (2012): 2

Scopus rating (2011): 0.601 0.965

Scopus rating (2010): 0.679 0.909

Scopus rating (2009): 0.697 0.825

Scopus rating (2008): 0.647 0.822

Scopus rating (2007): 0.678 0.931

Scopus rating (2006): 0.782 1.145

Scopus rating (2005): 0.779 0.912

Scopus rating (2004): 0.774 0.962

Scopus rating (2003): 0.816 1.067

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Scopus rating (2001): 0.964 1.157

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Molecular interactions on single-walled carbon nanotubes revealed by high-resolution transmission microscopy

The close solid-state structure-property relationships of organic pi - aromatic molecules have attracted interest due to their implications for the design of organic functional materials. In particular, a dimeric structure, that is, a unit consisting of two molecules, is required for precisely evaluating intermolecular interactions. Here, we show that the sidewall of a singlewalled carbon nanotube (SWNT) represents a unique molecular dimer platform that can be directly visualized using high-resolution transmission electron microscopy. Pyrene is chosen as the pi - aromatic molecule; its dimer is covalently linked to the SWNT sidewalls by aryl addition. Reflecting the orientation and separation of the two molecules, the pyrene dimer on the SWNT exhibits characteristic optical and photophysical properties. The methodology discussed here-form and probe molecular dimers-is highly promising for the creation of unique models and provides indispensable and fundamental information regarding molecular interactions.
Synthesis and Photophysical Properties of Two Diazaporphyrin-Porphyrin Hetero Dimers in Polar and Nonpolar Solutions

Two diazaporphyrin (DAP)-porphyrin hetero dimers, in β-meso and β-β 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 β-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 β-β 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.

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Authors: Abou-Chahine, F., Fujii, D., Imahori, H., Nakano, H., Tkachenko, N. V., Matano, Y., Lemmetyinen, H.
Number of pages: 10
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Scopus rating (2016): 1.348 1.02
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Scopus rating (2015): 1.367 1.096
Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
Publication Forum (2015): 1
Scopus rating (2014): 1.44 1.14
Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
Publication Forum (2014): 3
Scopus rating (2013): 1.494 1.2
Publication Forum (2013): 3
Scopus rating (2012): 1.92 1.251
Publication Forum (2012): 3
Scopus rating (2011): 1.78 1.226
Scopus rating (2010): 1.849 1.214
Scopus rating (2009): 2.232 1.349
Scopus rating (2008): 2.543 1.381
Scopus rating (2007): 2.346 1.282
Scopus rating (2006): 2.369 1.415
Catalytic effect of Ca and K on CO2 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 CO2 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 K2CO3 or physically mixing of CaC2O4. The prepared spruce samples were placed in a mesh holder and gasified in the TGA at 850°C in 100% CO2. The results demonstrate that the gasification rate of the char increased linearly with an increase in the concentration of Ca or K. Crystalline CaC2O4 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 CaCO3 and K2CO3 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.
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\(^{-3}\)). 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\(^{-3}\)). 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\(_3\) 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
Laser-pointer-induced self-focusing effect in hybrid-aligned dye-doped liquid crystals

Nonlinear optics deals with phenomena where "light controls light"; e.g., there is mediation by an intensity-dependent medium through which light propagates. This field has attracted much attention for its immense potential in applications dependent on nonlinear processes, such as frequency conversion, multiple-photon absorption, self-phase modulation, and so on. However, such nonlinearities are typically only observed at very high light intensities and thus they require costly lasers. Here, we report on a self-focusing effect induced with a 1 mW handheld laser pointer. We prepared polymer-stabilized dye-doped liquid crystals, in which the molecular director orientation gradually changes from homeotropic at one surface to homogeneous at the other. This is referred to as hybrid alignment. In such films, the threshold intensity needed to form diffraction rings was reduced by a factor of 8.5 compared to that in conventional homeotropic cells, which enabled the induction of the self-focusing effect with a laser pointer.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Tokyo Inst Technol, Tokyo Institute of Technology, Chem Resources Lab, Midori Ku, JST, Japan Science & Technology Agency (JST), PRESTO
Authors: Wang, J., Aihara, Y., Kinoshita, M., Mamiya, J., Priimagi, A., Shishido, A.
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Publication Forum (2016): 2
Scopus rating (2015): 2.057 1.684
Web of Science (2015): 5.228 5.525 2.1 0.559 0.2094 1.865
Publication Forum (2015): 2
Scopus rating (2014): 2.103 1.544
Web of Science (2014): 5.578 5.597 1.7 0.722 0.11476 2.075
Biomimetic collagen I and IV double layer Langmuir-Schaefer films as microenvironment for human pluripotent stem cell derived retinal pigment epithelial cells

The environmental cues received by the cells from synthetic substrates in vitro are very different from those they receive in vivo. In this study, we applied the Langmuir-Schaefer (LS) deposition, a variant of Langmuir-Blodgett technique, to fabricate a biomimetic microenvironment mimicking the structure and organization of native Bruch's membrane for the production of the functional human embryonic stem cell derived retinal pigment epithelial (hESC-RPE) cells. Surface pressure-area isotherms were measured simultaneously with Brewster angle microscopy to investigate the self-assembly of human collagens type I and IV on air-subphase interface. Furthermore, the structure of the prepared collagen LS films was characterized with scanning electron microscopy, atomic force microscopy, surface plasmon resonance measurements and immunofluorescent staining. The integrity of hESC-RPE on double layer LS films was investigated by measuring transepithelial resistance and permeability of small molecular weight substance. Maturation and functionality of hESC-RPE cells on double layer collagen LS films was further assessed by RPE-specific gene and protein expression, growth factor secretion, and phagocytic activity. Here, we demonstrated that the prepared collagen LS films have layered structure with oriented fibers corresponding to architecture of the uppermost layers of Bruch's membrane and result in increased barrier properties and functionality of hESC-RPE cells as compared to the commonly used dip-coated controls.
Gene expression profiles of Vibrio parahaemolyticus in viable but non-culturable state

Viable but non-culturable (VBNc) state is referred to as a dormant state of non-sporulating bacteria enhancing the survival in adverse environments. To our knowledge, only few studies have been conducted on whole genomic expression of Vibrio parahaemolyticus VBNc state. Since a degradation of nucleic acids in V. vulnificus non-culturable state has been detected, we hypothesize that gene regulation of VBNc cells is highly reduced, downregulation of gene expression is dominant and only metabolic functions crucial for survival are kept on a sustained basis. Hence, we performed the whole transcriptomic profiles of V. parahaemolyticus in three phases (exponential, early stationary phase and VBNc state). Compared with exponential and early stationary phase, in V. parahaemolyticus VBNc cells we found 509 induced genes and 309 repressed by more than 4-fold among 4820 investigated genes. Upregulation was dominant in most of non-metabolism functional categories, while five metabolism-related functional categories revealed downregulation in VBNc state. To our knowledge, this is the first study of comprehensive transcriptomic analyses of three phases of V. parahaemolyticus RIMD2210633. Although the mechanism of VBNc state is not yet clear, massive regulation of gene expression occurs in VBNc state compared with expression in other two phases, indicating VBNc cells are active.

General information

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Authors: Meng, L., Alter, T., Aho, T., Huehn, S.
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Light induced cytosolic drug delivery from liposomes with gold nanoparticles

Externally triggered drug release at defined targets allows site- and time-controlled drug treatment regimens. We have developed liposomal drug carriers with encapsulated gold nanoparticles for triggered drug release. Light energy is converted to heat in the gold nanoparticles and released to the lipid bilayers. Localized temperature increase renders liposomal bilayers to be leaky and triggers drug release. The aim of this study was to develop a drug releasing system capable of releasing its cargo to cell cytosol upon triggering with visible and near infrared light signals. The liposomes were formulated using either heat-sensitive or heat- and pH-sensitive lipid compositions with star or rod shaped gold nanoparticles. Encapsulated fluorescent probe, calcein, was released from the liposomes after exposure to the light. In addition, the pH-sensitive formulations showed a faster drug release in acidic conditions than in neutral conditions. The liposomes were internalized into human retinal pigment epithelial cells (ARPE-19) and human umbilical vein endothelial cells (HUVECs) and did not show any cellular toxicity. The light induced cytosolic delivery of calcein from the gold nanoparticle containing liposomes was shown, whereas no cytosolic release was seen without light induction or without gold nanoparticles in the liposomes. The light activated liposome formulations showed a controlled content release to the cellular cytosol at a specific location and time. Triggering with visual and near infrared light allows good tissue penetration and safety, and the pH-sensitive liposomes may enable selective drug release in the intracellular acidic compartments (endosomes, lysosomes). Thus, light activated liposomes with gold nanoparticles are an attractive option for time- and site-specific drug delivery into the target cells. (C) 2015 Elsevier B.V. All rights reserved.
Crystal structure of 2-methylpiperazine-1,4-dilium bis(hydrogen maleate)
In the title salt, $\text{C}_{5}\text{H}_{14}\text{N}_{2}^{2+} \cdot 2\text{C}_{4}\text{H}_{3}\text{O}_{4}^{-}$, 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 $\text{O} \cdot \cdot \cdot \text{O}$ hydrogen bonds generate S(7) rings. In the crystal, the four independent anions are linked to the 2-methylpiperazinium cations through $\text{N} \cdot \cdot \cdot \text{O}$ hydrogen bonds, forming two-dimensional layered structures lying parallel to (001).
The processes of charge generation, transport, and recombination are the main characteristics in organic photovoltaic systems. The triple layer structures, consisted of a primary electron donor layer (poly(3-hexylthiophene), P3HT), an electron acceptor layer (perylene diimide, PDI), and covalently linked porphyrin-fullerene donor acceptor dyad (D-A) layer (free base or Zn-porphyrin-fullerene dyad) were studied in this work by using a transient photocurrent method to monitor the electrical response in millisecond and second time scales. The active layers were in between two electrodes, which were insulated from them by several non-conductive octadecylamine films. Kinetics of charge generation, transport, and recombination was studied by monitoring light intensity dependent lifetimes of photocurrent signals. Both the signal intensities and lifetimes were increased by two orders of magnitude in the complete devices, H-(D-A)-E (or H vertical bar D-A vertical bar E), compared to the reference structures, H-(D-A) or (D-A)-A (or H vertical bar D-A and D-A vertical bar E), evidencing efficient charge separation in the triple layer. Relative yields for the charge separation were calculated from the excitation intensity dependent photocurrent lifetimes, according to a simple three state model. Recombination of the steady states in darkness followed second order kinetics. In the complete device with Zn-porphyrin dyad the longer lifetimes and lower quantum yields for the charge separation and recombination rates were observed, indicating a charge trapping inside the layers instead of complete separation.
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. $^1$H NMR spectroscopy and electrospray ionisation mass spectrometry were utilized in analysing the complexes in solution and in the gas phase, respectively. The $^1$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 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···π, CH···π and hydrogen bond interactions.

General information

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Organisations: Department of Chemistry and Bioengineering, University of Jyväskylä
Authors: Beyeh, N. K., Pan, F., Valkonen, A., Rissanen, K.
Number of pages: 7
Integrated in vitro-in silico screening strategy for the discovery of antibacterial compounds

Multidrug-resistant bacterial infections are an increasing source of healthcare problems, and the research for new antibiotics is currently unable to respond to this challenge. In this work, we present a screening strategy that integrates cell-based high-throughput screening (HTS) with in silico analogue search for antimicrobial small-molecule drug discovery. We performed an HTS on a diverse chemical library by using an assay based on a bioluminescent Escherichia coli K-12 (pTetLux1) strain. The HTS yielded eight hit compounds with >50% inhibition. These hits were then used for structural similarity-based virtual screening, and of the 29 analogues selected for in vitro testing, four compounds displayed potential activity in the pTetLux1 assay. The 11 most active compounds from combined HTS and analogue search were further assessed for antimicrobial activity against clinically important strains of E. coli and Staphylococcus aureus and for in vitro cytotoxicity against human cells. Three of the compounds displayed antibacterial activity and low human cell cytotoxicity. Additionally, two compounds of the set fully inhibited S. aureus growth after 24 h, but also exhibited human cell cytotoxicity in vitro.
Glycerol as an Efficient Medium for the Petasis Borono-Mannich Reaction

The multicomponent Petasis borono-Mannich (PBM) reaction is a useful tool for the preparation of complex molecules in a single step from boronic acids, aldehydes/ketones, and amines. Here, we describe the use of glycerol in the PBM reaction of salicylaldehydes or 2-pyridinecarbaldehyde with several boronic acids and secondary amines. From these readily available starting materials, alkylaminophenols, 2-substituted pyridines, and 2H-chromenes were prepared in reasonable to good yields. Glycerol was compared with other solvents, and in some cases, it provided the reaction product in higher yield. Crude glycerol, as generated by the biodiesel industry, was evaluated and found to be a suitable solvent for the PBM reaction, successfully expanding the potential use of this industry by-product. Based on density functional theory (DFT) calculations and the obtained experimental results, the involvement of glycerol-derived boronic esters in the reaction mechanism is suggested to be competitive with the free boronic acid pathway. Similar Gibbs free energies for the aryl migration from the boronate species to the iminium were determined for both mechanisms.
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 iodoethyl motif seems highly promising in future development of polymeric optical and photoactive materials driven by halogen bonding.
Photophysical Study of a Self-Assembled Donor-Acceptor Two-Layer Film on TiO2

The self-assembled monolayer (SAM) technique was employed to fabricate a two-layer donor-acceptor film on the surface of TiO2. The approach is based on using donor and acceptor compounds with anchoring groups of different lengths. The acceptor, a fullerene derivative, has a carboxyl anchor attached to the fullerene moiety via a short linker that places the fullerene close to the surface. The donor, a porphyrin derivative, is equipped with a long linker that can penetrate between the fullerenes and keep porphyrin on top of the fullerene layer. The two-layer fullerene-porphyrin structures were deposited on a mesoporous film of TiO2 nanoparticles by immersing the TiO2 film sequentially into fullerene and porphyrin solutions. Transient absorption spectroscopy studies of the samples revealed that after the selective photoexcitation of porphyrin a fast (}

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Tampere Univ Technol, Tampere University of Technology, Dept Chem & Bioengn
Authors: Stranius, K., George, L., Efimov, A., Ruoko, T., Pohjola, J., Tkachenko, N. V.
Keywords: (PHOTOINDUCED ELECTRON-TRANSFER, PORPHYRIN-FULLERENE DYADS, SOLAR-CELLS, CHARGE-SEPARATION, STATE, MONOLAYERS, DYNAMICS, ENERGY, PERFORMANCE, GENERATION)
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Controlled Regioselective Amination of Peryleneimides

Perylenedimides (PDIs) and perylenemonoimide diesters (PMIs) can be selectively substituted at the 1,6- or 7,12-positions of the bay region, respectively, by direct amination reactions. The reactions proceed by the formation of a perylene radical anion and its subsequent oxidation, and the yields range from 20-97%. The amination can be tuned to obtain either mono- or disubstituted perylenes by varying the oxidants involved. The presence of the imide cycle is crucial for the transformation, although the amination occurs regioselectively at the bay-region positions distant from the imide cycle.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
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Ratings:
Aryl end-capped quaterthiophenes applied as anode interfacial layers in inverted organic solar cells

Four aryl end-capped quaterthiophene derivatives were synthesized and their material properties were studied by computational, spectroscopic, electrochemical, and thermoanalytical methods. Compounds were applied as interfacial layers between the bulk heterojunction active layer and Ag anode in inverted organic solar cells. Results show that p-cyanophenyl end-capped quaterthiophene with hexyl side chains increases both the short circuit current density and power conversion efficiency notably compared to reference interlayer material, tris-(8-hydroxyquinoline)aluminum. The improved cell performance was attributed to the optimal positions of the highest occupied molecular orbital and the lowest unoccupied molecular orbital (LUMO) of this material, relative to those of the photoactive electron donor poly(3-hexythiophene) and Ag anode, and evenly distributed LUMO. In addition, the use of these materials as an anode interfacial layer increases the absorption of the solar cell, which could contribute to the formation of excitons and additional current production by the cell.
Photophysical properties of Sn (IV)tetraphenylporphyrin-pyrene dyad with a β-vinyl linker

A Sn(IV)tetraphenylporphyrin (T) has been functionalized with a β-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 λex = 340 nm, the fluorescence spectroscopy experiments indicate in all the studied solvents, an efficient quenching of the pyrene emission. When excited at either λex = 340 nm or λex = 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 λex = 425 nm, the fs transient absorption analysis shows two different intermediate species (~ 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 v(T-P)∗state, with a lifetime of 80-100 ps.

**General information**

State: Published

Ministry of Education publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Tampere University of Technology, Research group: Supramolecular photochemistry, Frontier Photonics, Inorganic and Physical Chemistry Division, CSIR-Indian Institute of Chemical Technology

Authors: Reeta, P. S., Khetubol, A., Jella, T., Chukharev, V., Abou-Chahine, F., Tkachenko, N. V., Giribabu, L., Lemmetyinen, H.

Keywords: (fs transient absorption, kinetics, optical properties, Sn (IV)tetraphenylporphyrin, β-vinyl pyrene donor)

Number of pages: 13

Pages: 288-300

Publication date: 1 Jan 2015

Peer-reviewed: Yes

ASJC Scopus subject areas: Chemistry(all)

**Publication information**

Journal: Journal of Porphyrins and Phthalocyanines

Volume: 19

Issue number: 1-3

ISSN (Print): 1088-4246

Ratings:

Publication Forum (2017): 1

Scopus rating (2016): 0.354 0.379

Publication Forum (2016): 1

Scopus rating (2015): 0.419 0.467

Web of Science (2015): 1.087 1.387 7.0 0.323 0.00257 0.267

Publication Forum (2015): 1

Scopus rating (2014): 0.486 0.545

Web of Science (2014): 1.397 1.603 6.7 0.179 0.00338 0.326

Publication Forum (2014): 1

Scopus rating (2013): 0.537 0.602

Publication Forum (2013): 1

Scopus rating (2012): 0.62 0.537

Publication Forum (2012): 1

Scopus rating (2011): 0.553 0.612

Scopus rating (2010): 0.564 0.46

Scopus rating (2009): 0.511 0.447

Scopus rating (2008): 0.572 0.481

Scopus rating (2007): 0.669 0.481

Scopus rating (2006): 0.625 0.529

Scopus rating (2005): 0.632 0.593

Scopus rating (2004): 0.646 0.667

Scopus rating (2003): 0.591 0.88

Scopus rating (2002): 0.86 1.153

Scopus rating (2001): 0.796 1.08

Scopus rating (2000): 0.863 0.759

Scopus rating (1999): 0.557 0.635

Original language: English

DOIs:

10.1142/S1088424615500108

Links:

http://www.scopus.com/inward/record.url?scp=84928483683&partnerID=8YFLogxK (Link to publication in Scopus)

Source: Scopus

Source-ID: 84928483683

Research output: Scientific - peer-review › Article
Branched thiophene oligomer/polymer bulk heterojunction organic solar cell

Thiophene small novel branched structures have been proposed as candidates for dopant agents transporting holes-electron in organic solar cell (OSC). Low-band gap of these branched oligothiophene have been obtained to be used in organic solar cells. Two branched thiophene oligomers, a sexithienylene vinylene (E)-Bis-l,2-(5,5‴-Dimethyl-(2,2′:3′,2″-terthiophene) vinylene ,(BSTV) and octathienylene vinylene (BOTV) (E)-Bis-l,2-(5,5‴-Dimethyl- (2,2′:5′,2″:3′,2‴-tetraphthalothiophene) vinylene oligomers, have been synthesized and used as electron donor or dopant in a bulk heterojunction poly(3-hexylthiophene) (P3HT), /[6,6]-phenyl C61-butyric acid methylester (PCBM), Organic Photovoltaic cell.

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Universidad de Chile
Authors: Martinez, F., Neculqueo, G., Vasquez, S. O., Lemmetyinen, H., Efimov, A., Vivo, P.
Number of pages: 7
Pages: 19-25
Publication date: 2015

Host publication information
Title of host publication: Materials Research Society Symposium Proceedings
Volume: 1737
Publisher: MATERIALS RESEARCH SOCIETY
ISBN (Print): 9781510806177
ASJC Scopus subject areas: Materials Science(all), Condensed Matter Physics, Mechanical Engineering, Mechanics of Materials
DOIs:
10.1557/opl.2015.529
Links:
http://www.scopus.com/inward/record.url?scp=84938866855&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source-ID: 84938866855
Research output: Scientific - peer-review › Conference contribution

Combination of a novel electrode material and artificial mediators to enhance power generation in an MFC

This study focuses on two main aspects: developing a novel cost-effective electrode material and power production from domestic wastewater using three different mediators. Methylene blue (MB), neutral red (NR) and 2-hydroxy-1,4-naphthoquinone (HNQ) were selected as electrode mediators with different concentrations. A tin-coated copper mesh electrode was tested as anode electrode. Maximum power density of the microbial fuel cell (MFC) with 300 μM MB was 636 mW/m². Optimal mediator concentrations with respect to the achieved maximum power output for MB, NR and HNQ were 300 μM, 200 μM and 50 μM, respectively. The results demonstrate that tin-coated copper mesh showed a higher biocompatibility and electrical conductivity.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Firat University
Authors: Taskan, E., Özkaya, B., Hasar, H.
Keywords: (Internal resistance, Mediator, Microbial fuel cell, Power output)
Number of pages: 9
Pages: 320-328
Publication date: 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Environmental Engineering, Water Science and Technology

Publication information
Journal: Water Science and Technology
Volume: 71
Issue number: 3
ISSN (Print): 0273-1223
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.394 0.621
Fe₂O₃-TiO₂ Nano-heterostructure Photoanodes for Highly Efficient Solar Water Oxidation

Harnessing solar energy for the production of clean hydrogen by photo-electrochemical water splitting represents a very attractive, but challenging approach for sustainable energy generation. In this regard, the fabrication of Fe₂O₃-TiO₂ photoanodes is reported, showing attractive performances [≈2.0 mA cm⁻² at 1.23 V vs. the reversible hydrogen electrode in 1 M NaOH] under simulated one-sun illumination. This goal, corresponding to a tenfold photoactivity enhancement with respect to bare Fe₂O₃, is achieved by atomic layer deposition of TiO₂ over hematite (α-Fe₂O₃) nanostructures fabricated by plasma enhanced-chemical vapor deposition and final annealing at 650 °C. The adopted approach enables an intimate Fe₂O₃-TiO₂ coupling, resulting in an electronic interplay at the Fe₂O₃/TiO₂ interface. The reasons for the photocurrent enhancement determined by TiO₂ overlayers with increasing thickness are unraveled by a detailed chemico-physical investigation, as well as by the study of photo-generated charge carrier dynamics. Transient absorption spectroscopy shows that the increased photoelectrochemical response of heterostructured photoanodes compared to bare hematite is due to an enhanced separation of photogenerated charge carriers and more favorable hole dynamics for water oxidation. The stable responses obtained even in simulated seawater provides a feasible route in view of the eventual large-scale generation of renewable energy.

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Halogen-bonded photoresponsive materials
The aim of the present review is to illustrate to the reader the state of the art on the construction of supramolecular azobenzene-containing materials formed by halogen bonding. These materials include several examples of polymeric, liquid crystalline or crystalline species whose performances are either superior to the corresponding performances of their hydrogen-bonded analogues or simply distinctive of the halogen-bonded species.

General information
State: Published
Ministry of Education publication type: A3 Part of a book or another research book
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, VTT Technical Research Centre of Finland, Politecnico di Milano, Aalto University
Authors: Saccone, M., Cavallo, G., Metrangolo, P., Resnati, G., Priimägi, A.
Keywords: (Azobenzene, Halogen bonding, Liquid crystals, Photoresponsive materials, Polymers)
Number of pages: 20
Pages: 147-166
Publication date: 2015
Host publication information
Title of host publication: Halogen Bonding II : Impact on Materials Chemistry and Life Sciences
Publisher: Springer International Publishing
ISBN (Print): 978-3-319-15731-3
ISBN (Electronic): 978-3-319-15732-0
ASJC Scopus subject areas: Chemistry(all)
Publication series
Name: Topics in Current Chemistry
Volume: 359
ISSN (Print): 0340-1022
DOIs:
10.1007/128_2014_615
Links:
http://www.scopus.com/inward/record.url?scp=84930627375&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note
JUFOID=68510
Source: Scopus
Source-ID: 84930627375
Halogen bonding enhances nonlinear optical response in poled supramolecular polymers

We demonstrate that halogen bonding strongly enhances the nonlinear optical response of poled supramolecular polymer systems. We compare three nonlinear optical chromophores with similar electronic structures but different bond-donating units, and show that both the type and the strength of the noncovalent interaction between the chromophores and the polymer matrix play their own distinctive roles in the optical nonlinearity of the systems.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research area: Optics, Research group: Nonlinear Optics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Tampere Univ Technol, Tampere University of Technology, Dept Phys, Univ Milan, Consiglio Nazionale delle Ricerche (CNR), University of Milan, Inst Mol Sci & Technol, CNR, ISTM, Politecn Milan, Polytechnic University of Milan, NFMLab, DCMIC Giulio Natta, Aalto University
Authors: Virkki, M., Tuominen, O., Forni, A., Saccone, M., Metrangolo, P., Resnati, G., Kauranen, M., Priimägi, A.
Keywords: (FILMS)
Number of pages: 4
Pages: 3003-3006
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Chemistry C
Volume: 3
ISSN (Print): 2050-7534
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.806 1.28
Publication Forum (2016): 1
Scopus rating (2015): 1.751 1.577
Web of Science (2015): 5.066 5.076 1.8 1.2 0.03679 1.119
Publication Forum (2015): 1
Scopus rating (2014): 1.505 1.36
Web of Science (2014): 4.696 4.701 1.3 1.139 0.01525 1.006
Publication Forum (2014): 3
Publication Forum (2013): 3
Original language: English
DOIs:
10.1039/c5tc00484e

Bibliographical note
AUX=orc,"Tuominen, Ossi"
ORG=fys,0.5
ORG=keb,0.5
Source: WOS
Source-ID: 000351601200002
Research output: Scientific - peer-review › Article

Microvesicle- and exosome-mediated drug delivery enhances the cytotoxicity of Paclitaxel in autologous prostate cancer cells

Background Extracellular vesicles (EVs) are naturally occurring membrane particles that mediate intercellular communication by delivering molecular information between cells. In this study, we investigated the effectiveness of two different populations of EVs (microvesicle- and exosome-enriched) as carriers of Paclitaxel to autologous prostate cancer cells. Methods EVs were isolated from LNCaP- and PC-3 prostate cancer cell cultures using differential centrifugation and characterized by electron microscopy, nanoparticle tracking analysis, and Western blot. The uptake of microvesicles and exosomes by the autologous prostate cancer cells was assessed by flow cytometry and confocal microscopy. The EVs were loaded with Paclitaxel and the effectiveness of EV-mediated drug delivery was assessed with viability assays. The distribution of EVs and EV-delivered Paclitaxel in cells was inspected by confocal microscopy. Results Our main finding was that the loading of Paclitaxel to autologous prostate cancer cell-derived EVs increased its cytotoxic effect. This capacity was independent of the EV population and the cell line tested. Although the EVs without the drug increased cancer cell viability, the net effect of enhanced cytotoxicity remained. Both EV populations delivered Paclitaxel to the
recipient cells through endocytosis, leading to the release of the drug from within the cells. The removal of EV surface proteins did not affect exosomes, while the drug delivery mediated by microvesicles was partially inhibited. Conclusions Cancer cell-derived EVs can be used as effective carriers of Paclitaxel to their parental cells, bringing the drug into the cells through an endocytic pathway and increasing its cytotoxicity. However, due to the increased cell viability, the use of cancer cell-derived EVs must be further investigated before any clinical applications can be designed.

**General information**

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Saari, H., Lázaro-Ibáñez, E., Viitala, T., Vuorimaa-Laukkanen, E., Siljander, P., Yliperttula, M.
Keywords: (Extracellular vesicles, Microvesicles, Exosomes, Paclitaxel, Drug delivery, Prostate cancer)
Number of pages: 11
Pages: 727-737
Publication date: 2015
Peer-reviewed: Yes

**Publication information**

Journal: Journal of Controlled Release
Volume: 220
ISSN (Print): 0168-3659
Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 2.393 1.84
Publication Forum (2016): 3
Scopus rating (2015): 2.725 2.08
Web of Science (2015): 7.441 8.407 6.9 1.33 0.05686 1.857
Scopus rating (2014): 2.416 2.092
Web of Science (2014): 7.705 8.097 7.0 1.138 0.05251 1.792
Publication Forum (2014): 2
Scopus rating (2013): 2.416 2.044
Publication Forum (2013): 2
Scopus rating (2012): 2.417 2.061
Publication Forum (2012): 2
Scopus rating (2011): 2.745 2.098
Scopus rating (2010): 3.194 2.306
Scopus rating (2009): 2.897 2.033
Scopus rating (2008): 2.25 1.886
Scopus rating (2007): 2.149 1.82
Scopus rating (2006): 1.771 1.779
Scopus rating (2005): 1.552 1.81
Scopus rating (2004): 1.475 1.778
Scopus rating (2003): 1.592 1.682
Scopus rating (2002): 1.393 1.534
Scopus rating (2001): 1.275 1.361
Scopus rating (2000): 1.067 1.384
Scopus rating (1999): 1.046 1.298
Original language: English
DOIs: 10.1016/j.jconrel.2015.09.031
Source: RIS
Source-ID: urn:1C9EE295CF4CF9BEC0AB245055AF777
Research output: Scientific - peer-review › Article

**Nano-graphite cold cathodes for electric solar wind sail**

**General information**
Role of the bridge in photoinduced electron transfer in porphyrin-fullerene dyads

The role of π-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-C₆₀ (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-C₆₀, introduces an additional 3,4-ethylenedioxythiophenylvinylene (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; 2) increased energy gap for through-bond electron transfer.
states; and 2) the disappearance of the intramolecular exciplex, which mediates photoinduced charge separation in the ZnP-Ph-C_{60} 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**

State: Published

Ministry of Education 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


Keywords: (Conjugated bridge, EDOT, Electron transfer, Fullerene, Porphyrin)

Number of pages: 12

Pages: 5814-5825

Publication date: 2015

Peer-reviewed: Yes

ASJC Scopus subject areas: Chemistry(all)

**Publication information**

Journal: Chemistry: A European Journal

Volume: 21

Issue number: 15

ISSN (Print): 0947-6539

Ratings:

Publication Forum (2017): 2

Scopus rating (2016): 2.247 1.046

Publication Forum (2016): 2

Scopus rating (2015): 2.416 1.184

Web of Science (2015): 5.771 5.572 4.6 1.338 0.19837 1.407

Publication Forum (2015): 2

Scopus rating (2014): 2.487 1.219

Web of Science (2014): 5.731 5.635 4.4 1.255 0.19743 1.433

Publication Forum (2014): 3

Scopus rating (2013): 2.604 1.239

Publication Forum (2013): 3

Scopus rating (2012): 2.884 1.294

Publication Forum (2012): 3

Scopus rating (2011): 2.726 1.336

Scopus rating (2010): 2.527 1.292

Scopus rating (2009): 2.499 1.365


Scopus rating (2007): 3.233 1.532

Scopus rating (2006): 2.911 1.505

Scopus rating (2005): 2.62 1.454

Scopus rating (2004): 2.32 1.472

Scopus rating (2003): 2.156 1.45


Scopus rating (2001): 2.834 1.612

Scopus rating (2000): 2.956 1.652

Scopus rating (1999): 3.013 1.73

Original language: English

DOIs:

10.1002/chem.201406514

Links:

http://www.scopus.com/inward/record.url?scp=84923917540&partnerID=8YFLogxK (Link to publication in Scopus)

Source: Scopus

Source-ID: 84923917540

Research output: Scientific - peer-review › Article
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-CH2CN and-CH2CO2Et 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 eukary-otic cells.

General information
State: Published
Ministry of Education 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
Keywords: (Cyclization, Fluorescence, Heterocycles, Pyrenes, Quinolines)
Number of pages: 6
Pages: 553-558
Publication date: 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Chemistry(all)

Publication information
Journal: Chemistry - An Asian Journal
Volume: 10
Issue number: 3
ISSN (Print): 1861-4728
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.584 0.773
Publication Forum (2016): 1
Scopus rating (2015): 1.766 0.911
Web of Science (2015): 4.592 4.28 3.7 1.202 0.0285 1.025
Publication Forum (2015): 1
Scopus rating (2014): 1.762 0.974
Web of Science (2014): 4.587 4.588 3.4 1.269 0.0282 1.106
Publication Forum (2014): 2
Scopus rating (2013): 1.767 0.872
Publication Forum (2013): 2
Scopus rating (2012): 2.267 1.026
Publication Forum (2012): 2
Scopus rating (2011): 2.31 1.017
Scopus rating (2010): 2.259 1.014
Scopus rating (2009): 2.372 1.019
Scopus rating (2008): 2.57 1.153
Scopus rating (2007): 1.566 0.669
Original language: English
DOIs: 10.1002/asia.201403339
Links:
http://www.scopus.com/inward/record.url?scp=84923364824&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source-ID: 84923364824
Research output: Scientific - peer-review › Article
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-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-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 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 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, C$_{60}$ can withdraw electrons from porphyrin if it is sufficiently close.

General information
State: Published
Ministry of Education 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
Authors: Karilainen, T., Cramariuc, O., Kuisma, M., Tappura, K., Hukka, T. I.
Keywords: (Car-Parrinello molecular dynamics, Fullerene, Porphyrin, Time-dependent-density functional theory)
Number of pages: 10
Pages: 612-621
Publication date: 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Chemistry(all), Computational Mathematics

Publication information
Journal: Journal of Computational Chemistry
Volume: 36
Issue number: 9
ISSN (Print): 0192-8651
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.428 1.297
Publication Forum (2016): 1
Web of Science (2015): 3.648 4.648 >10.0 1.013 0.02989 1.418
Publication Forum (2015): 1
Scopus rating (2014): 1.489 1.451
Web of Science (2014): 3.589 4.879 >10.0 0.909 0.03361 1.487
Publication Forum (2014): 2
Scopus rating (2013): 1.449 1.516
Publication Forum (2013): 2
Scopus rating (2012): 1.874 1.64
Publication Forum (2012): 2
Scopus rating (2011): 1.834 1.611
Scopus rating (2010): 1.745 1.366
Scopus rating (2009): 1.859 1.208
Scopus rating (2008): 2.482 1.655
Scopus rating (2007): 2.789 1.794
Scopus rating (2006): 2.201 1.561
Scopus rating (2005): 1.912 1.373
Scopus rating (2004): 1.695 1.321
Scopus rating (2003): 1.666 1.402
Scopus rating (2001): 1.711 1.237
π-Expanded α,β-unsaturated ketones: Synthesis, optical properties, and two-photon-induced polymerization

A library of π-expanded α,β-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-π-A-π-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.
Monoisomeric phthalocyanine-fullerene dyads with e- and cis-3 addition pattern; synthesis, modeling, photovoltage and solar cell experiments

Synthesis and characterization of two A(2)B(2)-type monoisomeric phthalocyanines and phthalocyanine-fullerene (Pc-C60) dyads, in which fullerene is regioselectively attached to phthalocyanine with two linkers, are described. H-1 NMR spectroscopy results clearly indicate an e addition pattern of the fullerene moiety in trans-dyad 9, and apparently a cis-3 addition pattern in cis-dyad 10. The possible spatial arrangements of 9 and 10 were further examined by molecular modeling. The dyads have polar (-OH) side chains on the fullerene side of the dyad providing a possibility to produce oriented donor-acceptor (D-A) Langmuir monolayers on aqueous subphase, which can be shifted onto a solid surface. When deposited on a solid electrode material, parallel vertical alignment of the phthalocyanine and fullerene moieties in 100% dyad monolayer was obtained and vertical electron transfer from Pc to C60 upon photoexcitation was demonstrated. Introduction of the dyads as an oriented interfacial monolayer between the photoactive layer and metal anode improved the power conversion efficiency in inverted organic solar cells.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Tampere Univ Technol, Tampere University of Technology, Dept Chem & Bioengn
Authors: Ranta, J., Niskanen, M., Kaunisto, K., Manninen, V., Mundy, M. E., Virkki, K., Hakola, H., Hukka, T. I., Lemmetyinen, H.
Keywords: (phthalocyanine, phthalocyanine-fullerene dyad, photovoltage, molecular modeling, solar cell, Langmuir-Schafer, PHOTOINDUCED ELECTRON-TRANSFER, MOLECULAR-FORCE FIELD, PORPHYRIN-FULLERENE, CHARGE SEPARATION, DENSITY, MMFF94, C-60, BISADDUCTS, ISOMERS, FILMS)
Number of pages: 17
Pages: 1108-1124
Publication date: Dec 2014
Peer-reviewed: Yes

Publication Information
Journal: Journal of Porphyrins and Phthalocyanines
Volume: 18
Issue number: 12
ISSN (Print): 1088-4246
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.354 0.379
Publication Forum (2016): 1
Photochemistry of self-assembled donor-acceptor architectures for photoactive supramolecular devices

Supramolecular donor-acceptor assemblies were prepared and studied with spectroscopic methods. The two main objectives of this work were: (i) fundamental study of photoinduced energy and electron transfer processes in self-assembled supramolecular donor-acceptor complexes in solutions and (ii) self-assembly and photophysical characterization of donor-acceptor films on titanium dioxide (TiO2) surface. The study of these systems aims to develop more complex architectures for artificial photosynthesis and understand factors that affect efficiency of the photoinduced energy and electron transfer processes in natural and artificial photosynthesis. This knowledge can be used for building photoactive molecular devices such as organic solar cells. The singlet excited state energy transfer in dyads formed via axial metal–ligand coordination of free-base porphyrin to metal (Mg, Ru) complexes of phthalocyanine was observed. The position of imidazole linker group on one of the meso-aryl groups of the free-base porphyrin was used to tune the rates of energy transfer. The two-point binding provides better control over complex geometry and it was implemented utilizing metal-ligand and crown-ether coordination in zinc chlorin– fullerene supramolecular dyads. This approach allowed to increase the binding efficiency and achieve a well-defined mutual orientation between the moieties. The electron transfer rate was found to depend on the donor-acceptor distance as well as the mutual orientation of the entities and could be manipulated by changing positions of binding groups. The donor-acceptor layers were assembled on TiO2 using two methods. First, a layer of covalently linked porphyrin-phthalocyanine dyads was formed on TiO2 via supramolecular approach. Then, a new method was developed to construct donor-acceptor two-layer films using separate porphyrin and fullerene molecules. In both cases, photo-excitation of donor molecules resulted in charge-separation (CS) inside the organic layer and sequential electron transfer towards the TiO2. Furthermore, the charge recombination (CR) process was found to be slower than for systems sensitized with single chromophores.
Molecular modifications of active and anode buffer layers of bulk heterojunction solar cell

In this work, new photoactive materials were tested in the active and anode buffer layers of the inverted ITO(ZnO)donor:PC60/70BM|Buffer|Au/Ag organic bulk heterojunction (BHJ) solar cell. The molecular properties of the materials synthesized for this work were designed in order to improve the efficiency of the inverted solar cell structure. In addition to testing the materials in the cells, their effect on the cell function was investigated. The work aimed to understand the effects of the studied buffer and active layer materials in the cell function and photovoltaic performance. Organometallic n-type tris-(8-hydroxyquinoline)aluminum (Alq3) derivatives, p-type aryl end-capped quaterthiophenes, and a combined p- and n-type Alq3 end-capped hexathiophene were tested as hole transporting anode buffer layer materials. As the various different materials provided a diverse buffer material selection, the properties of the materials for improved cell function were investigated by spectroscopic, electrochemical, computational and thermoanalytical methods. The studied Alq3 derivatives have electron donating amino substituents, either piperidine, pyrrolidine or morpholine rings, on the 5-position of the 8-hydroxyquinoline ligands, which ease the oxidation of the complexes and elevate the highest occupied molecular orbital (HOMO) energy levels. The higher HOMO levels of the derivatives, compared to that of Alq3, reduce the hole extraction barrier in the cell. Therefore, the cells with the derivatives as buffer layers had a higher short circuit current (Isc) compared to that with Alq3. Simultaneously, due to higher hole injection barrier, the cells with the derivatives as buffer layers had lower open circuit voltage (Voc) than the cell with Alq3. The derivative with the morpholine ring has ideal energy levels with respect to the created energy barriers. Thus, the cell with the morpholine derivative as buffer layer performed better than the cell with Alq3. The quaterthiophenes studied in this work have cyanophenyl or methoxyphenyl end-groups and methyl or hexyl side chains attached to the thiophene backbone. These structural differences affect their electronic distribution, absorption profile, energy levels and molecular packing, especially in the solid state. The use of p-cyano end-capped quaterthiophene with hexyl side chains as an anode buffer layer resulted in a better cell power conversion efficiency compared to that with Alq3. The use of the Alq3 end-capped hexathiophene as an anode buffer layer decreased the cell serial resistance (Rs) and increased Isc. Photoinduced reactions, such as energy or electron transfer, between the Alq3 or aryl end-capped oligothiophene buffer materials and photoactive layer partly explain the improved Isc. A synthesized benzodithiophene-benzotriazole donor-acceptor (D-A) copolymer was compared as donor material with three previously studied fluorine-benzotriazole D-A copolymers. The relation between donor polymer structural properties and photovoltaic performance was studied by combining computational and experimental methods. The cell with the benzodithiophene-benzotriazole copolymer as donor material had better efficiency than the cells with the fluorine-benzotriazole copolymers. Calculations on the molecular geometry, energy levels, molecular orbitals, and lowest energy excitations provided an additional perspective to understand the polymer’s function as donor material. Based on the calculations, the benzodithiophene-benzotriazole copolymer had a more planar backbone, continuous LUMO electron density, longer conjugation and better exciton and charge transport properties compared to those of the fluorine-benzotriazole copolymers. Bulky side groups in the fluorine-benzotriazole copolymers caused steric hindrance and twisting or bending of the backbone. As a result, the electron density concentrates in parts of the polymer structure and π-conjugation weakens or is broken. As the delocalization does not cover the whole polymer structure, excitons or charges are trapped in the gaps of the discontinuous molecular orbitals. Alq3, aryl and 8-phenoxyquinoline end-capped oligothiophenes were used as dopant materials in the P3HT:PC60BM BHJ photoactive layer. In the ternary blend of the dopant, P3HT and PC60BM molecules, intermolecular interactions are likely as the molecules are in close proximity in the solid photoactive layer. The effect of dopant molecules on the cell function was studied by solar cell experiments. To investigate the intermolecular interaction of the dopant molecules with the active layer components, P3HT donor and PC60BM acceptor, steady state and time resolved spectroscopic measurements were carried out in chloroform solutions.
Based on the measurements, Alq3 end-capped hexathiophene donates an electron to PC60BM. Photoinduced energy transfer was observed between the cyanophenyl end-capped quaterthiophene and PC60BM. The cell absorption increases with doping. Thus, dopant molecules function as additional light absorbers in the photoactive layer. After excitation, the dopant molecules transfer electrons or energy to PC60BM, which increases the cell Isc and power conversion efficiency. When a cyanophenyl end-capped oligothiophene with diketopyrrolopyrrole (DPP) core was used as dopant, the cell emission decreased. DPP-group inclusion broadens the dopant absorption to the near IR-region. Therefore, the absorption of the dopant overlaps with P3HT emission and the dopant molecules can reabsorb the light emitted by P3HT. In this case, the cell Isc and power conversion efficiency increased further.

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Ministry of Education publication type: G5 Doctoral dissertation (article)
Organisations: Department of Chemistry and Bioengineering
Authors: Manninen, V.
Publication date: 23 May 2014

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Publisher: Tampere University of Technology
Volume: 1214
ISSN (Print): 1459-2045
ISSN (Electronic): 1459-2045
Electronic versions: manninen.pdf
Links:

Bibliographical note
Awarding institution:Tampere University of Technology
Source: researchoutputwizard
Source-ID: 1024
Research output: Collection of articles > Doctoral Thesis

Binding Affinity and Mechanism of Polymer-DNA Polyplexes for Gene Delivery
The mechanism of polyethylenimine−DNA, poly(L-lysine)−DNA, peptide−DNA, and PBAE−DNA complex formation was studied by a time-resolved spectroscopic method. The data were analysed by a cooperative model for multivalent ligand binding to multisubunit substrate. The formation of polyplexes with polyethylenimines, poly(L-lysine) and peptide (KK)₂KGGC is observed to be positively cooperative and negatively cooperative with PBAEs. Polymers with positive cooperativity reach about 100% saturation in binding DNA, whereas for polymers with negative cooperativity, the saturation level remains at about 80–90%. The type of amine groups (primary, secondary and tertiary) of the polymers has an effect on the binding constants and the degree of cooperativity. The effects of pH, type of amine groups and polymer structure on the mechanism of the polyplex formation were studied with polyethylenimines (PEI) and poly(L-lysine) (PLL). At pH 5.2 and 7.4 for PEIs and PLL, the formation of the polyplex core was observed to be complete at N/P = 2, at which point nearly all DNA phosphate groups were bound by polymer amine groups. At higher N/P ratios, excess polymer binds to the core polyplex, forming a shell over the core. At pH 9.2, the core is formed at higher N/P ratios than at lower pH levels except for PLL, which behaves similarly at all pH levels. The overall cooperative binding constants are higher at pH 5.2 than at 9.2 due to the higher degree of amine group protonation at lower pH levels. The ionic strength and pH affect the binding mechanism with peptide (KK)₂KGGC polyplexes, but changing the buffer does not. Molecular weight shows a clear effect on the mechanism and efficiency of the polyplex formation: for the high-molecular weight polymers (BPEI and PLL), the saturation level is reached at lower N/P ratios than for low-molecular weight polymers (SPEI and peptide). In the absence of excess PEI, the transgene expression levels are lower than in the presence of it. However, the fluorescence properties of the polyplexes in the absence and the presence of excess PEI are similar. Hence, the original structure of the polyplex core is retained during the shell formation. The molecular structures of the poly(β-amino ester)s (PBAEs) can be modified in a controlled way with the accuracy of single carbon unit. The effect of very small changes in the polymer structure on the formation of the polyplexes was studied by changing the length of the backbone and the side chain, by adding end caps to the polymers and by changing the molecular weight of the polymers. For PBAEs without end caps, the highest saturation levels and overall binding constants were observed for the linear backbones and side chains when the number of carbons was four or five, respectively. The end-capping of PBAEs increases the amine density and the efficiency of polyplex formation, which is observed as higher saturation levels for the end-capped PBAEs. The presence of an OH-group in the end cap induces a change in the binding mechanism. The length of the backbone and the side chain
of PBAEs were observed to be important via amine density, hydrophobicity and steric hindrance to the complex formation. High-molecular weight PBAEs formed polyplexes more effectively than smaller ones.

**Are two azo groups better than one? Investigating the photoresponse of polymer-bisazobenzene complexes**

**General information**
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Authors: Vapaavuori, J., Goulet-Hanssens, A., Heikkinen, I. T., Barrett, C. J., Priimägi, A.
Number of pages: 8
Pages: 5089-5096
Publication date: 2014
Peer-reviewed: Yes

**Publication information**
Journal: Chemistry of Materials
Volume: 26
Issue number: 17
ISSN (Print): 0897-4756
Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 4.114 1.905
Publication Forum (2016): 3
Scopus rating (2015): 4.038 2.102
Web of Science (2015): 9.407 9.363 7.5 1.737 0.12692 2.376
Scopus rating (2014): 3.603 2.253
Web of Science (2014): 8.354 9.21 7.3 2.078 0.12128 2.2
Publication Forum (2014): 3
Scopus rating (2013): 3.658 2.277
Publication Forum (2013): 3
Scopus rating (2012): 4.169 2.264
Charge-Transfer Dynamics in Poly(3-hexylthiophene):Perylenedimid-C-60 Blend Films Studied by Ultrafast Transient Absorption

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Number of pages: 6
Pages: 10625-10630
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 118
Issue number: 20
ISSN (Print): 1932-7447
Ratings:
- Publication Forum (2017): 1
- Scopus rating (2016): 1.948 1.181
- Publication Forum (2016): 1
- Scopus rating (2015): 1.917 1.268
- Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
- Publication Forum (2015): 1
- Scopus rating (2014): 2.027 1.448
- Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
- Publication Forum (2014): 3
- Scopus rating (2013): 2.134 1.439
- Publication Forum (2013): 3
- Scopus rating (2012): 2.514 1.46
- Publication Forum (2012): 3
Deprotonation of resorcinarenes by mono- and diamine bases: complexation and intermolecular interactions in the solid state

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Beyeh, N. K., Valkonen, A., Rissanen, K.
Number of pages: 7
Pages: 3758-3764
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: CrystEngComm
Volume: 16
Issue number: 18
ISSN (Print): 1466-8033
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.043 0.904
Publication Forum (2016): 1
Scopus rating (2015): 1.063 0.999
Web of Science (2015): 3.849 3.801 3.4 0.928 0.05518 0.67
Publication Forum (2015): 1
Scopus rating (2014): 1.131 1.11
Web of Science (2014): 4.034 4.022 3.0 0.988 0.05187 0.717
Publication Forum (2014): 2
Scopus rating (2013): 1.079 1.11
Publication Forum (2013): 2
Scopus rating (2012): 1.253 1.142
Publication Forum (2012): 2
Scopus rating (2011): 1.174 1.191
Scopus rating (2010): 1.233 1.229
Scopus rating (2009): 1.227 1.257
Scopus rating (2008): 1.297 1.183
Scopus rating (2007): 1.42 1.704
Scopus rating (2005): 1.419 1.051
Scopus rating (2004): 1.0 0.951
Scopus rating (2003): 0.73 0.751
Scopus rating (2002): 0.228 0.509
Scopus rating (2001): 0.138 0.153
Dynamics of time-resolved photoluminescence in GaInNAs and GaNAsSb solar cells

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Optoelectronics Research Centre, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Gubanov, A., Polojärvi, V., Aho, A., Tukiainen, A., Tkachenko, N. V., Guina, M.
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Nanoscale Research Letters
Volume: 9
Article number: 80
ISSN (Print): 1931-7573
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.589 0.746
Publication Forum (2016): 1
Scopus rating (2015): 0.538 0.653
Web of Science (2015): 2.584 2.85 3.8 0.391 0.02704 0.644
Publication Forum (2015): 1
Scopus rating (2014): 0.748 1.019
Web of Science (2014): 2.779 3.008 3.3 0.324 0.02502 0.677
Publication Forum (2014): 1
Scopus rating (2013): 0.79 0.967
Publication Forum (2013): 1
Scopus rating (2012): 1.049 1.073
Publication Forum (2012): 1
Scopus rating (2011): 1.04 1.124
Scopus rating (2010): 1.062 1.007
Scopus rating (2009): 1.063 1.01
Scopus rating (2008): 0.828 0.632
Scopus rating (2007): 1.458 0.71
Original language: English
DOIs:
10.1039/c3ce42291g

Bibliographical note
Contribution: organisation=orc,FACT1=0.7<br/>Contribution: organisation=keb,FACT2=0.3<br/>Portfolio EDEND: 2014-04-29<br/>Publisher name: SpringerOpen
Source: researchoutputwizard
Source-ID: 371
Research output: Scientific - peer-review › Article

Effect of mutual position of electron donor and acceptor on photoinduced electron transfer in supramolecular chlorophyll-fullerene dyads
Formation of a stable polymer blue phase under UV irradiation of Langmuir-Schaefer films of dl-n N-arylcarbamate derivative

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Alekseev, A., Domnin, I., Ivanov, A., Vuorimaa-Laukkanen, E., Lemmetyinen, H., Tereshchenko, N.
Number of pages: 5
Pages: 160-164
Publication date: 2014
Peer-reviewed: Yes

Publication information
High-modulation-depth surface relief gratings using s-s polarization configuration in supramolecular polymer-azobenzene complexes

**General information**
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Authors: Sobolewska, A., Bartkiewicz, S., Priimagi, A.
Number of pages: 6
Pages: 23279-23284
Publication date: 2014
Peer-reviewed: Yes

**Publication information**
Journal: Journal of Physical Chemistry C
Volume: 118
Issue number: 40
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Scopus rating (2014): 2.027 1.448
Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
Publication Forum (2014): 3
Light-driven surface patterning of supramolecular polymers with extremely low concentration of photoactive molecules

Modeling of photoactive conjugated donor-acceptor copolymers: the effect of the exact HF exchange in DFT functionals on geometries and gap energies of oligomer and periodic models
Monoisomeric phthalocyanines and phthalocyanine-fullerene dyads with polar side chains: synthesis, modeling, and photovoltage

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Niskanen, M., Hukka, T.
Number of pages: 12
Pages: 13294-13305
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 16
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
Publication Forum (2016): 1
Scopus rating (2015): 1.771 1.244
Web of Science (2015): 4.449 4.273 4.1 1.017 0.19255 1.158
Publication Forum (2015): 1
Scopus rating (2014): 1.772 1.253
Web of Science (2014): 4.493 4.219 3.9 0.991 0.17937 1.209
Publication Forum (2014): 3
Scopus rating (2013): 1.715 1.216
Publication Forum (2013): 3
Scopus rating (2012): 1.916 1.184
Publication Forum (2012): 3
Scopus rating (2011): 1.697 1.203
Scopus rating (2010): 1.802 1.196
Scopus rating (2009): 2.127 1.369
Scopus rating (2008): 2.158 1.211
Scopus rating (2007): 1.84 1.138
Scopus rating (2006): 1.467 1.128
Scopus rating (2005): 1.389 1.104
Scopus rating (2004): 1.173 1.007
Scopus rating (2003): 1.093 0.925
Scopus rating (2002): 1.122 0.973
Scopus rating (2001): 1.09 0.914
Scopus rating (2000): 0.948 1.068
Scopus rating (1999): 0.121 0.0
Original language: English
DOIs:
10.1039/c4cp01165a
Additional files:
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Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-06-27<br/>Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 1150
Research output: Scientific - peer-review › Article

Monoisomeric phthalocyanines and phthalocyanine-fullerene dyads with polar side chains: synthesis, modeling, and photovoltage
Photo-induced electron transfer at nanostructured semiconductor-zinc porphyrin interface
Scopus rating (2016): 0.726 0.721
Publication Forum (2016): 1
Scopus rating (2015): 0.733 0.747
Web of Science (2015): 1.86 1.839 >10.0 0.493 0.03583 0.499
Publication Forum (2015): 1
Scopus rating (2014): 0.757 0.773
Web of Science (2014): 1.897 1.963 >10.0 0.475 0.04458 0.565
Publication Forum (2014): 2
Scopus rating (2013): 0.856 0.844
Publication Forum (2013): 2
Scopus rating (2012): 1.101 0.916
Publication Forum (2012): 2
Scopus rating (2011): 1.156 1.013
Scopus rating (2010): 1.207 0.94
Scopus rating (2009): 1.234 0.972
Scopus rating (2008): 1.296 0.937
Scopus rating (2007): 1.43 1.001
Scopus rating (2005): 1.503 1.086
Scopus rating (2004): 1.512 1.129
Scopus rating (2003): 1.556 1.156
Scopus rating (2002): 1.694 1.095
Scopus rating (2001): 1.706 1.102
Scopus rating (2000): 1.774 1.07
Scopus rating (1999): 1.4 1.0
Original language: English
DOIs:
10.1016/j.cplett.2013.11.028

Recognition of N-Alkyl and N-Aryl acetamides by N-Alkyl ammonium resorcinarene chlorides

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Beyeh, N. K., Ala-Korpi, A., Cetina, M., Valkonen, A., Rissanen, K.
Number of pages: 7
Pages: 15144-15150
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Chemistry: A European Journal
Volume: 20
Issue number: 46
ISSN (Print): 0947-6539
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.247 1.046
Publication Forum (2016): 2
Scopus rating (2015): 2.416 1.184
ROFRET: A Molecular-Scale Fluorescent Probe Displaying Viscosity-Enhanced Intramolecular Förster Energy Transfer

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Bai, S., Benniston, A. C., Whittle, V. L., Lemmetyinen, H., Tkachenko, N. V.
Number of pages: 8
Pages: 3089-3096
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: ChemPhysChem
Volume: 115
Issue number: 14
ISSN (Print): 1439-4235
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.264 0.771
Publication Forum (2016): 1
Scopus rating (2015): 1.334 0.912
Web of Science (2015): 3.138 3.13 5.5 0.857 0.0331 0.952
Publication Forum (2015): 1
Slow charge recombination and enhanced photoelectrochemical properties of Diazaporphyrin-Fullerene linked dyad

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Yamamoto, M., Takano, Y., Matano, Y., Stranius, K., Tkachenko, N. V., Lemmetyinen, H., Imahori, H.
Number of pages: 13
Pages: 1808-1820
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 118
Issue number: 4
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Scopus rating (2014): 2.027 1.448
Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
Solid state anion-pi interactions involving polyhalides

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Giese, M., Albrecht, M., Bohnen, C., Repenko, T., Valkonen, A., Rissanen, K.
Number of pages: 8
Pages: 1873-1880
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Dalton Transactions
Volume: 43
Issue number: 4
ISSN (Print): 1477-9234
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.243 0.931
Publication Forum (2016): 1
Scopus rating (2015): 1.351 1.026
Web of Science (2015): 4.177 4.003 4.5 1.088 0.10237 0.8
Publication Forum (2015): 1
Scopus rating (2014): 1.413 1.085
Web of Science (2014): 4.197 3.982 4.5 1.086 0.1013 0.824
Publication Forum (2014): 3
Scopus rating (2013): 1.436 1.083
Publication Forum (2013): 3
Scopus rating (2012): 1.554 1.001
Publication Forum (2012): 3
Scopus rating (2011): 1.505 1.013
Scopus rating (2010): 1.399 0.875
Scopus rating (2009): 0.928 0.783
Scopus rating (2008): 0.629 0.572
Scopus rating (2007): 0.669 0.539
Scopus rating (2006): 1.084 0.907
Scopus rating (2005): 1.128 0.815
Spectroscopic study of a synthesized Alq3 end-capped oligothiophene applied in organic solar cells

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Number of pages: 10
Pages: 8846-8855
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: RSC Advances
Volume: 4
Issue number: 17
ISSN (Print): 2046-2069
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.875 0.743
Publication Forum (2016): 1
Scopus rating (2015): 0.959 0.837
Web of Science (2015): 3.289 3.485 1.8 0.676 0.13014 0.628
Publication Forum (2015): 1
Scopus rating (2014): 1.144 0.965
Web of Science (2014): 3.84 3.907 1.7 0.597 0.0623 0.747
Publication Forum (2014): 1
Scopus rating (2013): 1.117 0.903
Publication Forum (2013): 1
Scopus rating (2012): 0.863 0.603
Original language: English
DOIs:
10.1039/c3ra47367h

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-09-30<br/>Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 1025
Research output: Scientific - peer-review › Article

Subcellular localization of bacteriophage PRD1 proteins in Escherichia coli

General information
Synthesis and characterization of monoisomeric phthalocyanines, phthalocyanine-fullerene dyads, and phthalocyanine-silicon complexes

General information
State: Published
Ministry of Education publication type: G5 Doctoral dissertation (article)
Organisations: Department of Chemistry and Bioengineering
The effect of diketopyrrolopyrrole (DPP) group inclusion in p-cyanophenyl end-capped oligothiophene used as a dopant in P3HT:PCBM BHJ solar cells
The effect of thiophene substituents of fulleropyrrolidine acceptors on the performance of inverted organic solar cells

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Number of pages: 8
Pages: 193-200
The effects of UV irradiation to polyetheretherketone fibres: Characterization by different techniques

The effects of UV irradiation on polyetheretherketone (PEEK) fibres were investigated in this study. PEEK fibres were manufactured with a melt spinning system and then artificially aged with simulated solar UV light. Fibres were then characterized by mechanical tests, Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), rheology, thermogravimetric analysis (TGA) and scanning electron microscopy (SEM). PEEK, best known for its excellent thermal stability, suffered greatly from the effects of UV irradiation. The low UV stability manifested as embrittlement of the fibres in the mechanical tests, increased crosslinking rate in the rheological tests, formation of carbonyl and hydroxyl groups and changes in the nature of the carbon-hydrogen bonds in the FTIR, diminished thermal properties in TGA, and transverse cracks in the SEM photos. DSC was found to be an inaccurate technique for estimating the degradation level of PEEK fibres, whereas the carbonyl index measured by FTIR was found to be the most convenient technique. © 2014 Elsevier Ltd. All rights reserved.
The Wolff Rearrangement

General information
State: Published
Ministry of Education publication type: A3 Part of a book or another research book
Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio)
Authors: Candeias, N., Trindade, A., Gois, P., Afonso, C.
Number of pages: 48
Pages: 944-991
Publication date: 2014

Host publication information
Title of host publication: Comprehensive Organic Synthesis II (Second Edition)
Place of publication: Oxford
Publisher: Elsevier
ISBN (Print): 978-0-08-097743-0
DOIs:
10.1016/B978-0-08-097742-3.00325-6

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-09-30
Source: researchoutputwizard
Source-ID: 205
Research output: Scientific - peer-review › Article

Ultrafast photophysical processes for Fe(III)-carboxylates

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Pozdnyakov, I. P., Melnikov, A. A., Tkachenko, N., Chekalin, S. V., Lemmetyinen, H., Plyusnin, V. F.
Number of pages: 6
Pages: 17590-17595
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Dalton Transactions
Volume: 43
Issue number: 47
ISSN (Print): 1477-9234
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.243 0.931
Publication Forum (2016): 1
Scopus rating (2015): 1.351 1.026
Web of Science (2015): 4.177 4.003 4.5 1.088 0.10237 0.8
Publication Forum (2015): 1
Scopus rating (2014): 1.413 1.085
Web of Science (2014): 4.197 3.982 4.5 1.086 0.1013 0.824
Publication Forum (2014): 3
Scopus rating (2013): 1.436 1.083
Publication Forum (2013): 3
Scopus rating (2012): 1.554 1.001
Publication Forum (2012): 3
Scopus rating (2011): 1.505 1.013
Scopus rating (2010): 1.399 0.875
Porphyrid 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-(porphyrin-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 π-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 π-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.
Bis(aryl)acenaphthenequinonedilimine substituent effect on the properties and coordination environment of ligands and their bis-chelate AgI complexes

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Papanikolaou, P., Gdaniec, M., Wicher, B., Akrivos, P. D., Tkachenko, N.
Number of pages: 10
Pages: 5196-5205
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: European Journal of Inorganic Chemistry
Volume: 2013
Issue number: 29
ISSN (Print): 1434-1948
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.791 0.633
Publication Forum (2016): 1
Chain processes in the photochemistry of PtIV halide complexes in aqueous solutions

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Glebov, E. M., Kolomeets, A. V., Pozdnyakov, I. P., Grivin, V. P., Plyusnin, V. F., Tkachenko, N. V., Lemmetyinen, H.
Number of pages: 9
Pages: 1540-1548
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Russian Chemical Bulletin
Volume: 62
Issue number: 7
ISSN (Print): 1066-5285
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.241 0.45
Publication Forum (2016): 1
Scopus rating (2015): 0.251 0.428
Charge transfer properties of a donor-acceptor dyad based on an expanded acridinium cation

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Benniston, A. C., He, X., Lemmetyinen, H., Tkachenko, N. V.
Number of pages: 8
Pages: 4995-5002
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: RSC Advances
Volume: 3
Issue number: 15
ISSN (Print): 2046-2069
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.875 0.743
Publication Forum (2016): 1
Scopus rating (2015): 0.959 0.837
Web of Science (2015): 3.289 3.485 1.8 0.676 0.13014 0.628
Chlorophyll tailored 20-trifluoroacetamide and its azacrown derivative as pH sensitive colorimetric sensor probe with response to AcO-, F- and CN- ions

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Authors: Iashin, V., Koso, T. V., Stranius, K., Muuronen, M., Heikkinen, S., Kavakka, J., Tkachenko, N. V., Helaja, J.
Number of pages: 4
Pages: 11485-11488
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: RSC Advances
Volume: 3
Issue number: 29
ISSN (Print): 2046-2069
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.875 0.743
Publication Forum (2016): 1
Scopus rating (2015): 0.959 0.837
Web of Science (2015): 3.289 3.485 1.8 0.676 0.130 0.628
Publication Forum (2015): 1
Scopus rating (2014): 1.114 0.965
Web of Science (2014): 3.84 3.907 1.7 0.597 0.0623 0.747
Publication Forum (2014): 1
Scopus rating (2013): 1.117 0.903
Publication Forum (2013): 1
Scopus rating (2012): 0.863 0.603
Original language: English
DOIs:
10.1039/c3ra41741g

Bibliographical note
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: RSC Publishing
Source-ID: 2365
Research output: Scientific - peer-review » Article

Complexation enhanced excited-state deactivation by lithium ion coordination to a borondipyrromethene (Bodipy) donor-bridge-acceptor dyad
Conjugated donor-acceptor (D-A) copolymers in inverted organic solar cells - a combined experimental and modelling study

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Benniston, A. C., Yang, S., Lemmetyinen, H., Tkachenko, N. V.
Number of pages: 11
Pages: 6859-6869
Publication date: 2013
Peer-reviewed: Yes

Publication information
Volume: 2013
Issue number: 30
ISSN (Print): 1434-193X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.133 0.653
Publication Forum (2016): 1
Scopus rating (2015): 1.198 0.758
Web of Science (2015): 3.068 2.971 5.5 0.777 0.04165 0.677
Publication Forum (2015): 1
Scopus rating (2014): 1.181 0.767
Web of Science (2014): 3.065 3.034 5.3 0.744 0.04326 0.703
Publication Forum (2014): 3
Scopus rating (2013): 1.292 0.796
Publication Forum (2013): 3
Scopus rating (2012): 1.471 0.811
Publication Forum (2012): 3
Scopus rating (2011): 1.536 0.857
Scopus rating (2010): 1.572 0.785
Scopus rating (2009): 1.497 0.778
Scopus rating (2008): 1.652 0.759
Scopus rating (2007): 1.711 0.84
Scopus rating (2006): 1.505 0.849
Scopus rating (2005): 1.246 0.763
Scopus rating (2004): 1.2 0.81
Scopus rating (2003): 1.19 0.802
Scopus rating (2002): 1.382 0.829
Scopus rating (2001): 1.159 0.816
Scopus rating (2000): 1.192 1.048
Scopus rating (1999): 0.877 0.976
Original language: English
DOIs:
10.1002/ejoc.201300867

Bibliographical note
Article first published online: 4 SEP 2013
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-11-29
Publisher name: WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
Source: researchoutputwizard
Source-ID: 1989
Research output: Scientific - peer-review Article
Demonstrating the mechanism and efficacy of water-induced shape memory and the influence of water on the thermal properties of oriented poly(d,l-lactide)

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Electronics and Communications Engineering, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Integrated Technologies for Tissue Engineering Research (ITTE)
Authors: Paakinaho, K., Hukka, T. I., Kastinen, T., Kellomäki, M.
Number of pages: 9
Pages: 4209-4218
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Applied Polymer Science
Volume: 130
Issue number: 6
ISSN (Print): 0021-8995
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.532 0.724
Publication Forum (2016): 1
Scopus rating (2015): 0.574 0.827
Web of Science (2015): 1.866 1.647 8.9 0.485 0.0441 0.315
Determination of preferential molecular orientation in porphyrin-fullerene dyad ZnDHD6ee monolayers by the X-ray standing-wave method and X-ray reflectometry

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Seregin, A., Dyakova, Y., Yakunin, S., Makhotkin, I., Alekseev, A., Klechkovskaya, V., Terechenko, E., Tkachenko, N., Lemmetyinen, H., Feigin, L., Kovalchuk, M.
Number of pages: 5
Pages: 934-938
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Crystallography Reports
Volume: 58
Issue number: 6
ISSN (Print): 1063-7745
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.313 0.644
Publication Forum (2016): 1
Scopus rating (2015): 0.286 0.583
Web of Science (2015): 0.561 0.572 >10.0 0.162 0.00176 0.137
Publication Forum (2015): 1
Dipyrrolidinyl-substituted perylene diimide as additive for poly(3-hexylthiophene): [6,6]-Phenyl C61 butyric acid methylester bulk-heterojunction blends

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Vivo, P., Dubey, R., Lehtonen, E., Kivistö, H., Vuorinen, T., Lemmetyinen, H.
Number of pages: 8
Pages: 398-405
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Thin Solid Films
Volume: 548
ISSN (Print): 0040-6090
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.64 0.897
Publication Forum (2016): 1
Scopus rating (2015): 0.705 0.98
Web of Science (2015): 1.761 1.79 9.0 0.356 0.04617 0.426
Publication Forum (2015): 1
Scopus rating (2014): 0.73 1.115
Web of Science (2014): 1.759 1.922 8.5 0.383 0.05315 0.456
Direct evidence of significantly different chemical behavior and excited-state dynamics of 1,7- and 1,6-regioisomers of pyrrolidinyl-substituted perylene diimide

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Dubey, R. K., Niemi, M., Kaunisto, K., Efimov, A., Tkachenko, N. V., Lemmetyinen, H.
Pages: 6791-6806
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Chemistry: A European Journal
Volume: 19
Issue number: 21
ISSN (Print): 0947-6539
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.247 1.046
Publication Forum (2016): 2
Scopus rating (2015): 2.416 1.184
Web of Science (2015): 5.771 5.572 4.6 1.338 0.19837 1.407
Publication Forum (2015): 2
Scopus rating (2014): 2.487 1.219
Web of Science (2014): 5.731 5.635 4.4 1.255 0.19743 1.433
Publication Forum (2014): 3
Scopus rating (2013): 2.604 1.239
Effect of anion coordination on electron transfer in double-linked zinc phthalocyanine-fullerene dyad

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Al-Subi, A. H., Efimov, A., Niemi, M., Tkachenko, N. V., Lemmetyinen, H.
Number of pages: 5
Pages: 96-100
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 572
ISSN (Print): 0009-2614
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.726 0.721
Publication Forum (2016): 1
Scopus rating (2015): 0.733 0.747
Web of Science (2015): 1.86 1.839 >10.0 0.493 0.03583 0.499
Publication Forum (2015): 1
Scopus rating (2014): 0.757 0.773
Web of Science (2014): 1.897 1.963 >10.0 0.475 0.04458 0.565
Publication Forum (2014): 2
Scopus rating (2013): 0.856 0.844
Publication Forum (2013): 2
Scopus rating (2012): 1.101 0.916
Publication Forum (2012): 2
Excited-state interaction of red and green perylene diimides with luminescent Ru(II) polypyridine complex

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Dubey, R. K., Niemi, M., Kaunisto, K., Stranius, K., Efimov, A., Tkachenko, N., Lemmetyinen, H.
Number of pages: 13
Pages: 9761-9773
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Inorganic Chemistry
Volume: 52
ISSN (Print): 0020-1669
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.774 1.198
Publication Forum (2016): 2
Scopus rating (2015): 1.805 1.239
Web of Science (2015): 4.82 4.62 8.0 1.101 0.11551 1.001
Publication Forum (2015): 2
Web of Science (2014): 4.762 4.64 7.8 1.029 0.12122 1.009
Publication Forum (2014): 3
Scopus rating (2013): 1.819 1.379
Publication Forum (2013): 3
Scopus rating (2012): 2.08 1.35
Publication Forum (2012): 3
Scopus rating (2011): 1.952 1.373
Scopus rating (2010): 1.98 1.323
Scopus rating (2009): 1.982 1.47
Scopus rating (2008): 2.025 1.412
Fluorescence properties of the chromophore-binding domain of bacteriophytochrome from Deinococcus radiodurans

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Lehtivuori, H., Rissanen, I., Takala, H., Bamford, J., Tkachenko, N. V., Ihalainen, J. A.
Pages: 11049-11057
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 117
ISSN (Print): 1520-6106
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.348 1.02
Publication Forum (2016): 1
Scopus rating (2015): 1.367 1.096
Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
Publication Forum (2015): 1
Scopus rating (2014): 1.44 1.14
Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
Publication Forum (2014): 3
Scopus rating (2013): 1.494 1.2
Publication Forum (2013): 3
Scopus rating (2012): 1.92 1.251
Publication Forum (2012): 3
Scopus rating (2011): 1.78 1.226
Scopus rating (2010): 1.849 1.214
Scopus rating (2009): 2.232 1.349
Scopus rating (2008): 2.543 1.381
Scopus rating (2007): 2.346 1.282
Scopus rating (2006): 2.369 1.415
Scopus rating (2005): 2.275 1.474
Scopus rating (2004): 2.148 1.511
Homoleptic Bis(aryl)acenaphthenediimine-CuI complexes - synthesis and characterization of a family of compounds with improved light-gathering characteristics

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Papanikolaou, P., Akrivos, P. D., Czapik, A., Wicher, B., Gdaniec, M., Tkachenko, N.
Number of pages: 14
Pages: 2418-2431
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: European Journal of Inorganic Chemistry
Volume: 2013
Issue number: 13
ISSN (Print): 1434-1948
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.791 0.633
Publication Forum (2016): 1
Scopus rating (2015): 0.971 0.701
Web of Science (2015): 2.686 2.68 6.1 0.701 0.02856 0.597
Publication Forum (2015): 1
Scopus rating (2014): 1.029 0.788
Web of Science (2014): 2.942 2.932 5.8 0.654 0.03239 0.665
Publication Forum (2014): 3
Scopus rating (2013): 1.037 0.78
Publication Forum (2013): 3
Scopus rating (2012): 1.188 0.855
Publication Forum (2012): 3
Scopus rating (2011): 1.176 0.824
Scopus rating (2010): 1.131 0.74
Scopus rating (2009): 1.106 0.839
Scopus rating (2008): 1.116 0.88
Scopus rating (2007): 1.221 1.027
Scopus rating (2006): 1.101 0.935
Scopus rating (2005): 1.091 0.811
Scopus rating (2004): 1.02 0.885
Scopus rating (2003): 0.991 0.863
Hydrolytic degradation of composites of poly(L-lactide-co-ε-caprolactone) 70/30 and beta-tricalcium phosphate

There is an increasing need for synthetic bone substitute materials that decrease the need for allografts and autografts. In this study, composites of β-TCP and a biodegradable poly(L-lactide-co-ε-caprolactone) were manufactured using extrusion to form biodegradable composites with high β-TCP contents for osteoconductivity. The hydrolytic degradation of the composites containing 0, 10, 20, 35 and 50% of β-TCP was studied in vitro for 52 weeks. During the study, it was observed that β-TCP did not have an effect on the degradation rate of the polymer matrix. However, the crystallinity of the materials increased throughout the test series and changes in Tgs were also observed as the comonomer ratio of the polymer matrix changed as the degradation proceeded. The results show that the materials have desirable degradation properties and, thus, possess great potential as bioabsorbable and osteoconductive bone filling materials.
Independent versus cooperative binding in polyethylenimine-DNA and poly(L-lysine)-DNA polyplexes

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Ketola, T., Hanzlikova, M., Leppänen, L., Ravina, M., Bishop, C. J., Green, J. J., Urtti, A., Lemmetyinen, H., Yliperttula, M., Vuorimaa-Laukkanen, E.
Number of pages: 9
Pages: 10405-10413
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 117
Issue number: 36
ISSN (Print): 1520-6106
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.348 1.02
Publication Forum (2016): 1
Scopus rating (2015): 1.367 1.096
Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
Publication Forum (2015): 1
Scopus rating (2014): 1.44 1.14
Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
Publication Forum (2014): 3
Scopus rating (2013): 1.494 1.2
Publication Forum (2013): 3
Scopus rating (2012): 1.92 1.251
Publication Forum (2012): 3
Scopus rating (2011): 1.78 1.226
Scopus rating (2010): 1.849 1.214
Influence of plasma chemistry on impurity incorporation in AlN prepared by plasma enhanced atomic layer deposition

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Authors: Pyymaki Perros, A., Hakola, H., Sajavaara, T., Huhtio, T., Lipsanen, H.
Number of pages: 8
Publication date: 2013
Peer-reviewed: Yes

Publication information
Volume: 46
Issue number: 50
Article number: 505502
ISSN (Print): 0022-3727
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.645 0.917
Publication Forum (2016): 1
Scopus rating (2015): 0.693 1.046
Web of Science (2015): 2.772 2.76 7.5 0.529 0.05347 0.838
Publication Forum (2015): 1
Scopus rating (2014): 1.069 1.383
Web of Science (2014): 2.721 2.711 7.0 0.632 0.06141 0.817
Publication Forum (2014): 2
Scopus rating (2013): 1.18 1.469
Publication Forum (2013): 2
Scopus rating (2012): 1.244 1.394
Publication Forum (2012): 2
Scopus rating (2011): 1.257 1.399
Scopus rating (2009): 1.283 1.337
Scopus rating (2008): 1.446 1.563
Scopus rating (2007): 1.385 1.633
Molecular dipole effects on tuning electron transfer in a porphine-quinone complex: A DFT and TDDFT study

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry, Computational Science X (CompX), Frontier Photonics
Authors: Cramariuc, O., Aittala, P., Hukka, T.
Pages: 697-704
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Molecular Modeling
Volume: 19
Issue number: 2
ISSN (Print): 1610-2940
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.447 0.482
Publication Forum (2016): 1
Scopus rating (2015): 0.454 0.589
Web of Science (2015): 1.438 1.508 4.2 0.406 0.01025 0.345
Publication Forum (2015): 1
Scopus rating (2014): 0.51 0.727
Web of Science (2014): 1.736 1.711 3.8 0.189 0.00979 0.374
Publication Forum (2014): 1
Scopus rating (2013): 0.523 0.734
Publication Forum (2013): 1
Scopus rating (2012): 0.571 0.679
Publication Forum (2012): 1
Scopus rating (2011): 0.52 0.773
Scopus rating (2010): 0.919 1.148
Scopus rating (2009): 0.752 1.025
Scopus rating (2008): 0.75 0.719
Scopus rating (2007): 0.637 0.75
Scopus rating (2006): 0.466 0.532
Scopus rating (2005): 0.542 0.668
Molecular weight distribution of a full-scale landfill leachate treatment by membrane bioreactor and nanofiltration membrane

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Campagna, M., Cakmakci, M., Busra Yaman, F., Özkaya, B.
Number of pages: 5
Pages: 866-870
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Waste Management
Volume: 33
Issue number: 4
ISSN (Print): 0956-053X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.354 2.044
Publication Forum (2016): 1
Scopus rating (2015): 1.739 2.256
Web of Science (2015): 3.829 4.297 6.1 0.7 0.01909 0.871
Publication Forum (2015): 1
Scopus rating (2014): 1.777 2.482
Web of Science (2014): 3.22 3.522 5.7 0.498 0.01945 0.804
Publication Forum (2014): 2
Scopus rating (2013): 1.822 2.435
Publication Forum (2013): 2
Scopus rating (2012): 1.611 2.184
Publication Forum (2012): 2
Scopus rating (2011): 1.698 2.085
Scopus rating (2010): 1.555 1.78
Scopus rating (2009): 1.502 1.899
Scopus rating (2007): 1.035 1.767
Scopus rating (2006): 1.046 1.749
Scopus rating (2005): 1.059 1.65
Scopus rating (2004): 1.289 1.939
Scopus rating (2003): 0.847 1.269
Photophysics of bis(ethylxanthato)nickel(II) \([\text{Ni(EtOCS}2])\] complex studied by femtosecond pump-probe spectroscopy

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Plyusnin, V., Kolomeets, A., Budkina, D., Pozdnyakov, I., Tkachenko, N., Lemmetyinen, H.
Number of pages: 6
Pages: 57-62
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Photochemistry and Photobiology, A: Chemistry
Volume: 251
Issue number: 1
ISSN (Print): 1010-6030
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.732 0.841
Publication Forum (2016): 1
Scopus rating (2015): 0.72 0.86
Web of Science (2015): 2.477 2.573 9.8 0.619 0.01027 0.521
Publication Forum (2015): 1
Scopus rating (2014): 0.782 0.97
Web of Science (2014): 2.495 2.549 9.4 0.609 0.01139 0.538
Publication Forum (2014): 1
Scopus rating (2013): 0.818 1.006
Publication Forum (2013): 1
Scopus rating (2012): 0.919 1.116
Publication Forum (2012): 1
Scopus rating (2011): 0.97 1.342
Scopus rating (2010): 1.021 1.05
Scopus rating (2009): 1.163 1.191
Scopus rating (2008): 1.04 1.137
Scopus rating (2007): 1.175 1.364
Scopus rating (2006): 0.996 1.263
Scopus rating (2005): 1.102 1.436
Scopus rating (2004): 0.952 1.213
Scopus rating (2003): 0.76 0.987
Scopus rating (2002): 0.646 0.864
Scopus rating (2001): 0.572 0.934
Scopus rating (2000): 0.782 0.945
Plasma-assisted chemical vapor deposition of Fe:TiO2 films for photoelectrochemical hydrogen production

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Mettenbörger, A., Merod, V., Singh, A., Lemmetyinen, H., Mathur, S.
Number of pages: 8
Pages: 81-88
Publication date: 2013

Host publication information
Title of host publication: Nanostructured Materials and Nanotechnology V - 36th International Conference on Advanced Ceramics and Composites, ICACC 2012, Daytona Beach, FL, USA, 22.-27.1.2013
Publisher: American Ceramic Society
ISBN (Print): 978-111820597-6

Publication series
Name: Ceramic Engineering and Science Proceedings
Volume: 33
No.: 7
ISSN (Print): 0196-6219
ISSN (Electronic): 1940-6339

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-12-29<br/>Publisher name: American Ceramic Society
Source: researchoutputwizard
Source-ID: 2921
Research output: Scientific - peer-review › Conference contribution

Probing the excited state dynamics of a new family of Cu(I)-complexes with an enhanced light absorption capacity: excitation-wavelength dependent population of states through branching

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Authors: Papanikolaou, P., Tkachenko, N.
Number of pages: 9
Pages: 13128-13136
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 15
Issue number: 31
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
Ring-expansion reaction of isatins with ethyl diazoacetate catalyzed by dirhodium(II)/DBU metal-organic system: En route to viridicatin alkaloids

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio)
Authors: Paterna, R., Andre, V., Duarte, M. T., Veiros, L. F., Rafael Candeias, N., Gois, P. M.
Number of pages: 11
Pages: 6280-6290
Publication date: 2013
Peer-reviewed: Yes

Publication information
Volume: 2013
Issue number: 28
ISSN (Print): 1434-193X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.133 0.653
Publication Forum (2016): 1
Scopus rating (2015): 1.198 0.758
Web of Science (2015): 3.068 2.971 5.5 0.777 0.04165 0.677
Sequential photoinduced energy and electron transfer directed improved performance of the supramolecular solar cell of a zinc porphyrin - zinc phthalocyanine conjugate modified TiO2 surface

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Number of pages: 11
Pages: 763-773
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 117
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Scopus rating (2014): 2.027 1.448
Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
Short synthesis of the natural product 3β-hydroxy-labd-8(17)-en-15-oic acid via microbial transformation of labdanolic acid

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Urban circular bioeconomy (UrCirBio), Former organisation of the author
Number of pages: 5
Pages: 165-169
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Phytochemistry Letters
Volume: 6
Issue number: 2
ISSN (Print): 1874-3900
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.543 0.81
Publication Forum (2016): 1
Scopus rating (2015): 0.524 0.852
Web of Science (2015): 1.353 1.451 3.2 0.338 0.0035 0.323
Publication Forum (2015): 1
Scopus rating (2014): 0.592 1.072
Web of Science (2014): 1.45 1.549 2.8 0.313 0.00285 0.342
Publication Forum (2014): 1
Scopus rating (2013): 0.647 1.014
Publication Forum (2013): 1
Scopus rating (2012): 0.545 0.944
Publication Forum (2012): 1
Scopus rating (2011): 0.544 0.776
Scopus rating (2010): 0.468 1.038
Scopus rating (2009): 0.375 0.87
Original language: English

Bibliographical note
Contribution: organisation=keb,FACT1=1&Portfolio EDEND: 2013-10-29
Source: researchoutputwizard

Publisher name: Elsevier

Source: researchoutputwizard
Studies on the structure of coumarin-modified dextran nanoparticles by fluorescence spectroscopy

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Wondraczek, H., Kotiaho, A., Niemi, M., Fardim, P., Heinze, T.
Number of pages: 7
Pages: 45-51
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Carbohydrate Polymers
Volume: 97
Issue number: 1
ISSN (Print): 0144-8617
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.404 1.745
Publication Forum (2016): 2
Scopus rating (2015): 1.46 1.842
Web of Science (2015): 4.219 4.689 4.6 1.029 0.05848 0.807
Publication Forum (2015): 2
Scopus rating (2014): 1.584 1.969
Web of Science (2014): 4.074 4.568 4.4 0.962 0.05081 0.783
Publication Forum (2014): 2
Scopus rating (2013): 1.346 1.967
Publication Forum (2013): 2
Scopus rating (2012): 1.409 2.045
Publication Forum (2012): 2
Scopus rating (2011): 1.287 1.991
Scopus rating (2010): 1.372 1.808
Scopus rating (2009): 1.43 1.718
Scopus rating (2008): 1.142 1.515
Scopus rating (2007): 0.879 1.369
Scopus rating (2006): 0.824 1.424
Scopus rating (2005): 0.816 1.349
Scopus rating (2004): 0.885 1.538
Scopus rating (2003): 0.937 1.41
Scopus rating (2002): 0.878 1.372
Scopus rating (2001): 0.828 1.062
Scopus rating (2000): 0.858 1.086
Scopus rating (1999): 0.764 1.074
Original language: English
DOIs:
10.1016/j.carbpol.2013.04.040

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-12-29<br/>Publisher name: Pergamon
Source: researchoutputwizard
Source-ID: 3748
Research output: Scientific - peer-review › Article
Study of structural order in porphyrin-fullerene dyad ZnDHD6ee monolayers by electron diffraction and atomic force microscopy

**General information**
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Number of pages: 7
Pages: 927-933
Publication date: 2013
Peer-reviewed: Yes

**Publication information**
Journal: Crystallography Reports
Volume: 58
Issue number: 6
ISSN (Print): 1063-7745
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.313 0.644
Publication Forum (2016): 1
Scopus rating (2015): 0.286 0.583
Web of Science (2015): 0.561 0.572 >10.0 0.162 0.00176 0.137
Publication Forum (2015): 1
Scopus rating (2014): 0.307 0.666
Web of Science (2014): 0.489 0.559 >10.0 0.148 0.00211 0.153
Publication Forum (2014): 1
Scopus rating (2013): 0.322 0.636
Publication Forum (2013): 1
Scopus rating (2012): 0.384 0.65
Publication Forum (2012): 1
Scopus rating (2011): 0.215 0.333
Scopus rating (2010): 0.477 0.583
Scopus rating (2009): 0.189 0.3
Scopus rating (2008): 0.22 0.202
Scopus rating (2007): 0.148 0.188
Scopus rating (2006): 0.236 0.62
Scopus rating (2005): 0.262 0.641
Scopus rating (2004): 0.209 0.446
Scopus rating (2003): 0.181 0.292
Scopus rating (2002): 0.128 0.132
Scopus rating (2001): 0.222 0.34
Scopus rating (2000): 0.258 0.399
Scopus rating (1999): 0.136 0.157
Original language: English
DOIs: 10.1134/S1063774513060096

**Bibliographical note**
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-12-29<br/>Publisher name: MAIK Nauka - Interperiodica
Source: researchoutputwizard
Source-ID: 2064
Research output: Scientific - peer-review » Article
Supramolecular assemblies of bay-substituted perylene diimides in solution and on a solid substrate

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Sariola-Leikas, E., Niemi, M., Lemmetyinen, H., Efimov, A.
Number of pages: 10
Pages: 6397-6406
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Organic and Biomolecular Chemistry
Volume: 11
ISSN (Print): 1477-0520
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.363 0.803
Publication Forum (2016): 1
Scopus rating (2015): 1.41 0.858
Web of Science (2015): 3.559 3.367 4.2 1.029 0.06052 0.797
Publication Forum (2015): 1
Scopus rating (2014): 1.387 0.903
Web of Science (2014): 3.562 3.382 3.9 0.966 0.05829 0.807
Publication Forum (2014): 3
Scopus rating (2013): 1.481 0.897
Publication Forum (2013): 3
Scopus rating (2012): 1.635 0.934
Publication Forum (2012): 3
Scopus rating (2011): 1.737 0.974
Scopus rating (2010): 1.775 0.951
Scopus rating (2009): 1.831 1.073
Scopus rating (2008): 1.936 1.042
Scopus rating (2007): 1.843 0.984
Scopus rating (2006): 1.557 0.957
Scopus rating (2005): 1.245 1.098
Scopus rating (2004): 1.274 0.999
Scopus rating (2003): 0.1
Original language: English
DOIs:
10.1039/c3ob41058g

Bibliographical note
ei vielä UT 2013-09-19<br/>

The Effect and Role of Carbon Atoms in Poly(ß-amino ester)s for DNA Binding and Gene Delivery

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Bishop, C. J., Ketola, T., Tzeng, S. Y., Sunshine, J. C., Urtti, A., Lemmetyinen, H., Vuorimaa-Laukkonen, E., Yliperttula, M., Green, J. J.
Triarylamine-substituted imidazole- and quinoxaline-fused push-pull porphyrins for dye-sensitized solar cells

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research group: Supramolecular photochemistry, Department of Chemistry and Bioengineering, Frontier Photonics
Authors: Hayashi, H., Touchy, A. S., Kinjo, Y., Kurotobi, K., Toude, Y., Ito, S., Saarenpää, H., Tkachenko, N., Lemmetyinen, H., Imahori, H.
Number of pages: 10
Pages: 508-517
Tuning the Förster overlap integral: energy transfer over 20 Ångstroms from a pyrene-based donor to borondipyrromethene (Bodipy)
Algorithm for In Silico Optimization of Production Strains

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Signal Processing, Department of Chemistry and Bioengineering, Research group: Computational Systems Biology
Authors: Heikkinen, E., Larjo, A., Santala, V., Yli-Harja, O., Aho, T.
Number of pages: 4
Pages: 1-4
Publication date: 2012

Host publication information
Title of host publication: Proceedings of Ninth International Workshop on Computational Systems Biology, WCSB 2012, 4-6 June, Ulm, Germany. TICSP Series
Place of publication: Tampere
Publisher: Tampere University of Technology
A Photoconductive, Thiophene-Fullerene Double-Cable Polymer, Nanorod Device

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Pages: 478-481
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Letters
Volume: 3
Issue number: 4
ISSN (Print): 1948-7185
Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 4.583 1.68
Publication Forum (2016): 3
Scopus rating (2015): 4.233 1.829
Web of Science (2015): 8.539 7.803 3.0 1.971 0.11885 2.482
Publication Forum (2015): 2
Web of Science (2014): 7.458 7.536 2.8 2.017 0.09524 2.425
Publication Forum (2014): 2
Scopus rating (2013): 3.515 1.61
Publication Forum (2013): 2
Scopus rating (2012): 3.943 1.751
Publication Forum (2012): 2
Scopus rating (2011): 3.244 1.602
Original language: English
DOIs: 10.1021/jz300015e

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society - ACS
Source: researchoutputwizard
Source-ID: 4305
Research output: Scientific - peer-review › Article

Asymmetric Intramolecular C-H Insertion of alpha-Diazoacetamides in Water by Dirhodium(II) Catalysts Derived from Natural Amino Acids
Azafullerene C59N-Phthalocyanine Dyad: Synthesis, Characterisation and Photoinduced Electron Transfer
Car-parrinello molecular dynamics study of a porphyrin-fullerene electron donor-acceptor dyad

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Research area: Computational Physics, Department of Chemistry and Bioengineering, Department of Physics
Authors: Karilainen, T., Cramariuc, O., Tappura, K., Hukka, T.
Number of pages: 1
Pages: 1-1
Publication date: 2012
Diaryl-Substituted Perylene Bis(imides): Synthesis, Separation, Characterization and Comparison of Electrochemical and Optical Properties of 1,7- and 1,6-Regioisomer
Directed electron transfer in Langmuir-Schäfer layers of porphyrin-fullerene and phthalocyanine-fullerene dyads in inverted organic solar cells

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Tolkki, A., Kaunisto, K., Efimov, A., Kivistö, H., Storbacka, L., Savikoski, R., Huttunen, K., Lehtimäki, S., Lemmetynen, H.
Pages: 3498-3504
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 14
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
Publication Forum (2016): 1
Scopus rating (2015): 1.771 1.244
Web of Science (2015): 4.449 4.273 4.1 1.017 0.19255 1.158
Publication Forum (2015): 1
Scopus rating (2014): 1.772 1.253
Web of Science (2014): 4.493 4.219 3.9 0.991 0.17937 1.209
Publication Forum (2014): 3
Scopus rating (2013): 1.715 1.216
Publication Forum (2013): 3
Scopus rating (2012): 1.916 1.184
Publication Forum (2012): 3
Scopus rating (2011): 1.697 1.203
Scopus rating (2010): 1.802 1.196
Scopus rating (2009): 2.127 1.369
Scopus rating (2008): 2.158 1.211
Scopus rating (2007): 1.84 1.138
Scopus rating (2006): 1.467 1.128
Scopus rating (2005): 1.389 1.104
Scopus rating (2004): 1.173 1.007
Scopus rating (2003): 1.093 0.925
Scopus rating (2002): 1.122 0.973
Scopus rating (2001): 1.09 0.914
Scopus rating (2000): 0.948 1.068
Scopus rating (1999): 0.121 0.0
Donor-acceptor alternating copolymer based on thermally converted isothianaphthene dimer and thiazolothiazole subunits

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Umeyama, T., Hirose, K., Noda, K., Matsushige, K., Shishido, T., Saarenpää, H., Tkachenko, N. V., Lemmetyinen, H., Ono, N., Imahori, H.
Pages: 17414-17423
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 116
Issue number: 33
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Scopus rating (2014): 2.027 1.448
Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
Publication Forum (2014): 3
Scopus rating (2013): 2.134 1.439
Publication Forum (2013): 3
Scopus rating (2012): 2.514 1.46
Publication Forum (2012): 3
Scopus rating (2011): 2.32 1.457
Scopus rating (2010): 2.438 1.356
Scopus rating (2009): 2.128 1.417
Scopus rating (2008): 1.856 1.033
Original language: English
DOIs: 10.1039/c2cp24022j

Bibliographical note
Contribution: organisation=keb kem,FACT1=1<Publisher name: RSC Publications
Source: researchoutputwizard
Source-ID: 5434
Research output: Scientific - peer-review › Article

Effect of halide binding on intramolecular exciplex of double-linked zinc porphyrin-fullerene dyad

General information
State: Published
Effect on Charge Transfer and Charge Recombination by Insertion of a Naphthalene-Based Bridge in Molecular Dyads Based on Borondipyrromethene (Bodipy)
Effects of Carbon-Metal-Carbon Linkages on the Optical, Photophysical, and Electrochemical Properties of Phosphametallacycle-Linked Coplanar Porphyrin Dimers

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Pages: 1825-1839
Publication date: 2012
Peer-reviewed: Yes
Excited State Intramolecular Proton Transfer in Electron-Rich and Electron-Poor Derivatives of 10-Hydroxybenzo[h]quinoline

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Piechowska, J., Huttunen, K., Wrobel, Z., Lemmetyinen, H., Tkachenko, N. V., Gryko, D.
Pages: 9614-9620
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 116
Issue number: 39
Exploring Förster electronic energy transfer in a decoupled anthracenyl-based borondipyrromethene (bodipy) dyad

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Bai, D., Benniston, A., Hagon, J., Lemmetyinen, H., Tkachenko, N. V., Clegg, W., Harrington, R.
Pages: 4447-4456
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 14
Issue number: 13
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
Hydrogen-Bonding Effects on the Formation and Lifetimes of Charge-Separated States in Molecular Triads

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Hankache, J., Niemi, M., Lemmetyinen, H., Wenger, O. S.
Pages: 8159-8168
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 116
Issue number: 31
ISSN (Print): 1089-5639
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.258 0.98
Publication Forum (2016): 1
Scopus rating (2015): 1.179 1.106
Web of Science (2015): 2.883 2.709 8.1 0.758 0.0807 0.729
In this work, the intramolecular C-H insertion of diazoacetamides catalyzed by dirhodium(II) complexes and using CO2 as solvent is disclosed. The expected lactams were obtained in yields over 97%. The asymmetric intramolecular C-H insertion was also achieved and the beta-lactam 14 was obtained in > 97% yield and 65% ee using the chiral dirhodium(II) catalyst Rh-2(S-PTTL)(4). Finally, the dirhodium(II) complex Rh-2(OAc)(4) was used in two consecutive cycles in which complete conversion to the lactam was observed.
Large Stokes Shift Fluorescent Dyes Based on a Highly Substituted Terephthalic Acid Core

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Benniston, A. C., Winstanley, T. P., Lemmetyinen, H., Tkachenko, N. V., Harrington, R. W., Wills, C.
Pages: 1374-1377
Publication date: 2012
Peer-reviewed: Yes

Publications information
Journal: Organic Letters
Volume: 14
Issue number: 6
ISSN (Print): 1523-7060
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.964 1.218
Publication Forum (2016): 2
Web of Science (2015): 6.732 6.033 5.5 1.566 0.17092 1.414
Publication Forum (2015): 2
Scopus rating (2014): 2.958 1.324
Web of Science (2014): 6.364 5.849 5.3 1.864 0.17383 1.407
Publication Forum (2014): 3
Scopus rating (2013): 3.144 1.329
Publication Forum (2013): 3
Scopus rating (2012): 3.312 1.355
Publication Forum (2012): 3
Scopus rating (2011): 3.271 1.377
Scopus rating (2010): 2.985 1.307
Scopus rating (2009): 3.048 1.37
Scopus rating (2007): 3.185 1.296
Making expensive dirhodium(II) catalysts cheaper: Rh(II) recycling methods

Dirhodium(II) catalysts have been widely used as a remarkable tool in organic synthesis, ultimately resulting in a myriad of transformations and formation of a wide variety of compounds, every so often intermediaries in drug synthesis. Aiming at a more sustainable chemistry, several methods suitable for the reutilisation of expensive dirhodium complexes have been developed. Herein, we provide a combined overview of the available methods for recovering and reusing dirhodium(II) metal complexes in catalysis, covering homogeneous catalysis as well as heterogenisation methods.
Meteorological parameters as an important factor on the energy recovery of landfill gas in landfills

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Uyanik, I., Özkaya, B., Demir, S., Cakmakci, M.
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Renewable and Sustainable Energy
Volume: 4
Issue number: 6
Article number: 063135
ISSN (Print): 1941-7012
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.418 0.523
Publication Forum (2016): 1
Scopus rating (2015): 0.372 0.52
Web of Science (2015): 0.961 1.141 2.9 0.287 0.00371 0.272
Publication Forum (2015): 1
Scopus rating (2014): 0.406 0.697
Web of Science (2014): 0.904 1.149 2.5 0.292 0.0028 0.25
Publication Forum (2014): 1
Scopus rating (2013): 0.441 0.856
Publication Forum (2013): 1
Scopus rating (2012): 0.575 1.246
Publication Forum (2012): 1
Scopus rating (2011): 0.344 1.024
Original language: English
DOIs:
10.1063/1.4769202

Bibliographical note
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: American Institute of Physics AIP
Source: researchoutputwizard
Source-ID: 5478
Research output: Scientific - peer-review › Article

Modulation of visible room temperature phosphorescence by weak magnetic fields

General information
State: Published
N-1-Functionalized Indole-Phosphane Oxazoline (IndPHOX) Ligands in Asymmetric Allylic Substitution Reactions

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Wang, Y., Vaismaa, M. J., Rissanen, K., Franzen, R.
Pages: 1569-1576
Publication date: 2012
Peer-reviewed: Yes

Publication information
Volume: 2012
Issue number: 8
ISSN (Print): 1434-193X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.133 0.653
Publication Forum (2016): 1
Scopus rating (2015): 1.198 0.758
Web of Science (2015): 3.068 2.971 5.5 0.777 0.04165 0.677
Nature's Nonlinear Optical Antennas

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Research group: Nonlinear Optics, Research area: Optics, Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Huttunen, M. J., Virkki, M., Bautista, G., Vuorimaa-Laukkonen, E., Der, A., Lemmetyinen, H., Kauranen, M.
Number of pages: 2
Pages: 1-2
Publication date: 2012

Host publication information
Title of host publication: CLEO 2012, San Jose, California, USA, 6-11 May 2012. Technical Digest
Publisher: OSA
Article number: QM4F.8
ISBN (Electronic): 978-146731839-6

Publication series
Name: Conference on Lasers and Electro-Optics

Bibliographical note
Contribution: organisation=fys,FACT1=0.5<br/>Contribution: organisation=keb kem,FACT2=0.5<br/>Publisher name: OSA
Source: researchoutputwizard
Source-ID: 4265
Research output: Scientific - peer-review › Conference contribution
Organometallic tris(8-hydroxyquinoline)aluminum complexes as buffer layers and dopants in inverted organic solar cells

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Pages: 4475-4481
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Thin Solid Films
Volume: 520
Issue number: 13
ISSN (Print): 0040-6090
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.64 0.897
Publication Forum (2016): 1
Scopus rating (2015): 0.705 0.98
Web of Science (2015): 1.761 1.79 9.0 0.356 0.04617 0.426
Publication Forum (2015): 1
Scopus rating (2014): 0.73 1.115
Web of Science (2014): 1.759 1.922 8.5 0.383 0.05315 0.456
Publication Forum (2014): 2
Scopus rating (2013): 0.818 1.215
Publication Forum (2013): 2
Scopus rating (2012): 0.899 1.162
Publication Forum (2012): 2
Scopus rating (2011): 0.995 1.337
Scopus rating (2010): 1.141 1.235
Scopus rating (2009): 1.142 1.221
Scopus rating (2008): 1.191 1.282
Scopus rating (2006): 1.147 1.318
Scopus rating (2005): 1.173 1.246
Scopus rating (2004): 1.188 1.308
Scopus rating (2003): 1.231 1.282
Scopus rating (2002): 1.175 1.14
Scopus rating (2001): 1.032 1.032
Scopus rating (2000): 0.99 0.924
Scopus rating (1999): 0.914 0.862
Original language: English
DOIs: 10.1016/j.tsf.2012.02.084

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Publisher name: Elsevier
Source: researchoutputwizard
Source-ID: 5435
Research output: Scientific - peer-review › Article

Photochemical properties and sensor applications of modified yellow fluorescent protein (YFP) covalently attached to the surfaces of etched optical fibers (EOFs)

General information
State: Published
Photoinduced Electron Transfer in Linear Triarylamine-Photosensitizer-Anthraquinone Triads with Ruthenium(II), Osmium(II), and Iridium(III)

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Hankache, J., Niemi, M., Lemmetyinen, H., Wenger, O. S.
Pages: 6333-6344
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Inorganic Chemistry
Volume: 51
Issue number: 11
ISSN (Print): 0020-1669
Photolysis and Quantum-Chemical Calculations of the Nalidixic Acid Radical States

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Department of Physics, Computational Science X (CompX)
Authors: Polischuk, A., Emelina, T., Cramariuc, O., Chukharev, V., Karaseva, T., Karasev, V.
Pages: 323-328
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Russian Journal of General Chemistry
Volume: 82
Issue number: 2
ISSN (Print): 1070-3632
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.202 0.5
Publication Forum (2016): 1
Scopus rating (2015): 0.212 0.541
Photophysics of Fe(III)-tartrate and Fe(III)-citrate complexes in aqueous solutions

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Pages: 45-48
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 530
ISSN (Print): 0009-2614
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.726 0.721
Publication Forum (2016): 1
Scopus rating (2015): 0.733 0.747
Web of Science (2015): 1.86 1.839 >10.0 0.493 0.03583 0.499
Publication Forum (2015): 1
Scopus rating (2014): 0.757 0.773
Preparation and Photophysical and Photoelectrochemical Properties of a Covalently Fixed Porphyrin–Chemically Converted Graphene Composite

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Pages: 4250-4257
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Chemistry: A European Journal
Volume: 18
Issue number: 14
ISSN (Print): 0947-6539
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.247 1.046
Publication Forum (2016): 2
Scopus rating (2015): 2.416 1.184
Web of Science (2015): 5.771 5.572 4.6 1.338 0.19837 1.407
Publication Forum (2015): 2
Scopus rating (2014): 2.487 1.219
Web of Science (2014): 5.731 5.635 4.4 1.255 0.19743 1.433
Publication Forum (2014): 3
Processing and sustained in vitro release of rifampicin containing composites to enhance the treatment of osteomyelitis

The objective in this study was to develop an osteoconductive, biodegradable and rifampicin releasing bone filling composite material for the treatment of osteomyelitis, a bacterial infection of bone that is very difficult and expensive to treat. The composite material will be used together with a ciprofloxacin releasing composite, because of the rapid development of resistant bacteria when rifampicin is used alone. Three composites were manufactured by twin-screw extrusion. The polymer matrix for the composites was poly(L-lactide-co-ε-caprolactone) 70/30 and all the composites contained 8 wt% (weight percent) of rifampicin antibiotic. The b-TCP contents of the composites were 0 wt%, 50 wt% and 60 wt%. The composites were sterilized by gamma irradiation before in vitro degradation and drug release tests. The hydrolytical degradation of the studied composites proceeded quickly and the molecular weight of the polymer component of the composites decreased rapidly. Rifampicin release occurred in four phases in which the high b-TCP content of the samples, polymer degradation and mass loss all played a role in determining the phases. The ceramic component was seen to have a positive effect on the drug release. The composite with 50 wt% of b-TCP showed the most promising rifampicin release profile and it also showed activity against a common osteomyelitis causing bacteria Pseudomonas aeruginosa. A clear inhibition zone was formed in 16 h incubation. Overall, the tested materials showed great potential to be developed into a bone filler material for the treatment of osteomyelitis or other bone related infections in combination with the ciprofloxacin releasing materials.
Quantitative Analysis of Intramolecular Exciplex and Electron Transfer in a Double-Linked Zinc Porphyrin-Fullerene Dyad

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Al-Subi, A., Niemi, M., Tkachenko, N., Lemmetyinen, H.
Pages: 9653-9661
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 116
Issue number: 39
ISSN (Print): 1089-5639
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.258 0.98
Publication Forum (2016): 1
Scopus rating (2015): 1.179 1.106
Web of Science (2015): 2.883 2.709 8.1 0.758 0.0807 0.729
Publication Forum (2015): 1
Scopus rating (2014): 1.154 1.071
Web of Science (2014): 2.693 2.713 7.6 0.676 0.09689 0.777
Publication Forum (2014): 3
Scopus rating (2013): 1.194 1.102
Publication Forum (2013): 3
Scopus rating (2012): 1.494 1.124
Publication Forum (2012): 3
Scopus rating (2011): 1.402 1.135
Scopus rating (2010): 1.466 1.102
Scopus rating (2009): 1.562 1.132
Redox processes in photochemistry of Pt(IV) hexahaloid complexes

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Glebov, E., Kolomeets, A., Pozdnyakov, I., Plyusnin, V., Grivin, V., Tkachenko, N., Lemmetyinen, H.
Pages: 5768-5778
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: RSC Advances
Volume: 2
Issue number: 13
ISSN (Print): 2046-2069
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.875 0.743
Publication Forum (2016): 1
Scopus rating (2015): 0.959 0.837
Web of Science (2015): 3.289 3.485 1.8 0.676 0.13014 0.628
Publication Forum (2015): 1
Scopus rating (2014): 1.114 0.965
Web of Science (2014): 3.84 3.907 1.7 0.597 0.0623 0.747
Publication Forum (2014): 1
Scopus rating (2013): 1.117 0.903
Publication Forum (2013): 1
Scopus rating (2012): 0.863 0.603
Original language: English
DOIs:
10.1039/c2ra20715j

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Publisher name: RSC Publications
Source: researchoutputwizard
Source-ID: 4091
Research output: Scientific - peer-review › Article
Rh-IndOlefOx catalyzed conjugate addition/Heck-type coupling of organoboronics to a lactam or a lactone

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Kuuloja, N., Vaismaa, M., Franzen, R.
Pages: 2313-2318
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Tetrahedron
Volume: 68
Issue number: 10
ISSN (Print): 0040-4020
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.907 0.742
Publication Forum (2016): 1
Scopus rating (2015): 0.954 0.84
Web of Science (2015): 2.645 2.621 9.6 0.609 0.04893 0.531
Publication Forum (2015): 1
Scopus rating (2014): 0.971 0.905
Web of Science (2014): 2.641 2.675 9.2 0.652 0.05691 0.575
Publication Forum (2014): 2
Scopus rating (2013): 1.101 0.92
Publication Forum (2013): 2
Scopus rating (2012): 1.32 0.999
Publication Forum (2012): 2
Scopus rating (2011): 1.476 1.094
Scopus rating (2010): 1.508 1.065
Scopus rating (2009): 1.534 1.124
Scopus rating (2008): 1.579 1.078
Scopus rating (2007): 1.639 1.116
Scopus rating (2006): 1.507 1.142
Scopus rating (2005): 1.354 1.138
Scopus rating (2004): 1.459 1.261
Scopus rating (2003): 1.448 1.265
Scopus rating (2002): 1.677 1.177
Scopus rating (2001): 1.46 1.178
Scopus rating (2000): 1.536 1.165
Scopus rating (1999): 1.37 1.172
Original language: English
DOIs:
10.1016/j.tet.2012.01.040

Bibliographical note
Contribution: organisation=keb kem,FACT1=1<br/>Publisher name: Elsevier Ltd.
Source: researchoutputwizard
Source-ID: 4578
Research output: Scientific - peer-review › Article

Self-Assembled Porphyrins on Modified Zinc Oxide Nanorods: Development of Model Systems for Inorganic-Organic Semiconductor Interface Studies

General information
Synthesis and characterization of tris-(5-amino-8-hydroxyquinoline)aluminum complexes and their use as anode buffer layers in inverted organic solar cells

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Pages: 22971-22982
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Chemistry
Volume: 22
Issue number: 43
ISSN (Print): 0959-9428
Ratings:
Publication Forum (2017): 3
Synthesis of 2-Aryl-Substituted Chromans by Intramolecular C-O Bond Formation

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Wang, Y., Franzen, R.
Pages: 925-929
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Synlett
Issue number: 6
ISSN (Print): 0936-5214
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.856 0.461
Publication Forum (2016): 1
Scopus rating (2015): 0.875 0.494
Web of Science (2015): 2.323 2.24 7.6 0.655 0.02219 0.533
Publication Forum (2015): 1
Scopus rating (2014): 0.956 0.574
Web of Science (2014): 2.419 2.279 7.3 0.514 0.0253 0.555
Publication Forum (2014): 2
Synthesis of porphyrinoids with silane anchors and their covalent self-assembling and metallation on solid surface

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Optoelectronics Research Centre, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Sariola-Leikas, E., Hietala, M., Veselov, A., Okhotnikov, O., Semjonov, S. L., Tkachenko, N. V., Lemmetyinen, H., Efimov, A.
Pages: 58-70
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Colloid and Interface Science
Volume: 369
Issue number: 1
ISSN (Print): 0021-9797
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.144 1.267
Publication Forum (2016): 1
Scopus rating (2015): 1.095 1.263
Web of Science (2015): 3.782 3.758 9.3 1.094 0.05491 0.805
Publication Forum (2015): 1
Scopus rating (2014): 1.166 1.406
Web of Science (2014): 3.368 3.637 8.9 0.827 0.06124 0.827
Publication Forum (2014): 2
Scopus rating (2013): 1.19 1.45
Publication Forum (2013): 2
Scopus rating (2012): 1.298 1.469
Synthesis of titanate nanostructures using amorphous precursor material and their adsorption/photocatalytic properties

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Ylhäinen, E. K., Nunes, M., Silvestre, A., Monteiro, O.
Pages: 4305-4312
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Science
Volume: 47
Issue number: 10
ISSN (Print): 0022-2461
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.762 1.064
Publication Forum (2016): 1
Scopus rating (2015): 0.811 1.081
Web of Science (2015): 2.302 2.288 >10.0 0.57 0.03898 0.566
Publication Forum (2015): 1
Scopus rating (2014): 0.985 1.431
Web of Science (2014): 2.371 2.32 9.8 0.532 0.04221 0.592
Publication Forum (2014): 1
Scopus rating (2013): 0.933 1.472
Publication Forum (2013): 1
Scopus rating (2012): 0.991 1.407
Publication Forum (2012): 1
Scopus rating (2011): 0.941 1.393
Scopus rating (2010): 0.965 1.097
Scopus rating (2009): 0.842 0.963
The fluorine effect: photophysical properties of borondipyrromethene (bodipy) dyes appended at the meso position with fluorinated aryl groups

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Alamiry, M. A., Benniston, A. C., Hagon, J., Winstanley, T. P., Lemmetyinen, H., Tkachenko, N. V.
Pages: 4944-4950
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: RSC Advances
Volume: 2
Issue number: 11
ISSN (Print): 2046-2069
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.875 0.743
Publication Forum (2016): 1
Scopus rating (2015): 0.959 0.837
Web of Science (2015): 3.289 3.485 1.8 0.676 0.13014 0.628
Publication Forum (2015): 1
Scopus rating (2014): 1.114 0.965
Web of Science (2014): 3.84 3.907 1.7 0.597 0.0623 0.747
Publication Forum (2014): 1
Scopus rating (2013): 1.117 0.903
Publication Forum (2013): 1
Scopus rating (2012): 0.863 0.603
Original language: English
DOI:
10.1039/c2ra20219k

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Publisher name: The Royal Society of Chemistry - RSC
Source: researchoutputwizard
Source-ID: 3840
Research output: Scientific - peer-review » Article
Construction of bispirooxindoles containing three quaternary stereocentres in a cascade using a single multifunctional organocatalyst

Single-step constructions of molecules with multiple quaternary carbon stereocentres are rare. The spirooxindole structural motif is common to a range of bioactive compounds; however, asymmetric synthesis of this motif is complicated due to the presence of multiple chiral centres. The development of organocatalytic cascade reactions has proven to be valuable for the construction of several chiral centres in one step. Here, we describe a newly designed organocatalytic asymmetric domino Michael-aldol reaction between 3-substituted oxindoles and methyleneindolinones that affords complex bispirooxindoles. This reaction was catalysed by a novel multifunctional organocatalyst that contains tertiary and primary amines and thiourea moieties to activate substrates simultaneously, providing extraordinary levels of stereocontrol over four stereocentres, three of which are quaternary carbon stereocentres. This new methodology provides facile access to a range of multisubstituted bispirocyclooxindole derivatives, and should be useful in medicinal chemistry and diversity-oriented syntheses of this intriguing class of compounds.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: Tan, B., Candeias, N. R., Barbas, C. F.
Keywords: (ENANTIOSELECTIVE CONJUGATE ADDITION, C BOND FORMATION, NATURAL-PRODUCTS, STEREOCONTROLLED CREATION, CINCHONA ALKALOIDS, DOMINO REACTIONS, ALDER REACTIONS, OXINDOLES, THIOUREA, DERIVATIVES)
Number of pages: 5
Pages: 473-477
Publication date: Jun 2011
Peer-reviewed: Yes

Publication information
Journal: Nature Chemistry
Volume: 3
Issue number: 6
ISSN (Print): 1755-4330
Ratings:
Core-Structure-Motivated Design of a Phosphine-Catalyzed [3+2] Cycloaddition Reaction: Enantioselective Syntheses of Spirocyclopenteneoxindoles

A novel organocatalytic asymmetric [3 + 2] cycloaddition reaction between methyleneindolinones and allylic compounds yielding complex spirocyclopenteneoxindoles has been developed. It provides extraordinary levels of enantioselective control involving a chiral phosphine as a nucleophilic organocatalyst. Simple precursors were used under mild conditions to construct oxindole derivatives with high enantiopurity and structural diversity. This method should be useful in medicinal chemistry and diversity-oriented syntheses of these intriguing compounds.
1,7- And 1,6-Regioisomers of Diphenoxy and Dipyrrolidinyl Substituted Perylene Dlimides: Synthesis, Separation, Characterization, and Comparison of Electrochemical and Optical Properties

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Dubey, R. K., Efimov, A., Lemmetyinen, H.
Pages: 778-788
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Chemistry of Materials
Volume: 23
Issue number: 3
ISSN (Print): 0897-4756
Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 4.114 1.905
Publication Forum (2016): 3
Scopus rating (2015): 4.038 2.102
Web of Science (2015): 9.407 9.363 7.5 1.737 0.12692 2.376
Scopus rating (2014): 3.603 2.253
Web of Science (2014): 8.354 9.21 7.3 2.078 0.12128 2.2
Publication Forum (2014): 3
Scopus rating (2013): 3.658 2.277
Publication Forum (2013): 3
Scopus rating (2012): 4.169 2.264
Publication Forum (2012): 3
Scopus rating (2011): 3.484 2.145
Anaerobic H-2 production at elevated temperature (60 °C) by enriched mixed consortia from mesophilic sources

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Karadag, D.
Pages: 458-465
Publication date: 2011
Peer-reviewed: Yes

Publication information
Volume: 36
Issue number: 1
ISSN (Print): 0360-3199
Ratings:
 Publication Forum (2017): 1
 Scopus rating (2016): 1.142 1.286
 Publication Forum (2016): 1
 Scopus rating (2015): 1.294 1.319
 Web of Science (2015): 3.205 3.419 4.6 0.651 0.08996 0.619
 Publication Forum (2015): 1
 Scopus rating (2014): 1.212 1.494
 Web of Science (2014): 3.313 3.659 4.3 0.539 0.08226 0.619
 Publication Forum (2014): 3
 Scopus rating (2013): 1.278 1.467
 Publication Forum (2013): 3
 Scopus rating (2012): 1.515 1.729
 Publication Forum (2012): 3
 Scopus rating (2011): 1.456 1.837
 Scopus rating (2010): 1.589 1.871
 Scopus rating (2009): 1.333 1.885
 Scopus rating (2008): 1.401 2.096
 Scopus rating (2007): 1.279 2.201
 Scopus rating (2006): 1.073 2.161
A solid phase extraction technique for HPLC analysis of short chain fatty acid fluxes during microbial degradation of plant polymers

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Carver, S., Munster, U., Tuovinen, O. H.
Pages: 1546-1555
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Liquid Chromatography and Related Technologies
Volume: 34
Issue number: 15
ISSN (Print): 1082-6076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.282 0.392
Publication Forum (2016): 1
Scopus rating (2015): 0.291 0.463
Web of Science (2015): 0.669 0.755 9.4 0.237 0.00237 0.157
Publication Forum (2015): 1
Scopus rating (2014): 0.297 0.527
Web of Science (2014): 0.606 0.652 9.4 0.143 0.00217 0.139
Publication Forum (2014): 1
Scopus rating (2013): 0.286 0.471
Publication Forum (2013): 1
Scopus rating (2012): 0.311 0.425
Publication Forum (2012): 1
Scopus rating (2011): 0.454 0.461
Scopus rating (2010): 0.5 0.553
Scopus rating (2009): 0.546 0.579
Scopus rating (2008): 0.483 0.583
Scopus rating (2007): 0.468 0.594
Scopus rating (2006): 0.455 0.401
Scopus rating (2005): 0.442 0.507
Scopus rating (2004): 0.415 0.606
Scopus rating (2003): 0.423 0.589
Scopus rating (2002): 0.485 0.666
Bay Region Borylation of Perylene Bisimides

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Dey, S., Efimov, A., Lemmetyinen, H.
Pages: 5955-5958
Publication date: 2011
Peer-reviewed: Yes

Publication information
Volume: 2011
Issue number: 30
ISSN (Print): 1434-193X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.133 0.653
Publication Forum (2016): 1
Scopus rating (2015): 1.198 0.758
Web of Science (2015): 3.068 2.971 5.5 0.777 0.04165 0.677
Publication Forum (2015): 1
Scopus rating (2014): 1.181 0.767
Web of Science (2014): 3.065 3.034 5.3 0.744 0.04326 0.703
Publication Forum (2014): 3
Scopus rating (2013): 1.292 0.796
Publication Forum (2013): 3
Scopus rating (2012): 1.471 0.811
Publication Forum (2012): 3
Scopus rating (2011): 1.536 0.857
Scopus rating (2010): 1.572 0.785
Scopus rating (2009): 1.497 0.778
Scopus rating (2008): 1.652 0.759
Scopus rating (2007): 1.711 0.84
Scopus rating (2006): 1.505 0.849
Scopus rating (2005): 1.246 0.763
Scopus rating (2004): 1.2 0.81
Scopus rating (2003): 1.19 0.802
Scopus rating (2002): 1.382 0.829
Scopus rating (2001): 1.159 0.816
Scopus rating (2000): 1.192 1.048
Scopus rating (1999): 0.877 0.976
Original language: English
Biohydrogen production in alkali-thermophilic conditions: Thermobrachium celere as a case study

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio)
Authors: Ciranna, A., Santala, V., Karp, M.
Pages: 8714-8722
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Bioresource Technology
Volume: 102
Issue number: 18
ISSN (Print): 0960-8524
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.191 1.91
Publication Forum (2016): 2
Scopus rating (2015): 2.255 1.908
Web of Science (2015): 4.917 5.744 5.0 1.012 0.13375 1.089
Publication Forum (2015): 2
Scopus rating (2014): 2.41 2.104
Web of Science (2014): 4.494 5.33 4.6 0.822 0.12645 1.042
Publication Forum (2014): 2
Scopus rating (2013): 2.412 2.503
Publication Forum (2013): 2
Scopus rating (2012): 2.389 2.465
Publication Forum (2012): 2
Scopus rating (2011): 2.314 2.508
Scopus rating (2010): 2.086 2.355
Scopus rating (2009): 1.912 2.231
Scopus rating (2008): 1.734 2.732
Scopus rating (2007): 1.529 2.423
Scopus rating (2006): 1.315 1.98
Scopus rating (2005): 1.269 2.006
Scopus rating (2004): 1.197 1.659
Scopus rating (2003): 0.948 1.639
Scopus rating (2002): 0.882 1.3
Scopus rating (2001): 0.541 1.208
Scopus rating (2000): 0.464 1.049
Scopus rating (1999): 0.669 1.061
Original language: English
DOIs:
10.1016/j.biortech.2011.01.028

Bibliographical note
Contribution: organisation=keb bio,FACT1=1
Source: researchoutputwizard
Carbon Nanotube Wiring of Donor-Acceptor Nanograins by Self-Assembly and Efficient Charge Transport

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Pages: 4615-4619
Publication date: 2011
Peer-reviewed: Yes

Publication information
Volume: 50
Issue number: 20
ISSN (Print): 1433-7851
Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 5.8 2.104
Publication Forum (2016): 3
Scopus rating (2015): 5.958 2.235
Web of Science (2015): 11.709 12.111 5.8 2.937 0.55213 3.432
Scopus rating (2014): 5.805 2.309
Web of Science (2014): 11.261 12.06 5.8 2.61 0.53069 3.39
Publication Forum (2014): 3
Scopus rating (2013): 5.681 2.204
Publication Forum (2013): 3
Scopus rating (2012): 6.362 2.338
Publication Forum (2012): 3
Scopus rating (2011): 6.062 2.387
Scopus rating (2010): 5.858 2.31
Scopus rating (2009): 5.52 2.218
Scopus rating (2008): 5.438 2.115
Scopus rating (2007): 4.406 1.87
Scopus rating (2006): 4.71 2.119
Scopus rating (2005): 4.7 2.295
Scopus rating (2004): 4.165 2.166
Scopus rating (2003): 3.41 2.126
Scopus rating (2002): 3.659 2.146
Scopus rating (2001): 3.695 2.07
Scopus rating (2000): 3.793 2.217
Scopus rating (1999): 3.59 2.156
Original language: English
DOIs:
10.1002/anie.201007065

Bibliographical note
Contribution: organisation=keb kemi
Source: researchoutputwizard
Source-ID: 7448
Research output: Scientific - peer-review › Article
Dynamics of Photoinduced Charge Transfer of Fullerene Based Donor-Acceptor Systems: From Solution to Organized Molecular Films
Effect of Anion Ligation on Electron Transfer of Double-Linked Zinc Porphyrin - Fullerene Dyad

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Al-Subi, A. H., Niemi, M., Tkachenko, N. V., Lemmetyinen, H.
Pages: 3263-3271
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 115
Issue number: 15
ISSN (Print): 1089-5639
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.258 0.98
Publication Forum (2016): 1
Scopus rating (2015): 1.179 1.106
Web of Science (2015): 2.883 2.709 8.1 0.758 0.0807 0.729
Publication Forum (2015): 1
Scopus rating (2014): 1.154 1.071
Web of Science (2014): 2.693 2.713 7.6 0.676 0.09689 0.777
Publication Forum (2014): 3
Scopus rating (2013): 1.194 1.102
Publication Forum (2013): 3
Scopus rating (2012): 1.494 1.124
Publication Forum (2012): 3
Scopus rating (2011): 1.402 1.135
Scopus rating (2010): 1.466 1.102
Scopus rating (2009): 1.562 1.132
Scopus rating (2008): 1.787 1.093
Scopus rating (2007): 1.907 1.136
Scopus rating (2006): 1.728 1.195
Scopus rating (2005): 1.789 1.215
Scopus rating (2004): 1.669 1.224
Scopus rating (2003): 1.75 1.241
Scopus rating (2002): 1.81 1.196
Scopus rating (2001): 1.732 1.224
Scopus rating (1999): 1.507 1.592
Original language: English
Effects of fullerene encapsulation on structure and photophysical properties of porphyrin-linked single-walled carbon nanotubes

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Umeyama, T., Mihara, J., Hayashi, H., Kadota, N., Chukharev, V., Tkachenko, N., Lemmetyinen, H., Yoshida, K., Isoda, S., Imahori, H.
Pages: 11781-11783
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Chemical Communications
Volume: 47
Issue number: 42
ISSN (Print): 1359-7345
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.506 1.159
Publication Forum (2016): 2
Scopus rating (2015): 2.664 1.314
Web of Science (2015): 6.567 6.628 4.6 1.713 0.36883 1.538
Publication Forum (2015): 2
Scopus rating (2014): 2.701 1.446
Web of Science (2014): 6.834 6.779 4.4 1.493 0.35082 1.58
Publication Forum (2014): 3
Scopus rating (2013): 2.755 1.38
Publication Forum (2013): 3
Scopus rating (2012): 3.09 1.347
Publication Forum (2012): 3
Scopus rating (2011): 2.857 1.322
Scopus rating (2010): 2.709 1.232
Scopus rating (2009): 2.588 1.252
Scopus rating (2008): 2.791 1.236
Scopus rating (2007): 2.851 1.237
Scopus rating (2006): 2.366 1.183
Scopus rating (2005): 2.129 1.15
Scopus rating (2004): 1.954 1.158
Scopus rating (2003): 1.644 1.098
Scopus rating (2002): 1.956 1.19
Scopus rating (2001): 1.817 1.098
Scopus rating (1999): 1.454 0.947
Original language: English
DOIs:
10.1039/c1cc15011a
Electronic Structure Manipulation of (Benzothiazole)zinc Complexes: Synthesis, Optical and Electrochemical Studies of 5-Substituted Derivatives

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Dey, S., Efimov, A., Giri, C., Rissanen, K., Lemmetyinen, H.
Pages: 6226-6232
Publication date: 2011
Peer-reviewed: Yes

Publication Information
Volume: 2011
Issue number: 31
ISSN (Print): 1434-193X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.133 0.653
Publication Forum (2016): 1
Scopus rating (2015): 1.198 0.758
Web of Science (2015): 3.068 2.971 5.5 0.777 0.04165 0.677
Publication Forum (2015): 1
Scopus rating (2014): 1.181 0.767
Web of Science (2014): 3.065 3.034 5.3 0.744 0.04326 0.703
Publication Forum (2014): 3
Scopus rating (2013): 1.292 0.796
Publication Forum (2013): 3
Scopus rating (2012): 1.471 0.811
Publication Forum (2012): 3
Scopus rating (2011): 1.536 0.857
Scopus rating (2010): 1.572 0.785
Scopus rating (2009): 1.497 0.778
Scopus rating (2008): 1.652 0.759
Scopus rating (2007): 1.711 0.84
Scopus rating (2006): 1.505 0.849
Scopus rating (2005): 1.246 0.763
Scopus rating (2004): 1.2 0.81
Scopus rating (2003): 1.19 0.802
Scopus rating (2002): 1.382 0.829
Scopus rating (2001): 1.159 0.816
Scopus rating (2000): 1.192 1.048
Scopus rating (1999): 0.877 0.976
Original language: English
DOIs:
10.1002/ejoc.201100186

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 5881
Enhanced performance and stability of inverted organic solar cells by using novel zinc-benzothiazole complexes as anode buffer layer

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Dey, S., Vivo, P., Efimov, A., Lemmetyinen, H.
Pages: 15587-15592
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Chemistry
Volume: 21
ISSN (Print): 0959-9428
Ratings:
Publication Forum (2017): 3
Publication Forum (2016): 3
Scopus rating (2015): 2.452 2.236
Scopus rating (2014): 2.457 2.296
Publication Forum (2014): 3
Scopus rating (2013): 2.249 1.84
Publication Forum (2013): 3
Scopus rating (2012): 2.771 1.523
Publication Forum (2012): 3
Scopus rating (2011): 2.616 1.565
Scopus rating (2010): 2.602 1.484
Scopus rating (2009): 2.526 1.529
Scopus rating (2008): 2.587 1.658
Scopus rating (2007): 2.623 1.591
Scopus rating (2006): 2.375 1.551
Scopus rating (2005): 1.983 1.501
Scopus rating (2004): 1.525 1.356
Scopus rating (2003): 1.509 1.39
Scopus rating (2002): 1.617 1.505
Scopus rating (2001): 1.479 1.552
Scopus rating (2000): 1.386 1.35
Scopus rating (1999): 1.263 1.423
Original language: English
DOIs:
10.1039/c1jm13256c

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 5883
Research output: Scientific - peer-review › Article

Excitation energy transfer in the LHC-II trimer: from carotenoids to chlorophylls in space and time

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Fused Alq3 derivatives: syntheses and photophysical characteristics

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Heiskanen, J. P., Tolkki, A. E., Lemmetyinen, H. J., Hormi, O. E. O.
Pages: 14766-14775
Publication date: 2011
Peer-reviewed: Yes
Indole-olefin-oxazoline (IndOlefOx)-ligands: synthesis and utilization in asymmetric Rh-catalyzed conjugate addition

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Kuuloja, N., Tois, J., Franzen, R.
Pages: 468-475
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Tetrahedron : Asymmetry
Volume: 22
Issue number: 4
ISSN (Print): 0957-4166
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.751 0.663
Publicaton Forum (2016): 1
Scopus rating (2015): 0.777 0.713
Optical, Electrochemical, and Photovoltaic Effects of an Electron-Withdrawing Tetrafluorophenylene Bridge in a Push-Pull Porphyrin Sensitizer Used for Dye-Sensitized Solar Cells

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Pages: 14415-14424
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 115
Issue number: 29
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Photochemical processes for dithiocarbamate metal complexes. Photochemistry of NiII(n-Bu2NCS2)2 complex in CCl4

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Kolomeets, A. V., Plyusnin, V. F., Grivin, V. P., Larionov, S. V., Lemmetyinen, H.
Pages: 164-172
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Photochemistry and Photobiology, A: Chemistry
Volume: 220
Issue number: 2-3
ISSN (Print): 1010-6030
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.732 0.841
Publication Forum (2016): 1
Scopus rating (2015): 0.72 0.86
Web of Science (2015): 2.477 2.573 9.8 0.619 0.01027 0.521
Publication Forum (2015): 1
Scopus rating (2014): 0.782 0.97
Web of Science (2014): 2.495 2.549 9.4 0.609 0.01139 0.538
Publication Forum (2014): 1
Scopus rating (2013): 0.818 1.006
Publication Forum (2013): 1
Scopus rating (2012): 0.919 1.116
Publication Forum (2012): 1
Scopus rating (2011): 0.97 1.342
Scopus rating (2010): 1.021 1.05
Scopus rating (2009): 1.163 1.191
Scopus rating (2008): 1.04 1.137
Scopus rating (2007): 1.175 1.364
Scopus rating (2006): 0.996 1.263
Scopus rating (2005): 1.102 1.436
Photochemistry of Dithiocarbamate Cu(II) Complex in CCl4

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Plyusnin, V. F., Kolomeets, A. V., Grivin, V. P., Larionov, S. V., Lemmetyinen, H.
Pages: 1763-1773
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 115
Issue number: 10
ISSN (Print): 1089-5639
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.258 0.98
Publication Forum (2016): 1
Scopus rating (2015): 1.179 1.106
Web of Science (2015): 2.883 2.709 8.1 0.758 0.0807 0.729
Publication Forum (2015): 1
Scopus rating (2014): 1.154 1.071
Web of Science (2014): 2.693 2.713 7.6 0.676 0.09689 0.777
Publication Forum (2014): 3
Scopus rating (2013): 1.194 1.102
Publication Forum (2013): 3
Scopus rating (2012): 1.494 1.124
Publication Forum (2012): 3
Scopus rating (2011): 1.402 1.135
Scopus rating (2010): 1.466 1.102
Scopus rating (2009): 1.562 1.132
Scopus rating (2008): 1.787 1.093
Scopus rating (2007): 1.907 1.136
Scopus rating (2006): 1.728 1.195
Scopus rating (2005): 1.789 1.215
Scopus rating (2004): 1.669 1.224
Scopus rating (2003): 1.751 1.241
Scopus rating (2002): 1.811 1.196
Scopus rating (2001): 1.732 1.224
Photochromic processes in di(mercaptoquinolinato)Ni(II) complex and perfluor diphenyl disulfide solutions

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Vorobyev, D., Kolomeets, A., Ivanov, Y., Bogdanchikov, G., Grivin, V., Plyusnin, V., Larionov, S., Lemmetyinen, H.
Pages: 1196-1202
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Photochemical & Photobiological Sciences
Volume: 10
Issue number: 7
ISSN (Print): 1474-905X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.722 0.799
Publication Forum (2016): 1
Scopus rating (2015): 0.805 0.811
Web of Science (2015): 2.235 2.673 6.0 0.823 0.01042 0.673
Publication Forum (2015): 1
Scopus rating (2014): 0.874 0.946
Web of Science (2014): 2.267 2.618 5.6 0.492 0.01153 0.699
Publication Forum (2014): 2
Scopus rating (2013): 0.989 1.006
Publication Forum (2013): 2
Scopus rating (2012): 1.049 0.919
Publication Forum (2012): 2
Scopus rating (2011): 1.013 0.962
Scopus rating (2010): 1.082 0.927
Scopus rating (2009): 0.983 1.115
Scopus rating (2008): 0.936 0.872
Scopus rating (2007): 1.09 0.957
Scopus rating (2006): 0.838 0.914
Scopus rating (2005): 0.938 1.061
Scopus rating (2004): 0.667 1.098
Scopus rating (2003): 0.492 0.793
Original language: English
DOIs:
10.1039/c1pp05061c

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 7536
Research output: Scientific - peer-review » Article
Photocurrent generation in fullerene-phthalocyanine composite by in situ cationic polymerization

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Lintinen, K., Storbacka, L., Efimov, A., Tolkki, A., Tkachenko, N., Lemmetyinen, H.
Pages: 909-916
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Solar Energy Materials and Solar Cells
Volume: 95
Issue number: 3
ISSN (Print): 0927-0248
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.587 1.71
Publication Forum (2016): 2
Web of Science (2015): 4.732 5.016 5.9 1.476 0.04281 1.16
Publication Forum (2015): 2
Scopus rating (2014): 2.204 2.396
Web of Science (2014): 5.337 5.755 5.6 1.042 0.04651 1.288
Publication Forum (2014): 2
Scopus rating (2013): 2.174 2.582
Publication Forum (2013): 2
Scopus rating (2012): 2.435 2.707
Publication Forum (2012): 2
Scopus rating (2011): 2.175 2.638
Scopus rating (2010): 2.524 2.121
Scopus rating (2009): 1.991 1.977
Scopus rating (2008): 1.654 1.458
Scopus rating (2007): 1.359 1.488
Scopus rating (2005): 1.141 1.619
Scopus rating (2004): 0.932 1.178
Scopus rating (2003): 0.992 1.34
Scopus rating (2002): 1.042 1.114
Scopus rating (2001): 0.896 1.235
Scopus rating (2000): 0.828 0.986
Scopus rating (1999): 0.701 0.75
Original language: English
DOIs:
10.1016/j.solmat.2010.11.018

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 6635
Research output: Scientific - peer-review » Article

Photoinduced electron transfer in a directly linked meso-triphenylamine zinc porphyrin-quinone dyad

General information
Photoinduced intra- and intermolecular electron transfer in solutions and in solid organized molecular assemblies

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Lemmetyinen, H., Tkachenko, N. V., Efimov, A., Niemi, M.

Publication information
Journal: Journal of Porphyrins and Phthalocyanines
Volume: 15
Issue number: 5-6
ISSN (Print): 1088-4246
Ratings:
Scopus rating (2017): 1
Scopus rating (2016): 0.354 0.379
Scopus rating (2015): 0.419 0.467
Web of Science (2015): 1.087 1.387 7.0 0.323 0.00257 0.267
Publication Forum (2015): 1
Scopus rating (2014): 0.486 0.545
Web of Science (2014): 1.397 1.603 6.7 0.179 0.00338 0.326
Publication Forum (2014): 1
Scopus rating (2013): 0.537 0.602
Publication Forum (2013): 1
Scopus rating (2012): 0.62 0.537
Publication Forum (2012): 1
Scopus rating (2011): 0.553 0.612
Scopus rating (2010): 0.564 0.46
Scopus rating (2009): 0.511 0.447
Scopus rating (2008): 0.572 0.481
Scopus rating (2007): 0.669 0.481
Scopus rating (2006): 0.625 0.529
Scopus rating (2005): 0.632 0.593
Scopus rating (2004): 0.646 0.667
Scopus rating (2003): 0.591 0.88
Scopus rating (2002): 0.86 1.153
Scopus rating (2001): 0.796 1.08
Scopus rating (2000): 0.863 0.759
Scopus rating (1999): 0.557 0.635
Original language: English
DOIs:
10.1142/S108842461100329X

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 7565
Research output: Scientific - peer-review › Article
Photoinduced processes in chromophore-gold nanoparticle assemblies

**General information**

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Kotiaho, A., Lahtinen, R., Lemmetyinen, H.
Pages: 813-821
Publication date: 2011
Peer-reviewed: Yes

**Publication information**

Journal: Pure and Applied Chemistry
Volume: 83
Photophysics and photoelectrochemical properties of nanohybrids consisting of fullerene-encapsulated single-walled carbon nanotubes and poly(3-hexylthiophene)

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Pages: 741-750
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Energy & Environmental Science
Volume: 4
Issue number: 3
ISSN (Print): 1754-5692
Ratings:
Poly(b-amino ester)-DNA complexes: Time-resolved fluorescence and cellular transfection studies

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Vuorimaa, E., Ketola, T., Green, J. J., Hanzlikova, M., Lemmetyinen, H., Langer, R., Anderson, D. G., Urtti, A., Yliperttula, M.
Pages: 171-176
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Controlled Release
Volume: 154
Issue number: 2
ISSN (Print): 0168-3659
Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 2.393 1.84
Publication Forum (2016): 3
Scopus rating (2015): 2.725 2.08
Web of Science (2015): 7.441 8.407 6.9 1.33 0.05686 1.857
Scopus rating (2014): 2.416 2.092
Web of Science (2014): 7.705 8.097 7.0 1.138 0.05251 1.792
Publication Forum (2014): 2
Scopus rating (2013): 2.416 2.044
Publication Forum (2013): 2
Scopus rating (2012): 2.417 2.061
Publication Forum (2012): 2
Preparation of triethylammonium tetra-arylborates (TETABs): coupling partners for the Suzuki reaction

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Kuuloja, N., Kymlälä, T. M., Tois, J. E., Sjöholm, R. E., Franzen, R. G.
Pages: 1052-1063
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Synthetic Communications
Volume: 41
Issue number: 7
ISSN (Print): 0039-7911
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.355 0.392
Publication Forum (2016): 1
Scopus rating (2015): 0.36 0.504
Web of Science (2015): 1.065 1.063 10.0 0.201 0.00534 0.181
Publication Forum (2015): 1
Scopus rating (2014): 0.306 0.462
Web of Science (2014): 0.929 0.995 >10.0 0.207 0.00562 0.174
Publication Forum (2014): 1
Scopus rating (2013): 0.367 0.52
Publication Forum (2013): 1
Scopus rating (2012): 0.425 0.567
Publication Forum (2012): 1
Scopus rating (2011): 0.432 0.543
Scopus rating (2010): 0.408 0.493
Scopus rating (2009): 0.459 0.55
Scopus rating (2008): 0.458 0.522
Scopus rating (2007): 0.47 0.605
Role of Polyplex Intermediate Species on Gene Transfer Efficiency: Polyethylenimine-DNA Complexes and Time-Resolved Fluorescence Spectroscopy

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Ketola, T., Hanzlikova, M., Urtti, A., Lemmetyinen, H., Yliperttula, M., Vuorimaa, E.
Pages: 1895-1902
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 115
Issue number: 8
ISSN (Print): 1520-6106
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.348 1.02
Publication Forum (2016): 1
Scopus rating (2015): 1.367 1.096
Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
Publication Forum (2015): 1
Scopus rating (2014): 1.44 1.14
Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
Publication Forum (2014): 3
Scopus rating (2013): 1.494 1.2
Publication Forum (2013): 3
Scopus rating (2012): 1.92 1.251
Publication Forum (2012): 3
Scopus rating (2011): 1.78 1.226
Scopus rating (2010): 1.849 1.214
Scopus rating (2009): 2.232 1.349
Scopus rating (2008): 2.543 1.381
Scopus rating (2007): 2.346 1.282
Scopus rating (2006): 2.369 1.415
Scopus rating (2005): 2.275 1.474
Scopus rating (2004): 2.148 1.511
Self-assembled monolayers (SAMs) of porphyrin deposited inside photonic crystal fibre (PCF)

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Optoelectronics Research Centre, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Veselov, A. A., Thur, C., Efimov, A., Guina, M., Lemmetyinen, H., Tkachenko, N. V.
Pages: 1858-1861
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Physica Status Solidi A: Applications And Materials Science
Volume: 208
Issue number: 8
ISSN (Print): 1862-6300
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.683 0.849
Publication Forum (2016): 1
Scopus rating (2015): 0.688 0.89
Web of Science (2015): 1.648 1.446 9.7 0.514 0.01361 0.404
Publication Forum (2015): 1
Scopus rating (2014): 0.692 0.901
Web of Science (2014): 1.616 1.481 9.5 0.385 0.01493 0.42
Publication Forum (2014): 1
Scopus rating (2013): 0.772 0.904
Publication Forum (2013): 1
Scopus rating (2012): 0.865 0.929
Publication Forum (2012): 1
Scopus rating (2011): 0.964 0.981
Scopus rating (2010): 0.872 0.794
Scopus rating (2009): 0.918 0.831
Scopus rating (2008): 0.818 0.791
Scopus rating (2007): 1.003 0.992
Scopus rating (2006): 0.833 0.791
Scopus rating (2005): 0.776 0.718
Scopus rating (2004): 0.697 0.632
Scopus rating (2003): 0.832 0.73
Scopus rating (2002): 0.824 0.806
Scopus rating (2001): 0.824 0.787
Scopus rating (2000): 1.107 0.914
Structure of porphyrin-fullerene dyad monolayer on the water surface and solid substrate

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Number of pages: 7
Pages: 157-163
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Crystallography Reports
Volume: 56
Issue number: 1
ISSN (Print): 1063-7745
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.313 0.644
Publication Forum (2016): 1
Scopus rating (2015): 0.286 0.583
Web of Science (2015): 0.561 0.572 >10.0 0.162 0.00176 0.137
Publication Forum (2015): 1
Scopus rating (2014): 0.307 0.666
Web of Science (2014): 0.489 0.559 >10.0 0.148 0.00211 0.153
Publication Forum (2014): 1
Scopus rating (2013): 0.322 0.636
Publication Forum (2013): 1
Scopus rating (2012): 0.384 0.65
Publication Forum (2012): 1
Scopus rating (2011): 0.215 0.333
Scopus rating (2010): 0.477 0.583
Scopus rating (2009): 0.189 0.3
Scopus rating (2008): 0.22 0.202
Scopus rating (2007): 0.148 0.188
Scopus rating (2006): 0.236 0.62
Scopus rating (2005): 0.262 0.641
Scopus rating (2004): 0.209 0.446
Scopus rating (2003): 0.181 0.292
Scopus rating (2002): 0.128 0.132
Scopus rating (2001): 0.222 0.34
Scopus rating (2000): 0.258 0.399
Scopus rating (1999): 0.136 0.157
Study of PEGylated Lipid Layers as a Model for PEGylated Liposome Surfaces: Molecular Dynamics Simulation and Langmuir Monolayer Studies

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry, Computational Science X (CompX), Frontier Photonics
Pages: 7788-7798
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Langmuir
Volume: 27
Issue number: 12
ISSN (Print): 0743-7463
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.55 1.188
Publication Forum (2016): 2
Scopus rating (2015): 1.686 1.308
Web of Science (2015): 3.993 4.21 7.6 0.67 0.16509 1.043
Publication Forum (2015): 2
Scopus rating (2014): 1.816 1.391
Web of Science (2014): 4.457 4.543 7.2 0.682 0.18462 1.096
Publication Forum (2014): 3
Scopus rating (2013): 1.895 1.356
Publication Forum (2013): 3
Scopus rating (2012): 2.177 1.382
Publication Forum (2012): 3
Scopus rating (2011): 2.051 1.357
Scopus rating (2010): 2.148 1.4
Scopus rating (2009): 2.156 1.351
Scopus rating (2008): 2.383 1.34
Scopus rating (2007): 2.449 1.434
Scopus rating (2006): 2.375 1.428
Scopus rating (2005): 2.157 1.463
Scopus rating (2004): 1.963 1.458
Scopus rating (2003): 1.953 1.4
Scopus rating (2002): 2.011 1.489
Scopus rating (2001): 2.01 1.382
Scopus rating (2000): 2.039 1.479
Scopus rating (1999): 1.719 1.496
Original language: English
DOIs:
Synthesis and photovoltaic properties of thiopheneimide-fused thiophene alternating copolymers with different alkyl side chains

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Umeyama, T., Oodoi, M., Yoshikawa, O., Sagawa, T., Yoshikawa, S., Evgenia, D., Tezuka, N., Matano, Y., Stranius, K., Tkachenko, N., Lemmetyinen, H., Imahori, H.
Pages: 12454-12461
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Chemistry
Volume: 21
Issue number: 33
ISSN (Print): 0959-9428
Ratings:
Publication Forum (2017): 3
Publication Forum (2016): 3
Scopus rating (2015): 2.452 2.236
Scopus rating (2014): 2.457 2.296
Publication Forum (2014): 3
Scopus rating (2013): 2.249 1.84
Publication Forum (2013): 3
Scopus rating (2012): 2.771 1.523
Publication Forum (2012): 3
Scopus rating (2011): 2.616 1.565
Scopus rating (2010): 2.602 1.484
Scopus rating (2009): 2.526 1.529
Scopus rating (2008): 2.587 1.658
Scopus rating (2007): 2.623 1.591
Scopus rating (2006): 2.375 1.551
Scopus rating (2005): 1.983 1.501
Scopus rating (2004): 1.525 1.356
Scopus rating (2003): 1.509 1.39
Scopus rating (2002): 1.617 1.505
Scopus rating (2001): 1.479 1.552
Scopus rating (2000): 1.386 1.35
Scopus rating (1999): 1.263 1.423
Original language: English
DOIs:
10.1039/C1JM11531F

Bibliographical note
Contribution: organisation=fys,FACT1=0.5
Source: researchoutputwizard
Source-ID: 7309
Research output: Scientific - peer-review › Article

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 7447
Research output: Scientific - peer-review › Article
Ultrafast pump-probe spectroscopy of IrCl62- complex in alcohol solutions

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Pages: 18168-18178
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 13
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
Publication Forum (2016): 1
Scopus rating (2015): 1.771 1.244
Web of Science (2015): 4.449 4.273 4.1 1.017 0.19255 1.158
Publication Forum (2015): 1
Scopus rating (2014): 1.772 1.253
Web of Science (2014): 4.493 4.219 3.9 0.991 0.17937 1.209
Publication Forum (2014): 3
Scopus rating (2013): 1.715 1.216
Publication Forum (2013): 3
Scopus rating (2012): 1.916 1.184
Publication Forum (2012): 3
Scopus rating (2011): 1.697 1.203
Scopus rating (2010): 1.802 1.196
Scopus rating (2009): 2.127 1.369
Scopus rating (2008): 2.158 1.211
Scopus rating (2007): 1.84 1.138
Scopus rating (2006): 1.467 1.128
Scopus rating (2005): 1.389 1.104
Scopus rating (2004): 1.173 1.007
Scopus rating (2003): 1.093 0.925
Scopus rating (2002): 1.122 0.973
Scopus rating (2001): 1.09 0.914
Scopus rating (2000): 0.948 1.068
Scopus rating (1999): 0.121 0.0
Original language: English
DOIs:
10.1039/c1cp90147h

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 5861
Research output: Scientific - peer-review › Article
Photopolymerizable liquid fullerene, phthalocyanine and porphyrin derivatives: synthesis, analysis and photocurrent generation

Photopolymerizable liquid monomers of fullerene, phthalocyanine and porphyrin were synthesized, polymerized and used as photoactive materials in organic solar cell structures. The design of the molecules requires the combination of three major parts: the functional core of the original molecules, alkylic side chains for liquid state and polymerizable end groups. The harsh conditions of the chromophore synthesis require a modular design, where the chromophore core and polymerizable tails are synthesized separately, and combined later by mild acylation. A means of ultra-thin-film polymerization, both photo and thermal, were devised. All of the chromophores could be polymerized as ultrathin films. Because of their high absorbances, it was possible to use UV-Vis spectroscopy to monitor polymerization indirectly; as the films were of only a few monomer units thick, it was possible to dissolve the unreacted monomer residues afterwards and thus determine polymerization degrees as a function of the absorbance of the polymerized film. The molecules were studied extensively to yield the parameters for thin film preparation, photopolymerization, and photocurrent generation. While the monomers were liquid at room temperature, the hardness of the polymers was that of crosslinked epoxy plastics. The porphyrin monomer was used to study photopolymerization kinetics due to its unique self-photoinitiating properties. Polarization modulation IR spectroscopy was used to study real-time photopolymerization of the porphyrin monomer at varying temperatures, yielding rate constants and the activation energy of the reaction. It was the first published study of ultra-thin-film polymerization kinetics. The monomers were polymerized in situ to form bilayers, bulk heterojunctions or hybrids of both, to create a photoactive structure for photocurrent generation. An extensive set of samples was prepared and studied. The monomers employed in this work were optimized for easy photopolymerizability and as such produced unoptimal power conversion efficiency. Nevertheless the basic structure of the polymer lends itself well to modification for improved organic photovoltaic performance.
Computational study of charge transfer in a porphine: quinone complex and novel alkoxypyridylindolizine derivatives

Finding ways to control electron transfer (ET) between molecules or molecular systems and to investigate efficient theoretical methods capable of describing ET is important for being able to design better molecular electronic devices. In this Thesis the capability of computational methods based on density functional theory (DFT) to describe charge transfer is studied in two molecular systems. In addition, the possibility to control ET by strong electric fields is investigated. The molecular structure and excited states of three alkoxypyridylindolizine derivatives are studied by using DFT and time-dependent DFT (TDDFT). In addition, the influence of an external electrostatic field of the order of magnitude of 109 V/m and of an electric field induced by ambient helical peptides on ET in a porphine–2,5-dimethyl-1,4-benzoquinone (PQ) complex is studied with TDDFT and the approximate coupled cluster singles and doubles (CC2) method. The calculations show that the absorption spectra of the studied indolizine derivatives are characterized by a band arising from the intramolecular CT between the indolizine ring and the pyridyl substituent attached to it and the hybrid functionals reproduce the experimental absorption spectra of the derivatives well within TDDFT. However, the same functionals are not as good in describing the fluorescence properties of the indolizine derivatives, namely the CT excited state of a derivative is obtained with too low an energy, which prevents the relaxation of the correct state. This problem can be circumvented by applying an exchange-correlation (XC) functional with a high fraction of Hartree–Fock (HF) exchange but this is done in the expense of the quantitative accuracy. According to the calculations, perturbation generated either by an external electrostatic field or by ambient Aib peptides affects the energies of the locally excited Q and B states of porphine in the PQ complex clearly less than the energy of the lowest CT state. Hence, it is possible to select a locally excited state (Q or B) of the PQ complex whose photoexcitation leads to ET from porphine to quinone. The results presented show that TDDFT applied with the current XC functionals provides an efficient way to study the qualitative picture of the excited states under the influence of an external electric field.
Multilayered thin films for organic photovoltaics

This work investigates the photoinduced interactions between different organic chromophores, thus identifying possible materials for organic photovoltaic applications. The intermolecular electron transfer (ET) in layered structures centered on a covalently bridged porphyrin–fullerene dyad (P–F) was studied by means of electrical and spectroscopic methods. When excited, the dyad initiates the vectorial ET in the films, and secondary processes take place after the charge separation between the porphyrin and fullerene moieties of P–F. This study showed that violanthrone-79 (V-79) and two different perylene derivatives (PDI and PTCDI) were capable to accept electrons from the photoinduced fullerene anion of P–F.

Longer-lived electrical and spectroscopic signals were achieved when the film structures were expanded to multilayered configurations containing an electron-donor, the P–F dyad, and an electron-acceptor. The electron-donor material used was poly(3-hexylthiophene) (PHT). The film deposition technique was switched from the Langmuir–Blodgett (LB) to Langmuir–Schäfer (LS) or thermal evaporation methods in order to achieve stronger photoelectrical signal amplitudes. As a result of the information gained in the ET studies, photovoltaic devices were prepared based on the studied compounds. The photocurrent generated from the ultrathin film systems studied in this Thesis can be easily measured with a three-electrode photoelectrochemical cell. In fact, the deposition of a metal top-electrode on the solar cell would damage the underlying organics, thus leading to short-circuiting problems. However, since the liquid cells suffer of poor performances and low stability, it was aimed to build layered cells with a metal top-electrode. The first step in this direction was the optimization of the organics|top-electrode junction, in order to protect the thin organic films. This was achieved with the introduction of a thin tris-8-hydroxy-quinolato aluminum (Alq3) layer in the cell, which successfully enhanced both the efficiency and the lifetime of the devices. Finally, multilayered cells based on a donor–acceptor pair sandwiched between an electron-donor and an electron-acceptor were developed, demonstrating that it is possible to design photovoltaic devices starting from the valuable information offered by the ET studies. The molecule chosen to this aim was the phthalocyanine-fullerene dyad, H2Pc–C60ee, which could be easily deposited as spin-coated layer.
Boronic Acids and Esters in the Petasis-Borono Mannich Multicomponent Reaction

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: Candeias, N. R., Montalbano, F., Cal, P. M. S. D., Gois, P. M. P.
Keywords: (ALPHA-AMINO-ACIDS, BETA-TURN MIMETICS, N-ACYLIMINIUM IONS, STEREOSELECTIVE-SYNTHESIS, ORGANOBORONIC ACIDS, SOLID-PHASE, 3-COMPONENT REACTION, PRACTICAL SYNTHESIS, HYDROXY ALDEHYDES, FORMAL SYNTHESIS)
Number of pages: 25
Pages: 6169-6193
Publication date: Oct 2010
Peer-reviewed: Yes

Publication information
Journal: Chemical Reviews
Volume: 110
Issue number: 10
ISSN (Print): 0009-2665
Ratings:
Publication Forum (2017): 2
Publication Forum (2016): 2
Scopus rating (2015): 18.373 11.51
Web of Science (2015): 37.369 51.56 8.1 8.87 0.24548 15.263
Publication Forum (2015): 2
Scopus rating (2014): 18.369 11.47
Web of Science (2014): 46.568 50.679 8.0 7.381 0.22401 14.711
Publication Forum (2014): 3
Scopus rating (2013): 22.176 12.915
Publication Forum (2013): 3
Scopus rating (2012): 20.511 11.43
Publication Forum (2012): 3
Scopus rating (2008): 16.038 8.682
Scopus rating (2004): 11.196 8.924
Scopus rating (2002): 11.825 10.102
Scopus rating (2001): 11.072 10.832
Scopus rating (2000): 11.55 10.154
Original language: English
DOIs:
10.1021/cr100108k
NHC-Iron-Catalyzed Aerobic Oxidative Aromatic Esterification of Aldehydes using Boronic Acids

NHC-Iron complexes prepared in situ very efficiently afforded benzoates via the aerobic oxidative aromatic esterification of aldehydes with boronic acids. This method uses equimolar amounts of both the aldehyde and the boronic acid allowing the preparation of benzoates in yields up to 97%.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Lisbon, Universidade de Lisboa, Fac Farm, iMed UL
Authors: Rosa, J. N., Reddy, R. S., Candeias, N. R., Cal, P. M. S. D., Gois, P. M. P.
Keywords: (N-HETEROCYCLIC CARBENES, BAEYER-VILLIGER OXIDATION, CROSS-COUPLING REACTIONS, MOLECULAR-OXYGEN, ZINC-OXIDE, COMPLEXES, EFFICIENT, KETONES, ESTERS, POLYMERIZATION)
Number of pages: 4
Pages: 2686-2689
Publication date: 18 Jun 2010
Peer-reviewed: Yes

Publication information
Journal: Organic Letters
Volume: 12
Issue number: 12
ISSN (Print): 1523-7060
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.964 1.218
Publication Forum (2016): 2
Web of Science (2015): 6.732 6.033 5.5 1.566 0.17092 1.414
Publication Forum (2015): 2
Scopus rating (2014): 2.958 1.324
Web of Science (2014): 6.364 5.849 5.3 1.864 0.17383 1.407
Publication Forum (2014): 3
Scopus rating (2013): 3.144 1.329
Publication Forum (2013): 3
Scopus rating (2012): 3.312 1.355
Publication Forum (2012): 3
Scopus rating (2011): 3.271 1.377
Scopus rating (2010): 2.985 1.307
Scopus rating (2009): 3.048 1.37
Scopus rating (2007): 3.185 1.296
Scopus rating (2006): 2.936 1.352
Scopus rating (2005): 2.552 1.329
Scopus rating (2004): 2.515 1.262
Scopus rating (2003): 2.451 1.325
Scopus rating (2002): 2.787 1.311
Scopus rating (2001): 2.266 1.427
Scopus rating (2000): 1.893 1.206
Original language: English
DOIs:
10.1021/ol100302e
Source: WOS
Source-ID: 000283395800014
Research output: Scientific - peer-review › Literature review
New dirhodium complex with activity towards colorectal cancer

A novel dirhodium complex (Rh(2)(L-PheAla)(2)(OAc)(2)) is reported with strong activity towards human colon adenocarcinoma cells. Its effect was not accompanied by generation of reactive oxygen species (ROS) neither by activation of caspase-3. (C) 2010 Elsevier Ltd. All rights reserved.
Dimeric Quinidine-Catalyzed Enantioselective Aminooxygenation of Oxindoles: An Organocatalytic Approach to 3-
Hydroxyoxindole Derivatives

3-Hydroxyoxindoles are common structural motifs found in a vast array of natural and biologically active molecules. Most catalytic methods for the asymmetric syntheses of these compounds require the use of transition-metal catalysts. In contrast, alternative catalytic procedures involving organocatalysis are scarce. Herein we disclose a novel aminooxygenation of oxindoles with nitrosobenzene catalyzed by a newly designed quinidine dimer to afford the desired products in good yields with enantioselectivities up to 96%. These reactions allow one to construct a C-O bond at the C(3) position of oxindoles with the creation of an oxygen-containing tetrasubstituted chiral center and provide a new, general organocatalytic approach to the synthesis of 3-hydroxyoxindole derivatives.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: Bui, T., Candeias, N. R., Barbas, C. F.
Keywords: (ASYMMETRIC ADDITION, ARYLBORONIC ACIDS, ISATINS, HYDROXYLATION, NITROALKENES, 2-OXINDOLES,ALKALOIDS, ACCESS)
Number of pages: 2
Pages: 5574-5575
Publication date: 28 Apr 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of the American Chemical Society
Volume: 132
Issue number: 16
ISSN (Print): 0002-7863
Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 7.368 2.584
Publication Forum (2016): 3
Web of Science (2015): 13.038 12.376 8.0 2.831 0.79612 3.527
Scopus rating (2014): 6.273 2.578
Web of Science (2014): 12.113 11.726 8.0 2.607 0.81323 3.286
Publication Forum (2014): 3
Scopus rating (2013): 5.953 2.455
Publication Forum (2013): 3
Scopus rating (2012): 6.141 2.379
Publication Forum (2012): 3
Scopus rating (2011): 5.447 2.336
Scopus rating (2010): 5.076 2.132
Scopus rating (2008): 4.936 2.116
Scopus rating (2007): 5.023 2.126
Scopus rating (2005): 4.284 2.207
Scopus rating (2004): 3.754 2.178
Scopus rating (2002): 3.527 2.346
Scopus rating (2001): 3.449 2.199
Scopus rating (2000): 3.573 2.224
Scopus rating (1999): 3.56 2.182
Original language: English
DOIs:
10.1021/ja101032j
Water as the reaction medium for multicomponent reactions based on boronic acids

Water is a suitable medium for the Petasis-borono-Mannich multicomponent reaction. Salicylaldehyde, glyoxalic acid, glycoaldehyde and glyoxal were reacted with several boronic acids and different amines affording alkylaminophenols, 2H-chromenes, alpha-amino acids, alpha-amino alcohols and 2-hydroxymorpholines in good to high yields. An efficient new one-pot method for the assembly of boron-heterocycles based on amino-acids, boronic acids and salicylaldehyde using water as the reaction media is presented. The mechanisms of these reactions were studied by means of OFF calculations, and the effect of solvent on the calculated energy barriers was addressed, for different aldehydes.

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General information

State: Published

Ministry of Education publication type: A1 Journal article-refereed

Organisations: Univ Lisbon, Universidade de Lisboa, Fac Farm, IMed UL, Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, Dept Engn Quim & Biol, Ctr Quim Estrutural

Authors: Candeias, N. R., Cal, P. M. S. D., Andre, V., Duarte, M. T., Veiros, L. F., Gois, P. M. P.

Keywords: (Boron, Multicomponent reactions, Petasis reaction, Boron heterocycles, MOLECULAR-ORBITAL METHODS , DIELS-ALDER REACTIONS, POLARIZABLE CONTINUUM MODEL, GAUSSIAN-TYPE BASIS, ALPHA-AMINO-ACIDS, ORGANIC-REACTIONS, EQUILIBRIUM GEOMETRIES, TRANSITION-STATES, MANNICH REACTIONS, SOLVATION MODELS)

Number of pages: 10

Pages: 2736-2745

Publication date: 3 Apr 2010

Peer-reviewed: Yes

Publication information

Journal: Tetrahedron

Volume: 66

Issue number: 14

ISSN (Print): 0040-4020

Ratings:

Publication Forum (2017): 1

Scopus rating (2016): 0.907 0.742

Publication Forum (2016): 1

Scopus rating (2015): 0.954 0.84

Web of Science (2015): 2.645 2.621 9.6 0.609 0.04893 0.531

Publication Forum (2015): 1

Scopus rating (2014): 0.971 0.905

Web of Science (2014): 2.641 2.675 9.2 0.652 0.05691 0.575

Publication Forum (2014): 2

Scopus rating (2013): 1.101 0.92

Publication Forum (2013): 2

Scopus rating (2012): 1.32 0.999

Publication Forum (2012): 2

Scopus rating (2011): 1.476 1.094

Scopus rating (2010): 1.508 1.065

Scopus rating (2009): 1.534 1.124

Scopus rating (2008): 1.579 1.078

Scopus rating (2007): 1.639 1.116

Scopus rating (2006): 1.507 1.142

Scopus rating (2005): 1.354 1.138

Scopus rating (2004): 1.459 1.261

Scopus rating (2003): 1.448 1.265

Scopus rating (2002): 1.677 1.177

Scopus rating (2001): 1.46 1.178

Scopus rating (2000): 1.536 1.165
Absolute probe of surface chirality based on focused circularly polarized light

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research group: Nonlinear Optics, Research area: Optics, Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry
Authors: Huttunen, M. J., Virkki, M., Erkintalo, M., Vuorimaa, E., Efimov, A., Lemmetyinen, H., Kauranen, M.
Pages: 1826-1829
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Letters
Volume: 1
Issue number: 12
ISSN (Print): 1948-7185
Ratings:
Scopus rating (2016): 4.583 1.68
Scopus rating (2015): 4.233 1.829
Web of Science (2015): 8.539 7.803 3.0 1.971 0.11885 2.482
Web of Science (2014): 7.458 7.536 2.8 2.017 0.09524 2.425
Scopus rating (2013): 3.515 1.61
Scopus rating (2012): 3.943 1.751
Scopus rating (2012): 2
Original language: English
DOIs:
10.1016/j.tet.2010.01.084

Bibliographical note
Contribution: organisation=fys,FACT1=0.5
Contribution: organisation=keb kem,FACT2=0.5
Source: researchoutputwizard
Source-ID: 8125
Research output: Scientific - peer-review › Article

Absolute probe of surface chirality based on focused circular polarizations

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Research group: Nonlinear Optics, Research area: Optics, Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry
Authors: Huttunen, M., Virkki, M., Erkintalo, M., Vuorimaa, E., Efimov, A., Lemmetyinen, H., Kauranen, M.
Pages: 1 p
Publication date: 2010
Absolute probe of surface chirality based on focusing circularly-polarized light

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Research group: Nonlinear Optics, Research area: Optics, Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry
Authors: Huttunen, M. J., Virkki, M., Erkintalo, M., Vuorimaa, E., Efimov, A., Lemmetyinen, H., Kauranen, M.
Pages: 47
Publication date: 2010

Acidity sensor based on porphyrin self-assembled monolayers covalently attached to the surfaces of tapered fibres

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Optoelectronics Research Centre, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Veselov, A., Thur, C., Efimov, A., Guina, M., Lemmetyinen, H., Tkachenko, N.
Number of pages: 10
Pages: 1-10
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Measurement Science and Technology
Volume: 21
Issue number: 11, 115205
ISSN (Print): 0957-0233
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 0.668 1.173
Publication Forum (2016): 2
Scopus rating (2015): 0.687 1.303
Web of Science (2015): 1.492 1.537 8.2 0.3 0.01728 0.505
Publication Forum (2015): 2
Scopus rating (2014): 0.657 1.319
Web of Science (2014): 1.433 1.534 7.9 0.302 0.01783 0.499
Publication Forum (2014): 2
Scopus rating (2013): 0.555 1.244
Aluminum doped zinc oxide films grown by atomic layer deposition for organic photovoltaic devices

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Optoelectronics Research Centre, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Saarenpää, H., Niemi, T., Tukiainen, A., Lemmetyinen, H., Tkachenko, N.
Pages: 1379-1383
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Solar Energy Materials and Solar Cells
Volume: 94
Issue number: 8
ISSN (Print): 0927-0248
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.587 1.71
Publication Forum (2016): 2
Web of Science (2015): 4.732 5.016 5.9 1.476 0.04281 1.16
Publication Forum (2015): 2
Scopus rating (2014): 2.204 2.396
Web of Science (2014): 5.337 5.755 5.6 1.042 0.04651 1.288
Publication Forum (2014): 2
Scopus rating (2013): 2.174 2.582
Publication Forum (2013): 2
Scopus rating (2012): 2.435 2.707
Publication Forum (2012): 2
A novel and efficient synthesis of 3-aminomethyl-N-tosyl-indazoles

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Kylmälä, T., Hämäläinen, A., Kuuloja, N., Tois, J., Franzen, R.
Pages: 8854-8861
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Tetrahedron
Volume: 66
Issue number: 46
ISSN (Print): 0040-4020
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.907 0.742
Publication Forum (2016): 1
Scopus rating (2015): 0.954 0.84
Web of Science (2015): 2.645 2.621 9.6 0.609 0.04893 0.531
Publication Forum (2015): 1
Scopus rating (2014): 0.971 0.905
Web of Science (2014): 2.641 2.675 9.2 0.652 0.05691 0.575
Publication Forum (2014): 2
Scopus rating (2013): 1.101 0.92
Publication Forum (2013): 2
Scopus rating (2012): 1.32 0.999
Publication Forum (2012): 2
Scopus rating (2011): 1.476 1.094
Scopus rating (2010): 1.508 1.065
Scopus rating (2009): 1.534 1.124
Scopus rating (2008): 1.579 1.078
Scopus rating (2007): 1.639 1.116
A TDDFT study of the fluorescence properties of three alkoxy pyridylindolizine derivatives

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry
Authors: Aittala, P. J., Cramariuc, O., Hukka, T. I., Vasilescu, M., Bandula, R., Lemmetyinen, H.
Pages: 7094-7101
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 114
Issue number: 26
ISSN (Print): 1089-5639
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.258 0.98
Publication Forum (2016): 1
Scopus rating (2015): 1.179 1.106
Web of Science (2015): 2.883 2.709 8.1 0.758 0.0807 0.729
Publication Forum (2015): 1
Scopus rating (2014): 1.154 1.071
Web of Science (2014): 2.693 2.713 7.6 0.676 0.09689 0.777
Publication Forum (2014): 3
Scopus rating (2013): 1.194 1.102
Publication Forum (2013): 3
Scopus rating (2012): 1.494 1.124
Publication Forum (2012): 3
Scopus rating (2011): 1.402 1.135
Scopus rating (2010): 1.466 1.102
Scopus rating (2009): 1.562 1.132
Scopus rating (2008): 1.787 1.093
Scopus rating (2007): 1.907 1.136
Scopus rating (2006): 1.728 1.195
Scopus rating (2005): 1.789 1.215
Scopus rating (2004): 1.669 1.224
Scopus rating (2003): 1.75 1.241
Carrier dynamics in 1300 nm AlGaInAs quantum wells metamorphically grown on GaAs

Catalytic asymmetric total synthesis of tangutorine
Close proximity dibenzo[a,c]phenazine-fullerene dyad: synthesis and photoinduced singlet energy transfer

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Dubey, R. K., Kumpulainen, T., Efimov, A., Tkachenko, N. V., Lemmetyinen, H.
Pages: 3428-3436
Publication date: 2010
Peer-reviewed: Yes

Publication information
Volume: 2010
Issue number: 18
ISSN (Print): 1434-193X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.133 0.653
Publication Forum (2016): 1
Scopus rating (2015): 1.198 0.758
Web of Science (2015): 3.068 2.971 5.5 0.777 0.04165 0.677
Publication Forum (2015): 1
Scopus rating (2014): 1.181 0.767
Web of Science (2014): 3.065 3.034 5.3 0.744 0.04326 0.703
Publication Forum (2014): 3
Scopus rating (2013): 1.292 0.796
Publication Forum (2013): 3
Scopus rating (2012): 1.471 0.811
Publication Forum (2012): 3
Scopus rating (2011): 1.536 0.857
Scopus rating (2010): 1.572 0.785
Copper-catalyzed cyclization of Z-oximes into 3-methyl-1,2-benzisoxazoles

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Udd, S., Jokela, R., Franzen, R., Tois, J.
Pages: 1030-1033
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Tetrahedron Letters
Volume: 51
ISSN (Print): 0040-4039
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.754 0.635
Publication Forum (2016): 1
Scopus rating (2015): 0.757 0.747
Web of Science (2015): 2.347 2.212 >10.0 0.58 0.05325 0.416
Publication Forum (2015): 1
Scopus rating (2014): 0.794 0.796
Web of Science (2014): 2.379 2.286 >10.0 0.558 0.06047 0.438
Publication Forum (2014): 2
Scopus rating (2013): 0.904 0.802
Publication Forum (2013): 2
Scopus rating (2012): 1.084 0.844
Publication Forum (2012): 2
Scopus rating (2011): 1.216 0.949
Scopus rating (2010): 1.232 0.916
Scopus rating (2009): 1.289 0.937
Scopus rating (2008): 1.325 0.881
Scopus rating (2007): 1.443 0.956
Scopus rating (2006): 1.301 0.925
Scopus rating (2005): 1.243 0.949
Directed photocurrent in Languir-Schaefer organic molecular films

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Alekseev, A., Efimov, A. V., Chukharev, V. I., Lemmetyinen, H.
Pages: 136-140
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Bulletin of the Lebedev Physics Institute
Volume: 37
Issue number: 5
ISSN (Print): 1068-3356
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.192 0.491
Publication Forum (2016): 1
Scopus rating (2015): 0.131 0.411
Web of Science (2015): 0.326 0.268 3.8 0.187 3.0E-4 0.056
Publication Forum (2015): 1
Scopus rating (2014): 0.128 0.203
Web of Science (2014): 0.246 0.181 4.6 0.057 2.1E-4 0.037
Publication Forum (2014): 1
Scopus rating (2013): 0.131 0.176
Publication Forum (2013): 1
Scopus rating (2012): 0.126 0.164
Publication Forum (2012): 1
Scopus rating (2011): 0.117 0.105
Scopus rating (2010): 0.104 0.002
Original language: English
DOIs:
10.3103/S1068335610050039

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 7667
Research output: Scientific - peer-review › Article
Effect of hot drawing on properties of wet-spun poly(L,D-lactide) copolymer multifilament fibers

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Department of Chemistry and Bioengineering, Department of Biomedical Engineering, Research group: Supramolecular photochemistry
Authors: Rissanen, M., Puolakka, A., Hukka, T., Ellä, V., Kellomäki, M., Nousiainen, P.
Pages: 608-615
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Applied Polymer Science
Volume: 115
Issue number: 1
ISSN (Print): 0021-8995
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.532 0.724
Publication Forum (2016): 1
Scopus rating (2015): 0.574 0.827
Web of Science (2015): 1.866 1.647 8.9 0.485 0.0441 0.315
Publication Forum (2015): 1
Scopus rating (2014): 0.658 0.964
Web of Science (2014): 1.768 1.662 8.5 0.378 0.04912 0.323
Publication Forum (2014): 2
Scopus rating (2013): 0.628 1.085
Publication Forum (2013): 2
Scopus rating (2012): 0.658 1.081
Publication Forum (2012): 2
Scopus rating (2011): 0.601 0.965
Scopus rating (2010): 0.679 0.909
Scopus rating (2009): 0.697 0.825
Scopus rating (2008): 0.647 0.822
Scopus rating (2007): 0.678 0.931
Scopus rating (2006): 0.782 1.145
Scopus rating (2005): 0.779 0.912
Scopus rating (2004): 0.774 0.962
Scopus rating (2003): 0.816 1.067
Scopus rating (2002): 0.866 1.084
Scopus rating (2001): 0.964 1.157
Scopus rating (2000): 0.864 1.157
Scopus rating (1999): 0.978 1.277
Original language: English
DOIs:
10.1002/app.31015

Bibliographical note
Contribution: organisation=mol,FACT1=0.34<br/>Contribution: organisation=keb kem,FACT2=0.33<br/>Contribution: organisation=bme,FACT3=0.33
Source: researchoutputwizard
Source-ID: 9121
Research output: Scientific - peer-review › Article

Effects of ð-elongation and the fused position of quinoxaline-fused porphyrins as sensitizers in dye-sensitized solar cells on optical, electrochemical, and photovoltaic properties

General information
Effects of meso-diarylamino group of porphyrins as sensitizers in dye-sensitized solar cells on optical, electrochemical, and photovoltaic properties

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Pages: 10656-10665
Publication date: 2010
Peer-reviewed: Yes
Electric-field-assisted electron transfer in a porphine-quinone complex: A theoretical study

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry
Authors: Aittala, P. J., Cramariuc, O., Hukka, T. I.
Pages: 805-816
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Theory and Computation
Volume: 6
Issue number: 3
ISSN (Print): 1549-9618
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.801 1.589
Publication Forum (2016): 2
Scopus rating (2015): 2.795 1.748
Web of Science (2015): 5.301 5.756 4.3 1.134 0.0635 1.768
Publication Forum (2015): 2
Scopus rating (2014): 2.777 1.603
Web of Science (2014): 5.498 5.76 3.9 1.195 0.05994 1.761
Publication Forum (2014): 2
Scopus rating (2013): 2.409 1.578
Publication Forum (2013): 2
Scopus rating (2012): 2.744 1.608
Publication Forum (2012): 2
Electronic energy harvesting multi BODIPY-zinc porphyrin dyads accommodating fullerene as photosynthetic composite of antenna-reaction center

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Maligaspe, E., Kumpulainen, T., Subbaiyan, N. K., Zandler, M. E., Lemmetyinen, H., Tkachenko, N. V., D'Souza, F.
Pages: 7434-7444
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 12
Issue number: 27
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
Publication Forum (2016): 1
Scopus rating (2015): 1.771 1.244
Web of Science (2015): 4.449 4.273 4.1 1.017 0.19255 1.158
Publication Forum (2015): 1
Scopus rating (2014): 1.772 1.253
Web of Science (2014): 4.493 4.219 3.9 0.991 0.17937 1.209
Publication Forum (2014): 3
Scopus rating (2013): 1.715 1.216
Publication Forum (2013): 3
Scopus rating (2012): 1.916 1.184
Publication Forum (2012): 3
Scopus rating (2011): 1.697 1.203
Scopus rating (2010): 1.802 1.196
Scopus rating (2009): 2.127 1.369
Scopus rating (2008): 2.158 1.211
Scopus rating (2007): 1.84 1.138
Scopus rating (2006): 1.467 1.128
Scopus rating (2005): 1.389 1.104
Scopus rating (2004): 1.173 1.007
Scopus rating (2003): 1.093 0.925
Scopus rating (2002): 1.122 0.973
Exciplex formation and excited state deactivation of difluoroborondipyrromethene (Bodipy) dyads

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Benniston, A. C., Copley, G., Lemmetyinen, H., Tkachenko, N. V.
Pages: 1685-1692
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 11
Issue number: 8
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
Publication Forum (2016): 1
Scopus rating (2015): 1.771 1.244
Web of Science (2015): 4.449 4.273 4.1 1.017 0.19255 1.158
Publication Forum (2015): 1
Scopus rating (2014): 1.772 1.253
Web of Science (2014): 4.493 4.219 3.9 0.991 0.17937 1.209
Publication Forum (2014): 3
Scopus rating (2013): 1.715 1.216
Publication Forum (2013): 3
Scopus rating (2012): 1.916 1.184
Publication Forum (2012): 3
Scopus rating (2011): 1.697 1.203
Scopus rating (2010): 1.802 1.196
Scopus rating (2009): 2.127 1.369
Scopus rating (2008): 2.158 1.211
Scopus rating (2007): 1.84 1.138
Scopus rating (2006): 1.467 1.128
Scopus rating (2005): 1.389 1.104
Scopus rating (2004): 1.173 1.007
Scopus rating (2003): 1.093 0.925
Scopus rating (2002): 1.122 0.973
Scopus rating (2001): 1.09 0.914
Scopus rating (2000): 0.948 1.068
Scopus rating (1999): 0.121 0.0
Original language: English
DOIs: 10.1039/c002757j
Excitation transfer in metal-ligand coordinated free-base porphyrin-magnesium phthalocyanine and free-base porphyrin-
magnesium naphthalocyanine dyads

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Stranius, K., Jacobs, R., Maligaspe, E., Lemmetyinen, H., Tkachenko, N. V., Zandler, M., D’Souza, F.
Pages: 948-961
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Porphyrins and Phthalocyanines
Volume: 14
Issue number: 11
ISSN (Print): 1088-4246
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.354 0.379
Publication Forum (2016): 1
Scopus rating (2015): 0.419 0.467
Web of Science (2015): 1.087 1.387 7.0 0.323 0.00257 0.267
Publication Forum (2015): 1
Scopus rating (2014): 0.486 0.545
Web of Science (2014): 1.397 1.603 6.7 0.179 0.00338 0.326
Publication Forum (2014): 1
Scopus rating (2013): 0.537 0.602
Publication Forum (2013): 1
Scopus rating (2012): 0.62 0.537
Publication Forum (2012): 1
Scopus rating (2011): 0.553 0.612
Scopus rating (2010): 0.564 0.46
Scopus rating (2009): 0.511 0.447
Scopus rating (2008): 0.572 0.481
Scopus rating (2007): 0.669 0.481
Scopus rating (2006): 0.625 0.529
Scopus rating (2005): 0.632 0.593
Scopus rating (2004): 0.646 0.667
Scopus rating (2003): 0.591 0.88
Scopus rating (2002): 0.86 1.153
Scopus rating (2001): 0.796 1.08
Scopus rating (2000): 0.863 0.759
Scopus rating (1999): 0.557 0.635
Original language: English
DOIs:
10.1142/S1088424610002847

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Good solvent effects of C70 cluster formations and their electron-transporting and photoelectrochemical properties

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Pages: 14287-14297
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 114
Issue number: 45
ISSN (Print): 1520-6106
Ratings:
  Publication Forum (2017): 1
  Scopus rating (2016): 1.348 1.02
  Publication Forum (2016): 1
  Scopus rating (2015): 1.367 1.096
  Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
  Publication Forum (2015): 1
  Scopus rating (2014): 1.44 1.14
  Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
  Publication Forum (2014): 3
  Scopus rating (2013): 1.494 1.2
  Publication Forum (2013): 3
  Scopus rating (2012): 1.92 1.251
  Publication Forum (2012): 3
  Scopus rating (2011): 1.78 1.226
  Scopus rating (2010): 1.849 1.214
  Scopus rating (2009): 2.232 1.349
  Scopus rating (2008): 2.543 1.381
  Scopus rating (2007): 2.346 1.282
  Scopus rating (2006): 2.369 1.415
  Scopus rating (2005): 2.275 1.474
  Scopus rating (2004): 2.148 1.511
  Scopus rating (2003): 2.034 1.47
  Scopus rating (2002): 2.118 1.496
  Scopus rating (2001): 2.053 1.508
  Scopus rating (2000): 2.145 1.527
  Scopus rating (1999): 1.713 1.8
Original language: English
DOIs:
10.1021/jp911141s

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 9397
Research output: Scientific - peer-review › Article
Langmuir-Schaeffer films from a π-π stacking perylenediimide dye: Organization and charge transfer properties
Micropolarity and microviscosity of Pluronics L62 and L64 core-shell aggregates in water at various concentrations and additives examined by absorption and fluorescence probes

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Vasilescu, M., Bandula, R., Lemmetyinen, H.
Pages: 1173-1184
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Colloid and Polymer Science
Volume: 288
Issue number: 10-11
ISSN (Print): 0303-402X
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.55 1.188
Publication Forum (2016): 2
Scopus rating (2015): 1.686 1.308
Web of Science (2015): 3.993 4.21 7.6 0.67 0.16509 1.043
Publication Forum (2015): 2
Scopus rating (2014): 1.816 1.391
Web of Science (2014): 4.457 4.543 7.2 0.682 0.18462 1.043
Publication Forum (2014): 3
Scopus rating (2013): 1.895 1.356
Publication Forum (2013): 3
Scopus rating (2012): 2.177 1.382
Publication Forum (2012): 3
Scopus rating (2011): 2.051 1.357
Scopus rating (2010): 2.148 1.4
Scopus rating (2009): 2.156 1.351
Scopus rating (2008): 2.383 1.34
Scopus rating (2007): 2.449 1.434
Scopus rating (2006): 2.375 1.428
Scopus rating (2005): 2.157 1.463
Scopus rating (2004): 1.963 1.458
Scopus rating (2003): 1.953 1.4
Scopus rating (2002): 2.011 1.489
Scopus rating (2001): 2.01 1.382
Scopus rating (2000): 2.039 1.479
Scopus rating (1999): 1.719 1.496
Original language: English
DOIs:
10.1021/la903978y

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 9416
Research output: Scientific - peer-review › Article
Mono-, bis- and tetrahydroxy phthalocyanines as building blocks for monomolecular layer assemblies

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Sariola, E., Kotiaho, A., Tkachenko, N. V., Lemmetyinen, H., Efimov, A.
Pages: 397-411
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Porphyrins and Phthalocyanines
Volume: 14
Issue number: 5
ISSN (Print): 1088-4246
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.354 0.379
Publication Forum (2016): 1
Scopus rating (2015): 0.419 0.467
Web of Science (2015): 1.087 1.387 7.0 0.323 0.00257 0.267
Publication Forum (2015): 1
Scopus rating (2014): 0.486 0.545
Web of Science (2014): 1.397 1.603 6.7 0.179 0.00338 0.326
Publication Forum (2014): 1
Multicomponent molecularly controlled Langmuir-Blodgett systems for organic photovoltaic applications

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Vivo, P., Vuorinen, T., Chukharev, V., Tolkki, A., Kaunisto, K., Ihalainen, P., Peltonen, J., Lemmetyinen, H.
Pages: 8559-8567
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 114
Issue number: 18
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Scopus rating (2014): 2.027 1.448
Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
Publication Forum (2014): 3
Scopus rating (2013): 2.134 1.439
Publication Forum (2013): 3
Scopus rating (2012): 2.514 1.46
Publication Forum (2012): 3
Scopus rating (2011): 2.32 1.457
Mutagen structure and transcriptional response: Induction of distinct transcriptional profiles in Salmonella TA100 by the drinking-water mutagen MX and its homologues

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Pages: 69-79
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Environmental and Molecular Mutagenesis
Volume: 51
Issue number: 1
ISSN (Print): 0893-6692
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.478 0.996
Publication Forum (2016): 1
Scopus rating (2015): 1.341 0.939
Web of Science (2015): 3.326 3.249 8.6 1.188 0.00518 0.924
Publication Forum (2015): 1
Scopus rating (2014): 0.948 0.831
Web of Science (2014): 2.63 2.938 9.0 0.743 0.00482 0.818
Publication Forum (2014): 1
Scopus rating (2013): 1.194 1.025
Publication Forum (2013): 1
Scopus rating (2012): 1.401 1.187
Publication Forum (2012): 1
Scopus rating (2011): 1.426 1.208
Scopus rating (2010): 1.0 1.07
Scopus rating (2009): 0.74 0.881
Scopus rating (2008): 0.776 1.006
Scopus rating (2007): 1.033 1.033
Scopus rating (2006): 0.982 0.887
Scopus rating (2005): 0.645 0.751
Scopus rating (2004): 0.744 0.877
Scopus rating (2003): 0.882 0.978
Scopus rating (2002): 0.833 0.915
Scopus rating (2001): 0.687 0.873
Scopus rating (2000): 0.762 0.983
Scopus rating (1999): 0.712 0.955
Original language: English
Off the back or on the side: Comparison of meso and 2-substituted donor-acceptor difluoroborondipyrromethene (Bodipy) dyads

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Benniston, A. C., Copley, G., Lemmetyinen, H., Tkachenko, N. V.
Pages: 2867-2877
Publication date: 2010
Peer-reviewed: Yes

Publication information
Volume: 2010
Issue number: 15
ISSN (Print): 1434-193X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.133 0.653
Publication Forum (2016): 1
Scopus rating (2015): 1.198 0.758
Web of Science (2015): 3.068 2.971 5.5 0.777 0.04165 0.677
Publication Forum (2015): 1
Scopus rating (2014): 1.181 0.767
Web of Science (2014): 3.065 3.034 5.3 0.744 0.04326 0.703
Publication Forum (2014): 3
Scopus rating (2013): 1.292 0.796
Publication Forum (2013): 3
Scopus rating (2012): 1.471 0.811
Publication Forum (2012): 3
Scopus rating (2011): 1.536 0.857
Scopus rating (2010): 1.572 0.785
Scopus rating (2009): 1.497 0.778
Scopus rating (2008): 1.652 0.759
Scopus rating (2007): 1.711 0.84
Scopus rating (2006): 1.505 0.849
Scopus rating (2005): 1.246 0.763
Scopus rating (2004): 1.2 0.81
Scopus rating (2003): 1.19 0.802
Scopus rating (2002): 1.382 0.829
Scopus rating (2001): 1.159 0.816
Scopus rating (2000): 1.192 1.048
Scopus rating (1999): 0.877 0.976
Original language: English
DOIs:
10.1002/ejoc.201000215

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Photodynamics of energy and electron transfers in solid films of porphyrin, phthalocyanine, and perylene diimide derivatives

General information
State: Published
Ministry of Education publication type: G5 Doctoral dissertation (article)
Organisations: Department of Chemistry and Bioengineering
Authors: Lehtivuori, H.
Publication date: 2010

Publication information
Place of publication: Tampere
Publisher: Tampere University of Technology
ISBN (Print): 978-952-15-2370-0
Original language: English

Publication series
Name: Tampereen teknillinen yliopisto. Julkaisu
Publisher: Tampere University of Technology
Volume: 896
ISSN (Print): 1459-2045

Bibliographical note
Awarding institution: Tampere University of Technology
Source: researchoutputwizard
Source-ID: 8594
Research output: Collection of articles › Doctoral Thesis

Photoinduced charge and energy transfer in phthalocyanine-functionalized gold nanoparticles

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Kotialho, A., Lahtinen, R., Efimov, A., Metsberg, H., Sariola, E., Lehtivuori, H., Tkachenko, N. V., Lemmetyinen, H.
Pages: 162-168
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 114
Issue number: 1
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Scopus rating (2014): 2.027 1.448
Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
Publication Forum (2014): 3
Scopus rating (2013): 2.134 1.439
Publication Forum (2013): 3
Scopus rating (2012): 2.514 1.46
Publication Forum (2012): 3
Scopus rating (2011): 2.32 1.457
Photoinduced electron transfer in thin films of porphyrin-fullerene dyad and perylenetetracarboxidiimide

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Vivo, P., Alekseev, A. S., Kaunisto, K., Pekkola, O., Tolkki, A., Chukharev, V., Efimov, A., Ihalainen, P., Peltonen, J., Lemmetyinen, H.
Pages: 12525-12532
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 12
Issue number: 39
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
Publication Forum (2016): 1
Scopus rating (2015): 1.771 1.244
Web of Science (2015): 4.449 4.273 4.1 1.017 0.19255 1.158
Publication Forum (2015): 1
Scopus rating (2014): 1.772 1.253
Web of Science (2014): 4.493 4.219 3.9 0.991 0.17937 1.209
Publication Forum (2014): 3
Scopus rating (2013): 1.715 1.216
Publication Forum (2013): 3
Scopus rating (2012): 1.916 1.184
Publication Forum (2012): 3
Scopus rating (2011): 1.697 1.203
Scopus rating (2010): 1.802 1.196
Scopus rating (2009): 2.127 1.369
Scopus rating (2008): 2.158 1.211
Scopus rating (2007): 1.84 1.138
Scopus rating (2006): 1.467 1.128
Scopus rating (2005): 1.389 1.104
Scopus rating (2004): 1.173 1.007
Scopus rating (2003): 1.093 0.925
Scopus rating (2002): 1.122 0.973
Scopus rating (2001): 1.09 0.914
Scopus rating (2000): 0.948 1.068
Scopus rating (1999): 0.121 0.0
Original language: English
Photoinduced vectorial electron transfer in multilayered Langmuir-Blodgett films of porphyrin and phtalocyanine derivatives

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Alekseev, A. S., Tkachenko, N. V., Efimov, A. V., Lemmetyinen, H.
Pages: 1230-1241
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Russian Journal of Physical Chemistry A
Volume: 84
Issue number: 7
ISSN (Print): 0036-0244
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.288 0.615
Publication Forum (2016): 1
Scopus rating (2015): 0.269 0.571
Web of Science (2015): 0.597 0.481 9.2 0.119 0.00286 0.09
Publication Forum (2015): 1
Scopus rating (2014): 0.294 0.628
Web of Science (2014): 0.562 0.492 8.7 0.097 0.00337 0.101
Publication Forum (2014): 1
Scopus rating (2013): 0.322 0.677
Publication Forum (2013): 1
Scopus rating (2012): 0.269 0.494
Publication Forum (2012): 1
Scopus rating (2011): 0.257 0.403
Scopus rating (2010): 0.232 0.346
Scopus rating (2009): 0.168 0.256
Scopus rating (2008): 0.151 0.205
Scopus rating (2007): 0.151 0.209
Scopus rating (2006): 0.205 0.444
Scopus rating (2005): 0.197 0.541
Scopus rating (2004): 0.205 0.464
Scopus rating (2003): 0.128 0.134
Scopus rating (2002): 0.133 0.156
Scopus rating (2001): 0.119 0.097
Scopus rating (2000): 0.105 0.026
Scopus rating (1999): 0.107 0.035
Original language: English
DOIs:
10.1134/S0036024410070253

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Preparation of indole-phosphine oxazoline (IndPHOX) ligands and their application in allylic alkylation

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Wang, Y., Hämäläinen, A., Tois, J., Franzen, R.
Pages: 2376-2384
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Tetrahedron : Asymmetry
Volume: 21
Issue number: 19
ISSN (Print): 0957-4166
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.751 0.663
Publication Forum (2016): 1
Scopus rating (2015): 0.777 0.713
Web of Science (2015): 2.108 1.973 9.7 0.531 0.00831 0.393
Publication Forum (2015): 1
Scopus rating (2014): 0.75 0.723
Web of Science (2014): 2.155 2.038 9.0 0.483 0.01076 0.426
Publication Forum (2014): 2
Scopus rating (2013): 0.965 0.725
Publication Forum (2013): 2
Scopus rating (2012): 1.037 0.748
Publication Forum (2012): 2
Scopus rating (2011): 1.288 0.839
Scopus rating (2010): 1.292 0.904
Scopus rating (2009): 1.275 0.84
Scopus rating (2008): 1.481 0.853
Scopus rating (2007): 1.534 0.868
Scopus rating (2006): 1.425 0.925
Scopus rating (2005): 1.275 0.902
Scopus rating (2004): 1.302 0.974
Scopus rating (2003): 1.181 0.966
Scopus rating (2002): 1.525 0.924
Scopus rating (2001): 1.533 1.074
Scopus rating (2000): 1.764 1.102
Scopus rating (1999): 1.599 1.036
Original language: English
DOIs:
10.1016/j.tetasy.2010.08.008

Bibliographical note
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source-ID: 9627
Research output: Scientific - peer-review › Article

Real-time IR study of ultra-thin film photopolymerization of liquid porphyrin monomer
Selective formation and efficient photocurrent generation of [70]fullerene-single-walled carbon nanotube composites

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Self-assembled monolayers (SAMs) of porphyrin deposited inside hollow-core photonic bandgap fiber (HCPBGF)

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Optoelectronics Research Centre, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Veselov, A., Thur, C., Efimov, A., Guina, M., Lemmetyinen, H., Tkachenko, N.
Pages: 45-45
Publication date: 2010

Host publication information
Title of host publication: Optics Days 2010 Proceedings, May 6-7, 2010, Tampere, Finland
Self-assembled monolayers (SAMs) of porphyrin deposited inside hollow-core photonic bandgap fiber (HCPBGF) and polarization maintaining fiber (PMF)

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Optoelectronics Research Centre, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Veselov, A., Thur, C., Efimov, A., Chamorovskiy, A., Guina, M., Okhotnikov, O. G., Lemmetyinen, H., Tkachenko, N.
Pages: 2 p
Publication date: 2010

Host publication information
Title of host publication: Optical Sensors, June 21, 2010, Karlsruhe, Germany
Publisher: OSA Optical Society of America

Synthesis and characterization of monoisomeric 1,8,15,22-substituted (A3B and A2B2) phthalocyanines and phthalocyanine-fullerene dyads

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Ranta, J., Kumpulainen, T., Lemmetyinen, H., Efimov, A.
Pages: 5178-5194
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Organic Chemistry
Volume: 75
Issue number: 15
ISSN (Print): 0022-3263
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.976 1.03
Publication Forum (2016): 2
Scopus rating (2015): 2.018 1.174
Web of Science (2015): 4.785 4.538 >10.0 1.289 0.10271 1.051
Publication Forum (2015): 2
Scopus rating (2014): 2.003 1.222
Web of Science (2014): 4.721 4.385 >10.0 1.073 0.10827 1.035
Publication Forum (2014): 3
Scopus rating (2013): 2.078 1.176
Publication Forum (2013): 3
Scopus rating (2012): 2.272 1.23
Synthesis and time-resolved fluorescence study of porphyrin-functionalized gold nanoparticles

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Kotiaho, A., Lahtinen, R., Efimov, A., Lehtivuori, H., Tkachenko, N. V., Kanerva, T., Lemmetyinen, H.
Pages: 129-134
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Photochemistry and Photobiology, A: Chemistry
Volume: 212
Issue number: 2-3
ISSN (Print): 1010-6030
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.732 0.841
Publication Forum (2016): 1
Scopus rating (2015): 0.72 0.86
Web of Science (2015): 2.477 2.573 9.8 0.619 0.01027 0.521
Publication Forum (2015): 1
Scopus rating (2014): 0.782 0.97
Web of Science (2014): 2.495 2.549 9.4 0.609 0.01139 0.538
Publication Forum (2014): 1
Scopus rating (2013): 0.818 1.006
Publication Forum (2013): 1
Scopus rating (2012): 0.919 1.116
Publication Forum (2012): 1
Scopus rating (2011): 0.97 1.342
Scopus rating (2010): 1.021 1.05
Scopus rating (2009): 1.163 1.191
Synthesis of chiral unsaturated aminolactones using Pd-catalyzed allylic amination

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Kallinen, A., Tois, J., Sjöholm, R., Franzen, R.
Pages: 2367-2371
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Tetrahedron Asymmetry
Volume: 21
Issue number: 19
ISSN (Print): 0957-4166
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.751 0.663
Publication Forum (2016): 1
Scopus rating (2015): 0.777 0.713
Web of Science (2015): 2.108 1.973 9.7 0.531 0.00831 0.393
Publication Forum (2015): 1
Scopus rating (2014): 0.75 0.723
Web of Science (2014): 2.155 2.038 9.0 0.483 0.01076 0.426
Publication Forum (2014): 2
Scopus rating (2013): 0.965 0.725
Publication Forum (2013): 2
Scopus rating (2012): 1.037 0.748
Publication Forum (2012): 2
Scopus rating (2011): 1.288 0.839
Scopus rating (2010): 1.292 0.904
Scopus rating (2009): 1.275 0.84
Scopus rating (2008): 1.481 0.853
Scopus rating (2007): 1.534 0.868
Scopus rating (2006): 1.425 0.925
Scopus rating (2005): 1.275 0.902
Scopus rating (2004): 1.302 0.974
Ultrafast singlet-singlet energy transfer in self-assembled via metal-ligand axial coordination of free-base porphyrin-zinc phthalocyanine and free-base porphyrin-zinc naphthalocyanine dyads

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Maligaspe, E., Kumpulainen, T., Lemmetyinen, H., Tkachenko, N. V., Subbaiyan, N., Zandler, M. E., D'Souza, F.
Pages: 268-277
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 114
Issue number: 1
ISSN (Print): 1089-5639
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.258 0.98
Publication Forum (2016): 1
Scopus rating (2015): 1.179 1.106
Web of Science (2015): 2.883 2.709 8.1 0.758 0.0807 0.729
Publication Forum (2015): 1
Scopus rating (2014): 1.154 1.071
Web of Science (2014): 2.693 2.713 7.6 0.676 0.09689 0.777
Publication Forum (2014): 3
Scopus rating (2013): 1.194 1.102
Publication Forum (2013): 3
Scopus rating (2012): 1.494 1.124
Publication Forum (2012): 3
Scopus rating (2011): 1.402 1.135
Scopus rating (2010): 1.466 1.102
Scopus rating (2009): 1.562 1.132
Scopus rating (2008): 1.787 1.093
Scopus rating (2007): 1.907 1.136
Scopus rating (2006): 1.728 1.195
Scopus rating (2005): 1.789 1.215
Scopus rating (2004): 1.669 1.224
Scopus rating (2003): 1.75 1.241
Scopus rating (2002): 1.81 1.196
Scopus rating (2001): 1.732 1.224
Unambiguous probe of surface chirality based on focused circularly-polarized light

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Research group: Nonlinear Optics, Research area: Optics, Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry
Authors: Huttunen, M., Virkki, M., Erkintalo, M., Kauranen, M., Vuorimaa, E., Efimov, A., Lemmetyinen, H.
Pages: 2 p
Publication date: 2010

Host publication information
Title of host publication: Conference on Lasers and Electro-Optics (CLEO) and the Quantum Electronics and Laser Science Conference (QELS) Citation Information, 16.-21.5.2010, San Jose, California, USA
Place of publication: Washington, DC
Publisher: OSA

Unambiguous probe of surface chirality based on focused circular polarizations

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Research group: Nonlinear Optics, Research area: Optics, Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry
Authors: Huttunen, M. J., Virkki, M., Erkintalo, M., Vuorimaa, E., Efimov, A., Lemmetyinen, H., Kauranen, M.
Pages: 32
Publication date: 2010

Host publication information
Editors: Sajavaara, T., Maasilta, I., Mätö, L., Julin, J., Rahkila, P.

Unambiguous probe of surface chirality based on focused circular polarizations

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Vivo, P., Kaunisto, K., Alekseev, A. S., Pekkola, O., Tolkki, A., Chukharev, V., Lemmetyinen, H.

Vectorial photoinduced electron transfer in multicomponent film systems of poly(3-hexylthiophene), porphyrin-fullerene dyad, and perylene-tetracarboxiimidide

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Vivo, P., Kaunisto, K., Alekseev, A. S., Pekkola, O., Tolkki, A., Chukharev, V., Lemmetyinen, H.
Z-Selective synthesis of o-bromoacetophenone N-tosylhydrazones and formation of 3-methylindazoles in aqueous ethanol

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Kylmäla, T., Udd, S., Tois, J., Franzen, R.
Pages: 3613-3615
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Tetrahedron Letters
Volume: 51
Issue number: 28
ISSN (Print): 0040-4039
Ratings:
Publication Forum (2017): 1
Cyclization of Diazoacetamides Catalyzed by N-Heterocyclic Carbene Dirhodium(II) Complexes

The axial coordination of N-heterocyclic carbene ligands onto dirhodium(II) complexes was examined, together with its role in the intramolecular C-H insertion reactions of alpha-diazoacetamides. The formation of a decarbonylated product occurs by a free-carbene mechanism in which the structures of the catalyst and the acetamide play a decisive role.
More Sustainable Approaches for the Synthesis of N-Based Heterocycles

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: Candeias, N. R., Branco, L. C., Gois, P. M. P., Afonso, C. A. M., Trindade, A. F.
Keywords: (SOLVENT-FREE CONDITIONS, ONE-POT SYNTHESIS, MICROWAVE-ASSISTED SYNTHESIS, DIELS-ALDER REACTIONS, TEMPERATURE IONIC LIQUIDS, 1,3-DIPOLAR CYCLOADDITION REACTIONS, SILICA SULFURIC-ACID, SOLID-PHASE EXTRACTION, ALPHA-AMINO-ACIDS, C-H INSERTION)
Number of pages: 100
Pages: 2703-2802
Publication date: Jun 2009
Peer-reviewed: Yes

Publication information
Journal: Chemical Reviews
Volume: 109
Issue number: 6
ISSN (Print): 0009-2665
Ratings:
Publication Forum (2017): 2
Developments in the Photochemistry of Diazo Compounds

This review focuses on photolytic reactions of diazo compounds, namely aryl-diazo alkanes and alpha-diazo carbonyl compounds, covering their synthetic applications such as Wolff rearrangement, 1,2-shift, X-H insertion, cyclopropanation, hydrogen abstraction and reaction with oxygen as well as physical organic studies, with special relevance to mechanistic considerations. Singlet-triplet gap studies and the solvent influence on the stability and reactivity of carbenes are also covered together in this review to provide a comprehensive interpretation of their reactivity. The mechanism of the synthetically important Wolff rearrangement, which remains to this day open to discussion, is evaluated in terms of the role of the diazo framework. 1,2-Shift photoinduced reactions, on the other hand, present well established mechanisms due to recent studies that have demonstrated the importance of photoexcited diazo species. The cyclopropanation reaction mechanism, which is used to demonstrate the spin multiplicity nature of a free carbene, is also well established. Contrary to these latter cases, O-H insertion and C-H insertion reactions continue to lack defined mechanisms inspite of recent studies. The few examples of diazo compounds reactions with molecular oxygen and hydrogen abstraction present in the literature are also covered.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Tecn Lisboa, Instituto Superior Tecnico, Universidade de Lisboa, Inst Nanosci & Nanotechnol, Ctr Quim Fis Mol & IN, Inst Super Tecn
Authors: Candeias, N. R., Afonso, C. A. M.
Keywords: (LASER-FLASH-PHOTOLYSIS, ALPHA-DIAZO CARBONYL COMPOUNDS, C-H ACTIVATION, PHOSPHONATE GROUP PARTICIPATION, TRIPLET ENERGY-GAP, WOLFF REARRANGEMENT, O-H, SUBSTITUTED CARBENES, RHODIUM CARBENOIDS, CARBONYL-COMPOUNDS)
Number of pages: 25
Pages: 763-787
Publication date: May 2009
Peer-reviewed: Yes
Water: A Suitable Medium for the Petasis Borono-Mannich Reaction

Water was used as the solvent in the Petasis borono-Mannich reaction. With the use of salicylaldehyde, secondary amines and boronic acids, several alkylaminophenols were obtained in considerably high yields in water. By using the same methodology, 2H-chromenes were prepared with the use of vinyl boronic acids. The reaction mechanism was studied by DFT calculations, and the results obtained corroborate the solvent effect experimentally observed. (© Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, Germany, 2009)
In this work we show that the intramolecular C-H insertion of diazo-acetamides catalysed by di-rhodium(II) complexes can be highly influenced by the axial ligand on the di-rhodium(II) complex. Axially monocoordinated NH-Cr(2)(OAc)(4) complexes have a distinct reactivity from the parent Rh(2)(OAc)(4) complex affording the cyclisation products in different rates and selectivities. Surprisingly, a new reaction mode emerged when using these complexes which led to a decarbonylation pathway. (C) 2008 Elsevier Ltd. All rights reserved.
C-H carbene insertion of alpha-diazo acetamides by photolysis in non-conventional media

Light from a mercury vapor high-pressure lamp was used to induce the photolytic decomposition of alpha-diazo acetamides in hexane and in nonconventional media such as water or a film. The corresponding beta- and/or gamma-lactams were obtained in reasonable yields and in some cases with good diastereoselectivities with no need to use a metallic catalyst. Experimental studies on chiral substrates demonstrated the occurrence of insertion with retention of configuration.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Tecn Lisboa, Instituto Superior Tecnico, Universidade de Lisboa, Inst Nanosci & Nanotechnol, Ctr Quim Fis Mol & IN, Inst Super Tecn, Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, Dept Engn Quim & Biol, Ctr Quim Estrutural, Univ Lisbon, Universidade de Lisboa, Fac Farm, iMed UL
Authors: Candeias, N. R., Gois, P. M. P., Veiros, L. F., Afonso, C. A. M.
Keywords: (CARBON-HYDROGEN INSERTION, ORGANIC-REACTIONS, AQUEOUS-MEDIA, WOLFF REARRANGEMENT, DIAZOCARBONYL COMPOUNDS, WATER, DECOMPOSITION, ESTERS, DIAZOACETAMIDES, STEREOCHEMISTRY)
Time-resolved fluorometry: typical methods, challenges, applications and standards

General information
State: Published
Ministry of Education publication type: A3 Part of a book or another research book
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Tkachenko, N., Lemmetyinen, H.
Pages: 195-214
Publication date: 2008

Host publication information
Title of host publication: Standardization and Quality Assurance in Fluorescence Measurements I Techniques. Springer Series on Fluorescence
Editor: Resch-Genger, U.
ISBN (Print): 978-3-540-75207-3
Efficient catalyst reuse by simple dissolution in non-conventional media
This feature article is a description of the achievements made on the development of attractive sustainable approaches to synthetic organic chemistry, namely, catalyst reuse by simple dissolution in water and ionic liquids and asymmetric transformations induced by readily available chiral ionic liquids.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Instituto Superior Tecnico, Lissabon, Portugal
Authors: Afonso, C. A. M., Branco, L. C., Candeias, N. R., Gois, P. M. P., Lourenco, N. M. T., Mateus, N. M. M., Rosa, J. N.
Keywords: (BAYLIS-HILLMAN REACTION, TEMPERATURE IONIC LIQUIDS, C-H INSERTION, NUCLEOPHILIC DISPLACEMENT-REACTIONS, SOLVENT-FREE TETRAHYDROPYRANYLATION, MICROWAVE-ASSISTED PREPARATION, CO2 PRODUCT RECOVERY, ONE-POT SYNTHESIS, ASYMMETRIC DIHYDROXYLATION, OSMIUM-TETROXIDE)
Number of pages: 11
Pages: 2669-2679
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Chemical Communications
Issue number: 26
ISSN (Print): 1359-7345
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.506 1.159
Publication Forum (2016): 2
Scopus rating (2015): 2.664 1.314
Web of Science (2015): 6.567 6.628 4.6 1.713 0.36883 1.538
Publication Forum (2015): 2
Scopus rating (2014): 2.701 1.446
Web of Science (2014): 6.834 6.779 4.4 1.493 0.35082 1.58
Publication Forum (2014): 3
Scopus rating (2013): 2.755 1.38
Publication Forum (2013): 3
Scopus rating (2012): 3.09 1.347
Publication Forum (2012): 3
Scopus rating (2011): 2.857 1.322
Scopus rating (2010): 2.709 1.232
Scopus rating (2009): 2.588 1.252
Scopus rating (2008): 2.791 1.236
Scopus rating (2007): 2.851 1.237
Scopus rating (2006): 2.366 1.183
Scopus rating (2005): 2.129 1.15
Scopus rating (2004): 1.954 1.158
Scopus rating (2003): 1.644 1.098
Scopus rating (2002): 1.956 1.19
Scopus rating (2001): 1.817 1.098
Rhodium (II) carbene C-H insertion in water and catalyst reuse

A five-session laboratory experiment is described for the synthesis of a P-lactam via Rh(II) catalysed intramolecular C-H insertion of an α-diazo-α-ethoxycarbonylacetamide. The metallo-carbene, responsible for the C-H bond activation, was generated from the diazo substrate and the catalyst Rh-2(OAc)(4). The high stability and solubility of the catalyst and the exclusive C-H insertion of the Rh-carbene allows the synthesis of this important heterocycle in water and the catalyst reutilization.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Instituto Superior Tecnico, Lissabon, Portugal
Authors: Candeias, N. R., Gois, P. M. P., Afonso, C. A. M.
Keywords: (dirhodium carbenoids, alpha-diazoacetamides, ORGANIC-SYNTHESIS, GREEN CHEMISTRY, ALPHA-DIAZOACETAMIDES, DIAZO-COMPOUNDS, ACTIVATION, TRANSFORMATIONS, DECOMPOSITION, STEREOCONTROL, SEPARATION, COMPOUND)
Number of pages: 5
Pages: 1768-1772
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Quimica Nova
Volume: 30
Issue number: 7
ISSN (Print): 0100-4042
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.217 0.386
Publication Forum (2016): 1
Scopus rating (2015): 0.264 0.476
Web of Science (2015): 0.617 0.765 7.7 0.079 0.034 0.014
Publication Forum (2015): 1
Scopus rating (2014): 0.284 0.62
Web of Science (2014): 0.661 0.916 7.2 0.086 0.005 0.189
Publication Forum (2014): 1
Scopus rating (2013): 0.291 0.521
Publication Forum (2013): 1
Scopus rating (2012): 0.354 0.689
Publication Forum (2012): 1
Scopus rating (2011): 0.319 0.587
Scopus rating (2010): 0.301 0.592
Scopus rating (2009): 0.29 0.56
Scopus rating (2008): 0.263 0.594
Scopus rating (2007): 0.317 0.654
Scopus rating (2006): 0.267 0.556
Scopus rating (2005): 0.255 0.568
Scopus rating (2004): 0.245 0.393
Scopus rating (2003): 0.236 0.476
Scopus rating (2002): 0.279 0.435
Rh(II)-catalyzed intramolecular C-H insertion of diazo substrates in water: Scope and limitations

Preferential Rh(II) carbenoid intramolecular C-H versus O-H insertion derived from R-diazo-acetamides can be achieved in water by using an appropriate combination of the catalyst and amide groups, which creates a larger hydrophobic environment around the reactive carbenoid center.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, CQFM
Authors: Candeias, N. R., Gois, P. M. P., Afonso, C. A. M.
Keywords: (RHODIUM(II) CATALYZED-REACTIONS, ORGANIC-REACTIONS, ALPHA-DIAZOACETAMIDES, N-ARYLDIAZOAMIDIES, YLIDE FORMATION, DIRHODIUM(II), CARBENOIDS, CYCLOPROPANATION, SOLVENT, ENANTIOSELECTIVITY)
Number of pages: 9
Pages: 5489-5497
Publication date: 21 Jul 2006
Peer-reviewed: Yes

Publication information
Journal: Journal of Organic Chemistry
Volume: 71
Issue number: 15
ISSN (Print): 0022-3263
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.976 1.03
Publication Forum (2016): 2
Scopus rating (2015): 2.018 1.174
Web of Science (2015): 4.785 4.538 >10.0 1.289 0.10271 1.051
Publication Forum (2015): 2
Scopus rating (2014): 2.003 1.222
Web of Science (2014): 4.721 4.385 >10.0 1.073 0.10827 1.035
Publication Forum (2014): 3
Scopus rating (2013): 2.078 1.176
Publication Forum (2013): 3
Scopus rating (2012): 2.272 1.23
Publication Forum (2012): 3
Scopus rating (2011): 2.27 1.261
Scopus rating (2010): 2.112 1.173
Scopus rating (2009): 2.186 1.254
Scopus rating (2008): 2.309 1.208
Scopus rating (2007): 2.37 1.309
Scopus rating (2006): 2.222 1.31
Scopus rating (2005): 1.995 1.3
Scopus rating (2004): 1.945 1.315
Scopus rating (2003): 1.865 1.355
Scopus rating (2002): 2.319 1.441
Scopus rating (2001): 2.064 1.406
Optical Spectroscopy: Methods and Instrumentations

General information
State: Published
Ministry of Education publication type: C1 Separate scientific books
Organisations: Materiaalioppi, Kemia
Authors: Tkachenko, N. V.
Number of pages: 307
Publication date: 2006

Publication information
Publisher: Unknown Publisher
ISBN (Print): 0-444-52126-7
Original language: English
Links:
http://catdir.loc.gov/catdir/enhancements/fy0634/2006044580-d.html

Bibliographical note
Contribution: organisation=kem,FACT1=0.5<br/>Contribution: organisation=mol,FACT2=0.5
Source: researchoutputwizard
Source-ID: 17750
Research output: Scientific - peer-review › Book

Preparation of non-fused heterocycles in zeolites and mesoporous materials
The use of zeolites and mesoporous materials in synthesis and industrial applications are extremely important due to their acidity properties and their reuse facility. In this review, is presented the use of zeolites and mesoporous materials in the preparation of non-fused heterocycles compounds, with particular emphasis in epoxidations, aziridinations and the Beckmann's rearrangement. (c) 2005 Elsevier B.V. All rights reserved.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Universidade de Lisboa
Authors: Candeias, N., Afonso, C.
Keywords: (zeolites, mesoporous materials, epoxidation, aziridination, Beckmann rearrangement, epsilon-caprolactam, catalyst reuse, immobilization, solid support, asymmetric catalyst, PHASE BECKMANN REARRANGEMENT, ASYMMETRIC HETEROGENEOUS AZIRIDINATION, CHIRAL ALLYLIC ALCOHOLS, H-BETA CATALYST, CYCLOHEXANONE-OXIME, EPSILON-CAPROLACTAM, HYDROGEN-PEROXIDE, MOLECULAR-SIEVES, ACTIVE-SITES, TITANIUM SILICALITE)
Number of pages: 23
Pages: 195-217
Publication date: 1 Dec 2005
Peer-reviewed: Yes

Publication information
Journal: Journal of Molecular Catalysis A: Chemical
Volume: 242
Issue number: 1-2
ISSN (Print): 1381-1169
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.006 1.095
Publication Forum (2016): 2
Preparation of enantioselective enriched alpha-(dialkoxyphosphoryl) lactams via intramolecular C-H insertion with chiral dirhodium(II) catalysts

The intramolecular C-H insertion on alpha-diazoacetamides is an extremely useful procedure for the preparation of a wide variety of heterocyclic compounds. In this work is presented a strategy for the preparation of enantioselective enriched alpha-(dialkoxyphosphoryl) lactams via dirhodium(II) catalyzed C-H insertion on alpha-diazo-alpha-(dialkoxyphosphoryl)acetamides, in which enantiomeric excess up to 40% is reported. Moreover, a systematic study was undertaken on the chiral dirhodium(II) catalyst and the alpha-diazo-alpha-(dialkoxyphosphoryl)acetamides influence on enantioselectivity. (C) 2004 Elsevier B.V. All rights reserved.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Nova Lisboa, Universidade Nova de Lisboa, REQUIMTE, Dept Quim, Fac Ciencias & Tecnol
Authors: Gois, P. M. P., Candeias, N. R., Afonso, C. A. M.
Keywords: (phosphonates, diazo compounds, rhodium catalysts, C-H insertion, lactams, ALPHA-DIAZOACETAMIDES, STEREOCONTROL, REGIOCONTROL)
Number of pages: 8
Pages: 17-24
Publication date: 1 Mar 2005
Peer-reviewed: Yes

Publication information
Journal: Journal of Molecular Catalysis A: Chemical
Volume: 227
Issue number: 1-2
ISSN (Print): 1381-1169
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.006 1.095
Growth-temperature-dependent bandgap of MBE-grown GaInNAs epilayers lattice matched to GaAs

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Kemia, Optoelectronics Research Centre, Research group: Supramolecular photochemistry
Authors: Pavelescu, E., Wagner, J., Kudrawiec, R., Dumitrescu, M., Konttinen, J., Dhaka, V., Lemmetyinen, H., Pessa, M.
Pages: 540-542
Publication date: 2005

Host publication information
Title of host publication: Proceedings 17th Indium Phosphide and Related Materials Conference (IPRM 2005), Glasgow, UK, May 8-12, 2005
ISBN (Print): 0-7803-8891-7
DOI: 10.1109/ICIPRM.2005.1517553

Bibliographical note
Verkko- ja paperijulkaisu<br/>&lt;br&gt;Contribution: organisation=orc,FACT1=0.5&lt;br&gt;Contribution: organisation=kem,FACT2=0.5
Source: researchoutputwizard
Source-ID: 19298
Research output: Scientific - peer-review › Conference contribution

Rh(II) catalysed intramolecular C-H insertion of diazo substrates in water: a simple and efficient approach to catalyst reuse

Water is an efficient solvent for the Rh-2(OAc)(4) catalysed intramolecular C - H insertion of a range of diazo substrates without competitive water insertion. Due to the high solubility and stability of the catalyst in water, the catalyst can be efficiently reused.
Comparison of the total mercury content in sediment samples with a mercury sensor bacteria test and Vibrio fischeri toxicity test

The suitability of a luminescent bacterial sensor strain Escherichia coli MC1061(pTOO11) [Virta, M.; Lampinen, J.; Karp, M. Anal Chem 1995, 67, 667-669] for the measuring of mercury from sediment samples was evaluated. The sensor strain is based on the control of expression of a reporter gene, firefly luciferase, by a mercury sensitive regulation unit. The sensor responds to mercury by increased luminescence as a consequence of increased production of the reporter protein luciferase. The method is simple to perform since the luminescence is recorded with a portable luminometer and the sensor bacteria are freeze-dried. The results obtained from river sediment samples were compared with the total mercury content of the samples, which was measured by atomic absorption spectrometry and Leco(R) Mercury analyzer and the
modified photobacteria luminescence inhibition test (Lappalainen, J.; Juvonen, R.; Vaajasaari, K.; Karp, M. Chemosphere 1999, 38, 1069-1083). The correlation between the bacterial sensor results with the total mercury content, ranging from 0.01 mg/kg to 16 mg/kg, was significant with 32 samples tested (R^2 UP to 0.8115). There was no correlation between the total mercury content and toxicity measured with Vibrio fischeri in this sample panel, (C) 2000 by John Wiley & Sons, Inc.

**General information**

State: Published

Ministry of Education publication type: A1 Journal article-refereed

Organisations: University of Turku

Authors: Lappalainen, J. O., Karp, M. T., Juvonen, R., Virta, M. P. J., Nurmi, J.

Keywords: (heavy metal, biosensor, mercury, sediment, REPORTER, ARSENITE, ENVIRONMENT, ANTIMONITE, BIOSENSOR, STRAIN)

Number of pages: 6

Pages: 443-448

Publication date: Dec 2000

Peer-reviewed: Yes

**Publication information**

Journal: Environmental Toxicology

Volume: 15

Issue number: 5

ISSN (Print): 1520-4081

Ratings:

Publication Forum (2017): 2
Scopus rating (2016): 0.688 0.829
Publication Forum (2016): 2
Scopus rating (2015): 0.804 0.848
Web of Science (2015): 2.868 2.637 7.8 0.612 0.00431 0.643
Publication Forum (2015): 2
Scopus rating (2014): 0.748 0.98
Web of Science (2014): 3.197 2.869 8.0 0.497 0.0039 0.671
Publication Forum (2014): 1
Scopus rating (2013): 0.767 0.897
Publication Forum (2013): 1
Scopus rating (2012): 0.828 0.94
Publication Forum (2012): 1
Scopus rating (2011): 0.765 0.807
Scopus rating (2010): 0.762 0.795
Scopus rating (2009): 0.683 0.888
Scopus rating (2008): 0.784 1.021
Scopus rating (2007): 0.766 0.963
Scopus rating (2006): 0.847 0.837
Scopus rating (2005): 0.574 0.722
Scopus rating (2004): 0.584 0.836
Scopus rating (2003): 0.612 0.783
Scopus rating (2002): 0.638 0.772
Scopus rating (2001): 0.564 0.764
Scopus rating (2000): 0.619 1.135
Scopus rating (1999): 0.658 0.823

Original language: English


Source: WOS

Source-ID: 000165446600012

Research output: Scientific › peer-review › Article

**Detecting bioavailable toxic metals and metalloids from natural water samples using luminescent sensor bacteria**

We have generated microbial sensors for analyzing the presence of various metals or metalloids by recombinant DNA technology. The strains are based on strictly regulated promoters controlling the expression of the firefly luciferase gene in microbial cells. The regulator-reporter constructs are located in shuttle plasmids capable of replicating in gram-negative or
-positive microbial organisms. The sensors developed are real-time indicators of metal responsive gene expression giving results in approximately 30 min, with optimal induction times ranging from 60 to 240 min. We describe here the performance of these metal sensing bacteria for the assessment of different water samples spiked with lead, arsenic, mercury or cadmium. We show that these bacteria are sensitive detectors of metal bioavailability, which is difficult or even impossible to measure by traditional analytical chemistry methods. All measurements were done using freeze-dried bacteria, which makes these sensors reagent-like and also easy to use in field conditions. (C) 2000 Elsevier Science Ltd. All rights reserved.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Turku, University of Turku, Dept Biotechnol
Authors: Tauriainen, S. M., Virta, M. P. J., Karp, M. T.
Keywords: (luciferase, luc-gene, environment, cadmium, mercury, arsenite, ESCHERICHIA-COLI, ARSENITE, LUCIFERASE, ANTIMONITE, MERCURY, LEAD, EXPRESSION, BIOSENSOR, CADMIUM, GENES)
Number of pages: 6
Pages: 2661-2666
Publication date: Jul 2000
Peer-reviewed: Yes

Publication information
Journal: Water Research
Volume: 34
Issue number: 10
ISSN (Print): 0043-1354
Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 2.629 2.558
Publication Forum (2016): 3
Scopus rating (2015): 2.689 2.507
Web of Science (2015): 5.991 6.769 8.3 1.04 0.0782 1.611
Scopus rating (2014): 2.957 2.727
Web of Science (2014): 5.528 6.279 8.2 0.966 0.07745 1.592
Publication Forum (2014): 3
Scopus rating (2013): 2.956 2.693
Publication Forum (2013): 3
Scopus rating (2012): 2.966 2.456
Publication Forum (2012): 3
Scopus rating (2011): 2.867 2.374
Scopus rating (2010): 2.582 2.196
Scopus rating (2009): 2.319 2.225
Scopus rating (2008): 2.065 2.19
Scopus rating (2007): 1.994 2.208
Scopus rating (2006): 1.895 2.214
Scopus rating (2005): 2.114 2.337
Scopus rating (2004): 2.227 2.106
Scopus rating (2003): 1.696 1.917
Scopus rating (2002): 1.54 1.775
Scopus rating (2001): 1.321 1.711
Scopus rating (2000): 1.305 1.688
Scopus rating (1999): 1.456 1.576
Original language: English
DOIs: 10.1016/S0043-1354(00)00005-1
Source: WOS
Source-ID: 000087436600004
Research output: Scientific - peer-review » Article
A recombinant Escherichia coli sensor strain for the detection of tetracyclines

A bioluminescent Escherichia coli K-12 strain for the specific detection of the tetracycline group of antibiotics is described. A sensor plasmid, containing five genes from bacterial luciferase operon of Photorhabdus luminescens inserted under the control of tetracycline-responsive elements of the transposon Tn10, was constructed. Usage of the full-length luciferase operon in the sensor resulted in tetracycline-dependent light production without additions, i.e., self-luminescent phenotype, since all the substrates were intrinsically produced by the recombinant organism. The time needed for optimal induction of light emission was 90 min. Maximal induction of similar to 100-fold over uninduced levels by using 20 ng of tetracycline, and picomole sensitivities for the seven different tetracyclines tested, were obtained without added Mg2+ ions. The higher the pH and the magnesium ion concentration in the assay medium the higher was the amount of membrane-impermeable tetracycline-Mg2+ chelate complex. In consequence, by adjusting the pH and the Mg2+ ion concentration, the sensitivity of the assay can be modified for different analytical purposes. Different non-tetracycline antibiotics did not cause induction of light emission.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Turku, University of Turku, Dept Biotechnol
Authors: Korpela, M. T., Kurittu, J. S., Karvinen, J. T., Karp, M. T.
Keywords: (XENORHABDUS-LUMINESCENS, EXPRESSION, ANTIMONITE, PROMOTER, ARSENITE, BACTERIA, BINDING, CLONING, GENES)
Number of pages: 6
Pages: 4457-4462
Publication date: 1 Nov 1998
Peer-reviewed: Yes

Publication information
Journal: Analytical Chemistry
Volume: 70
Issue number: 21
ISSN (Print): 0003-2700
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.255 1.491
Publication Forum (2016): 2
Scopus rating (2015): 2.277 1.57
Web of Science (2015): 5.886 5.922 7.6 1.107 0.15915 1.403
Publication Forum (2015): 2
Scopus rating (2014): 2.277 1.605
Web of Science (2014): 5.636 5.794 7.7 1.043 0.16427 1.449
Publication Forum (2014): 3
Scopus rating (2013): 2.395 1.7
Publication Forum (2013): 3
Scopus rating (2012): 2.674 1.715
Publication Forum (2012): 3
Scopus rating (2011): 2.61 1.665
Scopus rating (2010): 2.375 1.607
Scopus rating (2009): 2.318 1.656
Scopus rating (2008): 2.601 1.593
Scopus rating (2007): 2.59 1.772
Scopus rating (2006): 2.564 1.809
Scopus rating (2005): 2.497 2.016
Scopus rating (2004): 2.544 1.929
Scopus rating (2003): 2.331 1.837
Scopus rating (2002): 2.295 1.796
Scopus rating (2001): 2.545 2.022
Scopus rating (2000): 2.637 1.981
Scopus rating (1999): 2.577 2.059
Original language: English
DOIs: 10.1021/ac980740e
Simultaneous extraction and combined bioluminescent assay of oxidized and reduced nicotinamide adenine dinucleotide

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: University of Turku
Authors: Karp, M. T., Vuorinen, P. I.
Keywords: (Alcohol Dehydrogenase, Alcohol Oxidoreductases, Animals, Kinetics, Luminescent Measurements, NAD, Oxidation-Reduction, Potentiometry, Rats, Reagent Kits, Diagnostic)
Number of pages: 6
Pages: 147-152
Publication date: 1986
Peer-reviewed: Yes

Publication information
Journal: METHODS IN ENZYMOLOGY
Volume: 122
Issue number: Part G
ISSN (Print): 0076-6879
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.528 0.523
Publication Forum (2016): 1
Scopus rating (2015): 1.476 0.566
Publication Forum (2015): 1
Scopus rating (2014): 1.393 0.64
Web of Science (2014): 2.088 2.272 >10.0 0.322 0.02533 0.961
Publication Forum (2014): 1
Scopus rating (2013): 1.515 0.588
Publication Forum (2013): 1
Scopus rating (2012): 1.47 0.686
Publication Forum (2012): 1
Scopus rating (2011): 1.369 0.593
Scopus rating (2010): 1.368 0.534
Scopus rating (2009): 1.701 0.57
Scopus rating (2008): 1.707 0.663
Scopus rating (2007): 1.488 0.523
Scopus rating (2006): 1.411 0.47
Scopus rating (2005): 1.269 0.472
Scopus rating (2004): 1.049 0.463
Scopus rating (2003): 1.225 0.473
Scopus rating (2002): 1.187 0.489
Scopus rating (2001): 1.198 0.508
Scopus rating (2000): 3.164 1.327
Scopus rating (1999): 2.828 1.083
Original language: English
Links:
https://www.elsevier.com/books/vitamins-and-coenzymes-part-g/author/978-0-12-182022-0
Source: PubMed
Source-ID: 2939318
Research output: Scientific - peer-review › Article

Bioluminescent assay of lactate dehydrogenase and its isoenzyme-1 activity
A bioluminescent assay based on the bacterial luciferase reaction has been developed for the determination of total lactate dehydrogenase and heart-specific lactate dehydrogenase isoenzyme-1 activity in serum. The lactate
dehydrogenase-catalyzed reaction was measured in both directions, but NADH formation (lactate----pyruvate) is recommended because it allows the use of optimal reaction conditions. Internal calibration with a known amount of NADH accounts for possible interference from samples when both NADH formation and consumption are followed. The bioluminescent method is sensitive, has good precision, and is readily automated. Serum lactate dehydrogenase isoenzyme-1 was immunochemically isolated and the activity was assayed by bioluminescence. A good correlation between the bioluminescent assays and the conventional spectrophotometric procedure used as reference was obtained.

Fractionation of DNA with Sephacryl S-1000(R)
In this study the application of gel filtration for purification of heterogeneous DNA is described. The fractionation of partial restriction enzyme digests of bacterial chromosomal DNA on a Sephacryl S-1000 column is easy and rapid. Simultaneously intact chromosomal DNA and low molecular weight substances are eliminated in the run. The method is also applicable to the purification of plasmid DNA, as has been previously reported (3). Thus we are able to get pure DNA with yields over 80%.

Fractionation of DNA with Sephacryl S-1000(R)
In this study the application of gel filtration for purification of heterogeneous DNA is described. The fractionation of partial restriction enzyme digests of bacterial chromosomal DNA on a Sephacryl S-1000 column is easy and rapid. Simultaneously intact chromosomal DNA and low molecular weight substances are eliminated in the run. The method is also applicable to the purification of plasmid DNA, as has been previously reported (3). Thus we are able to get pure DNA with yields over 80%.
Time-resolved europium fluorescence in enzyme activity measurements: a sensitive protease assay

A method for incorporating into proteins a nonradioactive Eu3+ label, which exhibits fluorescence of a long decay time in the presence of suitable ligands, is described. As an example of the use of this label the method has been developed to work as a sensitive protease assay. By hydrolyzing the Eu3+-labeled casein, bound to an insoluble matrix (Sepharose 4B or Affi-Gel 10), with proteases and measuring the Eu3+ released with a pulsed time-resolved fluorometer it was possible to detect as low as 2.5, 1.0, or 1.0 ng of alpha-chymotrypsin, trypsin, or subtilisin, respectively.

Simultaneous extraction and combined bioluminescent assay of NAD+ and NADH

A new method for extracting pyridine nucleotides from tissue samples at room temperature that allows the simultaneous extraction of both the oxidized and reduced nucleotide when using a 70% buffered ethanol solution as the extractant has been developed. The extraction efficiencies for NAD+ and NADH were 91 and 102%, respectively. The extraction method was followed by a combined bioluminescent assay of both nucleotides. A bacterial bioluminescent system, which included luciferase and low levels of a NADH-specific oxidoreductase, was used to produce a constant light intensity directly proportional to the amount of NADH in the tissue extract sample. When the NADH had been measured, the NAD+ present in the extract was enzymatically converted to NADH by the addition of alcohol dehydrogenase, after which the second increase in light level was recorded. The sensitivity of the bioluminescent assay presented here is 5 X 10(-14) mol NADH or NAD+ per assay.