Electropolymerized polyazulene as active material in flexible supercapacitors

We report the capacitive behavior of electrochemically polymerized polyazulene films in different ionic liquids. The ionic liquids in this study represent conventional imidazolium based ionic liquids with tetrafluoroborate and bis(trifluoromethylsulfonyl)imide anions as well as an unconventional choline based ionic liquid. The effect of different ionic liquids on the polymerization and capacitive performance of polyazulene films is demonstrated by cyclic voltammetry and electrochemical impedance spectroscopy in a 3-electrode cell configuration. The films exhibit the highest capacitances in the lowest viscosity ionic liquid (92 mF cm\(^{-2}\)), while synthesis in high viscosity ionic liquid shortens the conjugation length and results in lower electroactivity (25 mF cm\(^{-2}\)). The obtained films also show good cycling stabilities retaining over 90% of their initial capacitance over 1200 p-doping cycles. We also demonstrate, for the first time, flexible polyazulene supercapacitors of symmetric and asymmetric configurations using the choline based ionic liquid as electrolyte. In asymmetric configuration, capacitance of 55 mF (27 mF cm\(^{-2}\)) with an equivalent series resistance of 19 \(\Omega\) is obtained at operating voltage of 1.5 V. Upon increasing the operating voltage up to 2.4 V, the capacitance increases to 72 mF (36 mF cm\(^{-2}\)).

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Electronics and Communications Engineering, Faculty of Biomedical Sciences and Engineering, Research area: Microsystems, Research area: Measurement Technology and Process Control, Research group: Sensor Technology and Biomeasurements (STB), Turun Yliopisto/Turun Biomateriaalikeskus
Authors: Suominen, M., Lehtimäki, S., Yewale, R., Damlin, P., Tuukkanen, S., Kvarnström, C.
Keywords: (Choline, Electropolymerization, Flexible supercapacitor, Ionic liquid, Polyazulene)
Number of pages: 10
Pages: 181-190
Publication date: 15 Jul 2017
Peer-reviewed: Yes

Publication information
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ISSN (Print): 0378-7753
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.945 1.483
Publication Forum (2016): 2
Scopus rating (2015): 1.945 1.686
Web of Science (2015): 6.333 6.098 5.4 1.681 0.13291 1.159
Publication Forum (2015): 2
Scopus rating (2014): 1.983 2.071
Web of Science (2014): 6.217 6.227 5.6 1.744 0.1163 1.128
Publication Forum (2014): 2
Scopus rating (2013): 1.985 2.138
Publication Forum (2013): 2
Scopus rating (2012): 2.293 2.016
Publication Forum (2012): 2
Scopus rating (2011): 2.247 2.181
Scopus rating (2010): 2.297 1.981
Scopus rating (2009): 2.117 1.793
Scopus rating (2008): 1.968 1.726
Scopus rating (2007): 1.597 1.489
Scopus rating (2006): 1.8 2.224
Scopus rating (2005): 1.65 1.825
Scopus rating (2004): 1.852 1.818
Scopus rating (2003): 1.66 1.583
Scopus rating (2002): 1.959 1.4
Scopus rating (2001): 1.115 1.492
Scopus rating (2000): 1.106 0.914
Scopus rating (1999): 0.854 0.998
Engineering and Characterization of Bacterial Nanocellulose Films as Low Cost and Flexible Sensor Material

Some bacterial strains such as Komagataeibacter xylinus are able to produce cellulose as an extracellular matrix. In comparison to wood-based cellulose, bacterial cellulose (BC) holds interesting properties such as biodegradability, high purity, water-holding capacity, and superior mechanical and structural properties. Aiming toward improvement in BC production titer and tailored alterations to the BC film, we engineered K. xylinus to overexpress partial and complete bacterial cellulose synthase operon that encodes activities for BC production. The changes in cell growth, end metabolite, and BC production titers from the engineered strains were compared with the wild-type K. xylinus. Although there were no significant differences between the growth of wild-type and engineered strains, the engineered K. xylinus strains demonstrated faster BC production, generating 2–4-fold higher production titer (the highest observed titer was obtained with K. xylinus-bcsABCD strain producing 4.3 ± 0.46 g/L BC in 4 days). The mechanical and structural characteristics of cellulose produced from the wild-type and engineered K. xylinus strains were analyzed with a stylus profilometer, in-house built tensile strength measurement system, a scanning electron microscope, and an X-ray diffractometer. Results from the profilometer indicated that the engineered K. xylinus strains produced thicker BC films (wild type, 5.1 μm, and engineered K. xylinus strains, 6.2–10.2 μm). Scanning electron microscope revealed no principal differences in the structure of the different type BC films. The crystallinity index of all films was high (from 88.6 to 97.5%). All BC films showed significant piezoelectric response (5.0–20 pC/N), indicating BC as a promising sensor material.

General information
State: E-pub ahead of print
Ministry of Education publication type: A1 Journal article-refereed
Authors: Mangayil, R., Rajala, S., Pammo, A., Sarlin, E., Luo, J., Santala, V., Karp, M., Tuukkanen, S.
Number of pages: 9
Publication date: 18 May 2017
Peer-reviewed: Yes

Publication information
Journal: ACS Applied Materials & Interfaces
ISSN (Print): 1944-8244
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.524 1.528
Publication Forum (2016): 2
Scopus rating (2015): 2.299 1.568
Web of Science (2015): 7.145 7.332 2.4 1.18 0.1479 1.462
Publication Forum (2015): 2
Scopus rating (2014): 2.126 1.64
Web of Science (2014): 6.723 6.813 2.3 0.991 0.09406 1.373
Publication Forum (2014): 1
Scopus rating (2013): 1.979 1.543
Publication Forum (2013): 1
Scopus rating (2012): 2.18 1.309
Publication Forum (2012): 1
Scopus rating (2011): 2.017 1.396
Scopus rating (2010): 1.571 0.931
Original language: English
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.
Fluorescence spectroscopy "knife" for polyplex "cakes": taste the filling

General information
State: Published
Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials
Authors: Vuorimaa-Laukkanen, E., Lisitsyna, E. S., Ketola, T., Morin-Pickardat, E., Liang, H., Hanzlikova, M., Urtti, A., Yliperttula, M. L.
Publication date: 2017
Peer-reviewed: Unknown
ASJC Scopus subject areas: Chemistry(all), Pharmaceutical Science
Event: Paper presented at 30 Years of Drug Delivery Research, Kuopio, Finland.
Research output: Scientific › Paper, poster or abstract

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.

General information
State: Accepted/In press
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Computational Systems Biology, Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Molecular Signaling Lab
Authors: Karjalainen, A., Doan, P., Sandberg, O., Chandraseelan, J. G., Yli-Harja, O., R. Candeias, N., Kandhavelu, M.
Publication date: 2017
Peer-reviewed: Yes

Publication information
Journal: Anti-Cancer Agents in Medicinal Chemistry
Volume: 17
ISSN (Print): 1871-5206
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.769 0.796
Publication Forum (2016): 1
Scopus rating (2015): 0.969 0.854
Web of Science (2015): 2.722 2.849 4.4 0.489 0.00598 0.678
Publication Forum (2015): 1
Scopus rating (2014): 0.949 0.777
Web of Science (2014): 2.469 2.974 4.2 0.744 0.0059 0.697
Publication Forum (2014): 1
Scopus rating (2013): 1.087 0.822
Publication Forum (2013): 1
Scopus rating (2012): 1.007 0.945
Publication Forum (2012): 1
Scopus rating (2011): 1.33 1.118
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

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Journal: Waste Management
Volume: 57
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
UPS and DFT investigation of the electronic structure of gas-phase trimesic acid

Benzene-1,3,5-tricarboxylic acid (trimesic acid, TMA) molecules in gas-phase have been investigated by using valence band photoemission. The photoelectron spectrum in the binding energy region from 9 to 22 eV is interpreted based on the density functional theory calculations. The electronic configuration that makes contribution to each transition is demonstrated. Furthermore, electronic structure of TMA is compared with benzene and benzoic acid (BA) in order to demonstrate changes in molecular orbital energies induced by addition of carboxyl groups to benzene ring.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Optoelectronics Research Centre, Research group: Surface Science, University of Tartu, MAX IV Laboratory, Lund University
Authors: Reisberg, L., Pärna, R., Kikas, A., Kuusik, I., Kisand, V., Hirsimäki, M., Valden, M., Nõmmiste, E.
Keywords: (trimesic acid, molecules, electronic structure, synchrotron radiation, MAX IV Laboratory, UPS, DFT, organic acids, gas-phase, spectroscopy, photoemission)
Number of pages: 6
Pages: 11-16
Publication date: Nov 2016
Peer-reviewed: Yes
ASJC Scopus subject areas: Organic Chemistry, Atomic and Molecular Physics, and Optics

Publication information
Journal: Journal of Electron Spectroscopy and Related Phenomena
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ISSN (Print): 0368-2048
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.962 0.837
Publication Forum (2016): 1
Scopus rating (2015): 0.813 0.923
Web of Science (2015): 1.561 1.679 >10.0 0.44 0.00536 0.553
Publication Forum (2015): 1
Scopus rating (2014): 0.778 0.815
Web of Science (2014): 1.436 1.631 >10.0 0.258 0.00506 0.544
Publication Forum (2014): 1
Scopus rating (2013): 0.91 0.954
Publication Forum (2013): 1
Scopus rating (2012): 1.047 0.954
Thermo-catalytic decomposition of methane: The effect of reaction parameters on process design and the utilization possibilities of the produced carbon

The study presents a path for selecting the reaction and reactor parameters of a process applying thermo-catalytic decomposition of methane (TDM). Temperature and catalyst are the main reaction parameters affecting the type of TDM carbon and defining the reaction’s theoretical heat requirement. Secondly, the reaction parameters affect the reactor design including the selection of reactor type and heating source as well as the reactor dimensioning. The reactor dimensioning is discussed by highlighting the methane residence time requirement at different reaction conditions. Finally, the economic value of the TDM products is analyzed. According to the analyses, the reaction temperature and catalyst have a significant effect on reactor design and on the value and utilization possibilities of the TDM carbon. The prices of carbon products vary greatly as does the global demand of those. The utilization possibilities of carbon highly affect the overall viability of the TDM process and therefore should be carefully considered during process design.

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: Keipi, T., Tolvanen, K. E., Tolvanen, H., Konttinen, J.
Keywords: (Carbon capture, Process design, Natural gas, Methane decomposition, Hydrogen production)
Number of pages: 12
Pages: 923-934
Publication date: Oct 2016
Peer-reviewed: Yes

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Journal: Energy Conversion and Management
Volume: 126
ISSN (Print): 0196-8904
Ratings:
Scopus rating (2011): 1.06 0.842
Scopus rating (2010): 0.742 0.658
Scopus rating (2009): 0.682 0.663
Scopus rating (2008): 0.786 0.68
Scopus rating (2007): 0.774 0.807
Scopus rating (2006): 0.863 0.725
Scopus rating (2005): 0.779 0.784
Scopus rating (2004): 0.754 0.759
Scopus rating (2003): 1.093 0.8
Scopus rating (2002): 1.008 0.771
Scopus rating (2001): 0.872 0.785
Scopus rating (2000): 0.623 0.593
Scopus rating (1999): 0.891 0.663
Original language: English
DOIs: 10.1016/j.elspec.2016.10.004
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
Peer-reviewed: Unknown
Research output: Scientific › Paper, poster or abstract

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.

General information
State: E-pub ahead of print
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Department of Physics, Research area: Computational Physics, Research group: Electronic Structure Theory, Department of Physics, Imperial College London, South Kensington Campus, London SW7 2AZ, U.K.
Authors: Kontkanen, O., Niskanen, M., Hukka, T., Rantala, T.
Pages: 14382-14389
Publication date: 12 May 2016
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
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.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Department of Physics, Research area: Computational Physics
Authors: Kastinen, T., Niskanen, M., Risko, C., Cramariuc, O., Hukka, T. I.
Keywords: (density functional theory, DFT, time-dependent DFT, donor-acceptor copolymer, benzodithiophene)
Number of pages: 14
Pages: 1051-1064
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

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
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.

General information

State: Published
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Carraro, G., Maccato, C., Gasparotto, A., Kaunisto, K., Sada, C., Barreca, D.
Keywords: (Co₃O₄, Fe₂O₃, plasma-enhanced chemical vapor deposition (PE-CVD), sputtering, water splitting)
Number of pages: 10
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
A study on raw, torrefied, and steam-exploded wood: Fine grinding, drop-tube reactor combustion tests in N$_2$/O$_2$ and CO$_2$/O$_2$ atmospheres, particle geometry analysis, and numerical kinetics modelling

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 O$_2$ concentrations used in the measurements were 3–21 vol-% in either N$_2$ or CO$_2$ 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.
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).
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.
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 S0 was provided for the bacteria to produce H2SO4. 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.
Corrosion Losses in Sintered (Nd,Dy)-Fe-B Magnets vs. Magnet geometry

Sintered Nd-Fe-B magnets with cube and flat geometries were exposed to pressurized heat-humidity corrosion tests for the durations of 96 and 240 hours. Parallel measurements of weight and flux losses were performed after the corrosion tests. The corroded specimens were further characterized using scanning electron microscopy and optical profilometry. The microcrystalline anisotropy of sintered magnets gave rise to heterogeneous corrosion behavior, where the pole faces degraded preferentially to the side faces. The magnetic field by the magnet itself thus contributed to the amount and location of detached ferromagnetic grains. The magnets with cube geometry suffered greater losses than the flat magnets, even though the flat magnets had a higher relative amount of the pole face. The higher total flux (due to a larger volume)
of the cube-shaped magnets led to the higher overall losses. In the flat magnets, the corrosion concentrated heavily on areas near the corners.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Materials Characterization
Authors: Isotahdon, E., Huttunen-Saarivirta, E., Kuokkala, V., Paju, M.
Keywords: (Corrosion, Hard Magnetic Materials, Nd-Fe-B magnets)
Publication date: 2016
Peer-reviewed: Yes
Early online date: 1 Jan 2015

Publication information
Journal: IEEE Magnetics Letters
Volume: 7
Article number: 5500504
ISSN (Print): 1949-307X
Publications Forum (2017): 1
Scopus rating (2016): 0.39 0.454
Publication Forum (2016): 1
Scopus rating (2015): 0.452 0.689
Web of Science (2015): 1.978 1.776 2.8 0.204 0.00115 0.772
Scopus rating (2014): 0.76 0.745
Web of Science (2014): 1.692 1.833 3.0 0.154 9.0E-4 0.789
Scopus rating (2013): 0.68 0.664
Scopus rating (2012): 0.705 0.936
Scopus rating (2011): 0.558 0.399
Original language: English
DOI: 10.1109/LMAG.2015.2501404
Source: Bibtex
Source-ID: urn:eda200522672923bb11d236d61a3260f
Research output: Scientific - peer-review Article

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
State: E-pub ahead of print
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
Publications Forum (2017): 1
Scopus rating (2016): 1.13 0.906
Publication Forum (2016): 1
Scopus rating (2015): 1.148 0.905
Remarkable Dependence of the Final Charge Separation Efficiency on the Donor-Acceptor Interaction in Photoinduced Electron Transfer

The unprecedented dependence of final charge separation efficiency as a function of donor-acceptor interaction in covalently-linked molecules with a rectilinear rigid oligo-p-xylene bridge has been observed. Optimization of the donor-acceptor electronic coupling remarkably inhibits the undesirable rapid decay of the singlet charge-separated state to the ground state, yielding the final long-lived, triplet charge-separated state with circa 100% efficiency. This finding is extremely useful for the rational design of artificial photosynthesis and organic photovoltaic cells toward efficient solar energy conversion.
Corrosion products of carbonation induced corrosion in existing reinforced concrete facades

Active corrosion in reinforced concrete structures is controlled by environmental conditions and material properties. These factors determine the corrosion rate and type of corrosion products which govern the total achieved service life. The type and critical amount of corrosion products were studied by electron microscopy and X-ray diffractometry on concrete and reinforcement samples from existing concrete facades on visually damaged locations. The corrosion products in outdoor environment exposed concrete facades are mostly hydroxides (Feroxyhite, Goethite and Lepidocrocite) with a volume ratio to Fe of approximately 3. The results can be used to calibrate calculation of the critical corrosion penetration of concrete facade panels.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Civil Engineering, Research group: Service Life Engineering of Structures, Department of Materials Science, Research group: Materials Characterization, Research area: Structural Engineering, Research group: Structures and Their Behaviour, Engineering materials science and solutions (EMASS), Life Cycle Effectiveness of the Built Environment (LCE@BE)
Authors: Köliö, A., Honkanen, M., Lahdensivu, J., Vippola, M., Pentti, M.
Keywords: (B. SEM, B. X-ray diffraction, C. Corrosion, D. Reinforcement, E. Concrete)
Number of pages: 8
Pages: 200-207
Publication date: Dec 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Materials Science(all), Building and Construction
Enhanced pre-treatment of cellulose pulp prior to dissolution into NaOH/ZnO

As a result of the constantly growing demand for textile fibres interest in utilising cellulose pulps for manufacturing regenerated cellulose fibres is growing. One promising water-based process for the manufacture of regenerated cellulosic products is the Biocelsol process based on an NaOH/ZnO solvent system. The drawback of the Biocelsol process is the need for pre-treatment of the pulp, i.e. long mechanical pre-treatment (up to 5 h) followed by a 2–3-h enzymatic hydrolysis utilising a rather high amount of cellulolytic enzymes. In this work more efficient conditions to carry out the pre-treatment of cellulose pulp prior to dissolution into NaOH/ZnO are presented. Based on the results, cellulase treatment, when carried out in an extruder, can be used to effectively open up and fibrillate the fibres without completely destroying the fibre structure. The molar mass of the pulp treated enzymatically in an extruder was 14 % lower as compared to the state-of-the-art-treated cellulose. As a consequence, the alkaline solutions prepared from the pulp treated enzymatically in an extruder had clearly lower dope viscosities regarding the cellulose content than the solutions prepared from the state-of-the-art-treated pulp. This enabled increasing the cellulose content in the dope up to 7 % (w/w) without increasing the dope viscosity.
Graphene-intercalated Fe₂O₃/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-Fe\(_2\)O\(_3\) 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-Fe\(_2\)O\(_3\)/TiO\(_2\) 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-Fe\(_2\)O\(_3\) and TiO\(_2\) layers resulted in reduced recombination in the α-Fe\(_2\)O\(_3\) layer. The results showed that graphene intercalation improved the charge separation and the photocurrent density of the FTO/α-Fe\(_2\)O\(_3\)/FLG/TiO\(_2\) system.

**Power generation in fed-batch and continuous up-flow microbial fuel cell from synthetic wastewater**

Up-flow bioreactors have the advantages of retaining very high cell density and having high mass transfer efficiency. The recirculation rate could improve the up-flow rate in up-flow bioreactor. A two-chamber UFMFC (up-flow microbial fuel cell) is constructed with flat graphite electrodes and anion exchange membrane for electricity generation. The anode chamber is seeded with compost culture enriched on xylose and operated on synthetic wastewater with 0.5 g/L xylose, external resistance of 100 Ω, at pH 7.0 and 37 °C in fed-batch mode. The cathode chamber in the top of the UFMFC is filled with potassium ferricyanide (pH 7.0) as the electron acceptor. The effects of different recirculation rates of 1.2, 2.4, 4.8 and 7.2 RV (reactor-volumes)/h to increase the mass transfer and electricity production are determined in fed-batch mode. At a recirculation rate of 4.8 RV/h, a power density of 356 ± 24 mW/m\(^2\) with CE (coulombic efficiency) of 21.3 ± 1.0% is obtained. Decreasing HRT (hydraulic retention time) could improve the electricity production performance of UFMFC in continuous mode. The power generation is increased to 372 ± 20 mW/m\(^2\), while CE remains at 13.4 ± 0.5% with HRT of
1.7 d and optimum recirculation rate of 4.8 RV/h on continuous mode. Microbial communities were characterized with PCR (polymerase chain reaction) - DGGE (denaturing gradient gel electrophoresis). In the end of the experiment, the biofilm contained both fermenting and exoelectrogenic bacteria, while fermenting and nitrate-reducing bacteria were mainly present in the anodic solutions. Moreover, some changes occurred in the microbial communities of the anodic solutions when the MFCs were switched from fed-batch to continuous mode, while the differences were minor between different recirculation rates in fed-batch mode.
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.
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.

General information

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Engineering materials science and solutions (EMASS)
Authors: Mylläri, V., Ruoko, T., Vuorinen, J., Lemmetyinen, H.
Keywords: (Fibre, PEEK, Thermal degradation)
Number of pages: 8
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Peer-reviewed: Yes
Early online date: 6 Aug 2015

Publication information

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Volume: 120
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Scopus rating (2016): 1.029 1.582
Publication Forum (2016): 1
Scopus rating (2015): 1.22 1.634
Web of Science (2015): 3.12 3.553 8.3 0.507 0.01691 0.688
Publication Forum (2015): 1
Scopus rating (2014): 1.278 1.888
Web of Science (2014): 3.163 3.722 8.0 0.348 0.01798 0.725
Publication Forum (2014): 2
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
Scopus rating (2010): 1.237 1.642
Characterization of thermally aged polyetheretherketone fibres_pre-print

DOI:
10.1016/j.polymdegradstab.2015.08.003

Links:
http://urn.fi/URN:NBN:fi:tty-201612024835

Characterization of thermally aged polyetheretherketone fibres

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.

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), 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.
Keywords: (Eicosapentaenoic acid, Nannochloropsis, Paper mill, Pulp mill, Wastewater)
Number of pages: 8
Pages: 469-476
Publication date: 1 Oct 2015
Peer-reviewed: Yes
Early online date: 2 Jul 2015
ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

Publication information
Journal: Bioresource Technology
Volume: 193
ISSN (Print): 0960-8524
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.191 1.91
The Effect of Phosphorus Exposure on Diesel Oxidation Catalysts—Part I: Activity Measurements, Elementary and Surface Analyses

The effects of phosphorus poisoning on the activity of PtPd and Pt diesel oxidation catalysts and on the activity of the support material were investigated using the gas phase laboratory-scale-aging procedure. The catalysts were treated using two different phosphorus concentrations (0.065 and 0.13 mol/L (NH4)(2)HPO). The deactivation was studied by inductively coupled plasma optical emission spectroscopy, electron microscopy, X-ray diffractometry, X-ray photoelectron spectrometry and Fourier-transform infrared reflectance, N-2-physisorption, and activity measurements with CO, C3H6 and NO. The amount of accumulated phosphorus was higher on the Pt catalyst surface than on the PtPd catalyst and significantly higher on the surface of the bare support material. Phosphorus concentration was uniform throughout the support layer (down to the 10 mu m), and phosphorus was found as phosphate, although it can also form compounds like AlPO(4) with the support. The treatment with low phosphorus concentration was found to have a clear deactivation effect only for C3H6 oxidation activity on PtPd catalysts above 200 degrees C. The treatment with high phosphorus concentration significantly decreased the activity of both the PtPd and Pt catalysts. In particular, the C3H6 and NO oxidation activities of the fresh and P-treated Pt catalysts were higher than those of the PtPd catalysts for the entire temperature range.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Materials Characterization, Univ Oulu, University of Oulu, Fac Technol, Environm & Chem Engn, Aalto University, Dinex Ecocat Oy, Catalyst Res
Authors: Kärkkäinen, M., Kolli, T., Honkanen, M., Heikkinen, O., Huuhtanen, M., Kallinen, K., Lepistö, T., Lahtinen, J., Vippola, M., Keiski, R. L.
Keywords: (Phosphorus, Deactivation, Poisoning, Diesel oxidation catalyst, Platinum, Palladium, NO OXIDATION, THERMAL-STABILITY, DEACTIVATION, REDUCTION, MECHANISMS, BEHAVIOR, EXHAUST)
Number of pages: 10
The Effect of Phosphorus Exposure on Diesel Oxidation Catalysts-Part II: Characterization of Structural Changes by Transmission Electron Microscopy

Phosphorus poisoning and its effect on the diesel oxidation catalysts morphology was studied by transmission electron microscopy (TEM). The studied catalyst samples were PtPd or Pt supported on the alumina-based washcoat including additives. The laboratory-scale phosphorus exposures were carried out with two different phosphorus concentrations. The cross-sectional TEM samples were prepared from the fresh and phosphorus-treated catalysts. After phosphorus exposures, significant structural changes were observed compared to the fresh catalysts. The shape of the noble metal particles had changed from irregular to more spherical-shaped particles. In addition, phosphorus was detected throughout the catalyst TEM samples but the amount varied depending on the local composition of the support. Phosphorus accumulated mainly in the alumina-containing areas of the support and indications of dense and amorphous aluminium phosphates were found. Based on the results gained, cross-sectional TEM characterization is essential to observe these kinds of morphological changes in the catalysts caused e.g. by phosphorus exposures. In addition, cross-sectional TEM samples are needed to study the effect of local variation in the support composition on the phosphorus accumulation.

General information
State: Published
Protective Spinel Coatings for Solid Oxide Fuel Cell Interconnectors by Thermal Spray Processes: From Conventional Dry Powder to Novel Solution Precursor Thermal Spraying

Protective coatings are used on ferritic stainless steel interconnectors to prevent the transport of the harmful CrO3(g) and Cr2O7(OH)2(g) compounds in solid oxide fuel cells. These compounds are transported on the triple-phase boundary of the cathode, and electrically reduce back to Cr2O3 causing degradation of the cell. The most promising materials to be used as protective coatings are (Mn,Co)3O4 spinels. However, in order to provide good protectiveness in long-term use (5 years or more), these coatings should have a dense microstructure, good adhesion with the substrate and good chemical stability at high temperature in an oxidizing atmosphere. Several deposition techniques have been studied, for example various wet-ceramic processes and thin film techniques. However, the studies have shown that the coatings produced with
these methods are not dense, and therefore their long-term protectiveness is questionable.

In this study, protective (Mn,Co)₃O₄ and (Mn,Co,Fe)₃O₄ spinel coatings were manufactured with conventional atmospheric plasma spraying (APS) and novel high velocity solution precursor flame spraying (HVSPFS). The aim was to obtain a dense microstructure. Since the HVSPFS process is a novel deposition method, the coating build-up mechanism and materials synthesis were studied more closely. The as-sprayed coatings were oxidized in order to obtain more detailed information about the Cr barrier and electrical properties during the oxidation cycles.

The spinel coatings with a dense microstructure were sprayed using the APS and the HVSPFS processes. The deposition methods caused the as-sprayed coatings to sinter during the oxidation cycles. The sintering was a consequence of the metastable phase structure and the small particle and crystallite size. Due to the dense microstructure and fully recovered spinel phases, the coatings provided a good Cr barrier and electrical properties, even in a relatively harsh environment. It can be stated that Mn₁.₅Co₁.₅O₄ and MnCo₁.₉Fe₀.₁O₄ spinel coatings, manufactured either by conventional thermal spraying using agglomerated cermet powder, or by solution precursor thermal spraying, are good candidates for use as protective coatings on metallic interconnectors.

**General information**
State: Published
Ministry of Education publication type: G5 Doctoral dissertation (article)
Organisations: Department of Materials Science, Research group: Surface Engineering
Authors: Puranen, J.
Number of pages: 81
Publication date: 18 Sep 2015

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Publisher: Tampere University of Technology
Original language: English

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Publisher: Tampere University of Technology
Volume: 1322
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Electronic versions:
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Versio ok 16.12.2015
Research output: Collection of articles » Doctoral Thesis

**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/m²<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.

**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)
Measuring synthesis yield in graphene oxide synthesis by modified hummers method

Synthesis of graphene oxide by the modified Hummers method and measuring the synthesis yield were investigated. Based on the results, a comprehensive method to measure graphene oxide synthesis yield was proposed, which will allow comparison of future literature results. In addition, changes are proposed to the exfoliation procedure to improve the yield of the modified Hummers synthesis. With the proposed method, systematic error of the concentration measurement was calculated to be ±0.08 × 10^{-3} g mL^{-1}. In addition, changes proposed to the graphene oxide exfoliation process can improve the synthesis yield by up to 70%.

General information
State: Published
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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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), University of Jyväskylä, Valmet Technologies Oy, VTT Technical Research Centre of Finland, Department of Chemistry, Renewable Natural Resources and Chemistry of Living Environment, Stora Enso
Authors: Bajamundi, C. J. E., Vainikka, P., Hedman, M., Silvennoinen, J., Heinanen, T., Taipale, R., Konttinen, J.
Keywords: (Alkali chloride mitigation, Corrosion, SRF, Waste-to-energy)
Number of pages: 12
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Peer-reviewed: Yes
ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

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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
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
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.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Padova University, Padova University and INSTM, Department of Physics and Astronomy, University of Turku, Univ Antwerp, University of Antwerp, EMAT, CNR-IENI and INSTM, Department of Chemistry, Department of Chemical and Pharmaceutical Sciences, ICCOM-CNR Trieste Research Unit - INSTM Research Unit, Trieste University
Number of pages: 8
Pages: 6219-6226
Publication date: 28 Aug 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics

Publication information

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Issue number: 32
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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
Electrospun Black Titania Nanofibers: Influence of Hydrogen Plasma-Induced Disorder on the Electronic Structure and Photoelectrochemical Performance

This work encompasses a facile method for tailoring surface defects in electrospun TiO2 nanofibers by employing hydrogen plasma treatments. This amiable processing method was proven with SQUID, EPR, and XPS to be highly effective in generating oxygen vacancies, accompanied by the reduction of Ti4+ centers to Ti3+, resulting in the formation of black titania. The treatment temperature was found to affect the Ti3+/Ti4+ ratios and surface valence, while preserving the original 1D morphology of the titania fibers. Ab initio DFT calculations showed that a high concentration of oxygen vacancies is highly efficient in producing midgap states that enhance the system absorption over the whole visible range, as observed with UV/vis/NIR diffuse reflectance spectroscopy. Pristine TiO2 nanofibers produced a photocurrent density of similar to 0.02 mA/cm2 at 1.23 V vs RHE, whereas the hydrogen plasma treatment resulted in up to a 10-fold increase in the photoelectrochemical performance.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Universita degli Studi di Padova, Italy, Univ Cologne, University of Cologne, Dept Chem, Chair Inorganic & Mat Chem, Padova University, INSTM, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Institute of Inorganic Chemistry, Catalonia Institute for Energy Research (IREC), Multiscale Materials Modelling and Tribology Simulation, CNR-IENI
Authors: Lepcha, A., Maccato, C., Mettenbörger, A., Andreu, T., Mayrhofer, L., Walter, M., Olthof, S., Ruoko, T. P., Klein, A., Moseler, M., Meerholz, K., Morante, J. R., Barreca, D., Mathur, S.
Keywords: (ROOM-TEMPERATURE, WATER, SURFACE, NANOSTRUCTURES, NANOPARTICLES, PHOTOCATALYSIS, INSULATORS, CONVERSION, DEFECTS, ARRAYS)
Number of pages: 8
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Peer-reviewed: Yes
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

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Volume: 119
Issue number: 33
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
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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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Industrial Bioengineering and Applied Organic Chemistry, Frontier Photonics, Urban circular bioeconomy (UrCirBio)
Authors: George Abraham, B., Sarkisyan, K. S., Mishin, A. S., Santala, V., Tkachenko, N. V., Karp, M.
Keywords: (RESONANCE ENERGY-TRANSFER, IMAGING MICROSCOPY, FORSTER DISTANCES, MONOMERIC RED, LIVING CELLS, LIVE CELLS, BIOSENSORS, SENSOR, FLIM, ENVIRONMENT)
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Volume: 10
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Article number: e0134436
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Ratings:
Photoinduced electron transfer (ET) in CdSe/ZnS core-shell quantum dot (QD) – fullerene (COOH-C<sub>60</sub>) hybrids was studied by the means of time-resolved emission and absorption spectroscopy techniques. A series of four QDs with emission in the range 540-630 nm was employed to investigate the dependence of the electron transfer rate on the QD size. Emission of the QDs is quenched upon hybrid formation, and the quenching mechanism is identified as photoinduced electron transfer from the QD to the fullerene moiety due to the fullerene anion signature observed in transient absorption. In order to obtain quantitative information on the ET reaction, several kinetic data analysis techniques were used, including a conventional multiexponential fitting and a maximum entropy method for emission decay analysis, as well as a distributed decay model based on the Poisson distribution of fullerenes in the hybrids. The latter gradually simplifies the interpretation of the transient absorption spectra and indicates that the spectra of QD cations are essentially similar to those of neutral QDs, differing only by a minor decrease in the intensity and broadening. Furthermore, only a minor decrease in the ET rate with the increasing QD size was observed, the time constants being in the range 100-200 ps for all studied QDs. The charge recombination is extended to 10 ns or longer for all hybrids.

**General information**

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Virkki, K., Demir, S., Lemmetyinen, H., Tkachenko, N. V.
Number of pages: 12
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Publication date: 23 Jul 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

**Publication information**

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Volume: 119
Issue number: 31
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
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:α-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.

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, 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., Lemmetyinen, H.
Keywords: (FILM ELECTRODES, IRON-OXIDE, SEMICONDUCTOR ELECTRODES, WATER OXIDATION, VISIBLE-LIGHT, ALPHA-FE2O3, PHOTOELECTRODES, TIO2, RECOMBINATION, ELECTROLYSIS)
Number of pages: 6
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ASJC Scopus subject areas: Materials Science(all)

Publication information
Journal: Journal of Physical Chemistry Letters
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Ratings:
Publication Forum (2017): 3
Scopus rating (2016): 4.583 1.68
Publication Forum (2016): 3
Synthesis and study of electrochemical and optical properties of substituted perylenemonoimides in solutions and on solid surfaces

A new and efficient methodology towards the synthesis of 7-pyrrolidinyl and 7,12-bispyrrolidinyl perylenemonoimide monoanhydrides (PMI monoanhydrides) and their corresponding dicarboxylic acids is devised. The high yields (70-96%) and facile synthesis of PMI monoanhydrides, as compared to traditional methodologies, make the method attractive and versatile. The reported 7,12-bispyrrolidinyl PMI monoanhydrides are a new family of peryleneimides, where both the bay-substituents are located towards the anhydride cycle. The electrochemical and optical properties of target molecules and their precursors were investigated using UV-Vis spectroscopy and differential pulse voltammetry. Atomic charges and electronic properties were calculated using density functional theory (DFT). In addition, self-assembling monolayers of the PMI monoanhydrides and their corresponding diacids were successfully formed over ZnO and TiO<sub>2</sub> films. The results of the current study indicate that these molecules are potentially good candidates for various applications in the fields of organic electronics and solar cells.

General information
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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Ahmed, Z., George, L., Hiltunen, A., Lemmetyinen, H., Hukka, T., Efimov, A.
Number of pages: 8
Pages: 13332-13339
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Peer-reviewed: Yes
ASJC Scopus subject areas: Chemistry(all), Renewable Energy, Sustainability and the Environment, Materials Science(all)

Publication information
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Volume: 3
Issue number: 25
ISSN (Print): 2050-7488
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 3.037 1.468
Publication Forum (2016): 2
Scopus rating (2015): 2.672 1.663
We describe novel tools, bioluminescent whole-cell reporter gene assays, for facilitating the use of natural products in antimicrobial drug discovery. As proof-of-concept, a plant extract library was screened and follow-up experiments were carried out. Primary results can be obtained in 2-4 h with high sensitivity, leading to significant improvements of the process.

**Bioluminescent whole-cell reporter gene assays as screening tools in the identification of antimicrobial natural product extracts**

We describe novel tools, bioluminescent whole-cell reporter gene assays, for facilitating the use of natural products in antimicrobial drug discovery. As proof-of-concept, a plant extract library was screened and follow-up experiments were carried out. Primary results can be obtained in 2-4 h with high sensitivity, leading to significant improvements of the process.

**General information**

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Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Centre for Drug Research, Helsinki University, Division of Pharmaceutical Biosciences
Authors: Nybond, S., Karp, M., Yrjönen, T., Tammela, P.
Keywords: (Antibacterial, Bioluminescence, Cell-based assay, Escherichia coli, Natural products, Screening)
Number of pages: 3
Pages: 54-56
Publication date: 1 Jul 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Microbiology, Molecular Biology, Microbiology (medical), Biotechnology

**Publication information**

Journal: Journal of Microbiological Methods
Volume: 114
ISSN (Print): 0167-7012
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.723 0.8
Publication Forum (2016): 1
Scopus rating (2015): 0.816 0.873
Web of Science (2015): 1.857 2.247 9.1 0.333 0.01149 0.625
Publication Forum (2015): 1
Scopus rating (2014): 0.903 1.037
Web of Science (2014): 2.026 2.338 8.4 0.237 0.01275 0.672
Publication Forum (2014): 1
Scopus rating (2013): 0.917 1.019
Publication Forum (2013): 1
Scopus rating (2012): 0.87 1.004
Publication Forum (2012): 1
Scopus rating (2011): 0.9 0.972
Scopus rating (2010): 0.945 1.05
Scopus rating (2009): 0.993 1.156
Scopus rating (2008): 0.926 1.031
Scopus rating (2007): 0.942 1.111
Scopus rating (2006): 1.138 1.251
Low temperature temporal and spatial atomic layer deposition of TiO2 films

Titanium dioxide films were grown by atomic layer deposition (ALD) using titanium tetraisopropoxide as a titanium precursor and water, ozone, or oxygen plasma as coreactants. Low temperatures (80-120 degrees C) were used to grow moisture barrier TiO2 films on polyethylene naphthalate. The maximum growth per cycle for water, ozone, and oxygen plasma processes were 0.33, 0.12, and 0.56 angstrom/cycle, respectively. X-ray photoelectron spectrometry was used to evaluate the chemical composition of the layers and the origin of the carbon contamination was studied by deconvoluting carbon C1s peaks. In plasma-assisted ALD, the film properties were dependent on the energy dose supplied by the plasma. TiO2 films were also successfully deposited by using a spatial ALD (SALD) system based on the results from the temporal ALD. Similar properties were measured compared to the temporal ALD deposited TiO2, but the deposition time could be reduced using SALD. The TiO2 films deposited by plasma-assisted ALD showed better moisture barrier properties than the layers deposited by thermal processes. Water vapor transmission rate values lower than 5 x 10(-4) g day(-1) m(-2) (38 degrees C and 90% RH) was measured for 20 nm of TiO2 film deposited by plasma-assisted ALD. (C) 2015 American Vacuum Society.
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 single-walled 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 \( \beta \)-meso and \( \beta \)-\( \beta \) configurations, were prepared to study their photoinduced intramolecular electron transfer properties. The two meso nitrogen atoms in the porphyrin ring of DAP change its redox potential, making DAP more easily reduced, compared to its porphyrin counterpart. A charge-transfer from porphyrin to DAP in both hetero dimers was verified by versatile optical spectroscopic methods. The steady-state fluorescence spectra indicated an efficient intramolecular exciplex formation for both dimers. For the \( \beta \)-meso dimer, ultrafast time-resolved spectroscopic methods revealed the subpicosecond formation of two types of primary short-living (1-18 ps) intramolecular exciplexes, which relaxed in toluene to form a long-living final exciplex (1.4 ns) followed by a
longer-living charge transfer complex (>5 ns). However, in benzonitrile, the lifetime of the final exciplex was longer (660 ps) as was that of the charge transfer complex (180 ps). The 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.
Catalytic effect of Ca and K on CO$_2$ gasification of spruce wood char

Gasification is one route to produce chemicals and liquid fuels from biomass. The gasification of the char is catalyzed by alkali and alkaline earth metals in the biomass. In this work the catalytic effect of calcium (Ca) and potassium (K) on CO$_2$ gasification of spruce wood was studied using a thermo gravimetric analyzer (TGA). The ash-forming elements were first removed from the wood using an acid leaching method. Then, various concentrations of K and Ca were absorbed to the wood by ion-exchange to carboxylic and phenolic groups, impregnation of K$_2$CO$_3$ or physically mixing of CaC$_2$O$_4$. The prepared spruce samples were placed in a mesh holder and gasified in the TGA at 850°C in 100% CO$_2$. The results demonstrate that the gasification rate of the char increased linearly with an increase in the concentration of Ca or K. Crystalline CaC$_2$O$_4$ distributed only at the surface of the wood particles resulted in low catalytic activity. The catalytic activity of Ca was higher than K in the beginning of char gasification but the catalytic effect of Ca decreased earlier than the catalytic effect of potassium. Further, the char structure was investigated by SEM-EDX. The SEM analysis from interrupted gasification experiments showed the formation of CaCO$_3$ and K$_2$CO$_3$ 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.

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Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), Abo Akademi University, Åbo Akademi University, University of Jyväskylä, Process Chemistry Center, VTT Technical Research Centre of Finland
Authors: Perander, M., DeMartini, N., Brink, A., Kramb, J., Karlström, O., Hemming, J., Moilanen, A., Konttinen, J., Hupa, M.
Keywords: (Biomass, Calcium, Char reactivity, CO, Gasification, Potassium)
Number of pages: 9
Pages: 464-472
Publication date: 15 Jun 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

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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
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 CHCl₃ 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.
Dissolution of enzyme-treated cellulose using freezing thawing method and the properties of fibres regenerated from the solution

The rapid coagulation of NaOH-based cellulose solution during the wet spinning process leads to a low stretching ratio and, consequently, the low mechanical properties of the fibres. The aim of this work was to slow down the coagulation by replacing the sulphuric acid spin bath with an acetic acid bath. The spin dope was prepared by dissolving the enzyme-treated dissolving pulp in aqueous sodium zincate using a freezing thawing method. The optimal zinc oxide and sodium hydroxide concentrations were studied first. The most thermally stable cellulose solution contained 6.5 wt% NaOH and 1.3 wt% ZnO with 6 wt% enzyme-treated dissolving pulp. The spin dope was prepared accordingly. Coagulation of the cellulose solution slowed down in the acetic acid bath, resulting in a significantly higher stretching ratio for the fibres than with the sulphuric acid bath. However, the acetic acid spun fibres shrunk strongly during drying, and the possibly aligned order of the molecular chains due to the high stretch was partly lost. As a consequence, the high stretch was not transferred to high tenacity of the fibres in this study. However, the result suggests attractive potential to develop processing conditions to increase fibre tenacity.
High temperature oxidation tests for the high velocity solution precursor flame sprayed manganese-cobalt oxide spinel protective coatings on SOFC interconnector steel

High velocity solution precursor flame spray process was used to deposit MnCo1.9Fe0.1O4 and Mn1.5Co1.5O4 coatings on Crofer 22 APU ferritic stainless steel samples. The solution precursors were manufactured by diluting metal nitrates into deionized water. The as-sprayed coatings were oxidized at 850 degrees C for 500 h to evaluate Cr-barrier and electrical properties.

The post-mortem studies were performed with various qualitative and quantitative elemental analysis methods and a four-point measurement was used for the area specific resistance studies. The as-sprayed coatings were formed of single crystallite nanoparticles (10-20 nm) and polycrystalline sub-micron particles (100-500 nm). The small particle and crystallite size showed strong sintering behavior during the oxidation cycle. Cr-migration was fully prevented thought the oxidized coatings. The surface topography and grain growth dominated the electrical properties during the test cycle.

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General information
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Organisations: Department of Materials Science, Research group: Surface Engineering, Research group: Materials Characterization, Research group: Ceramic materials, Engineering materials science and solutions (EMASS), Univ Toronto, University of Toronto, Dept Mat Sci & Engn, Univ Toronto, University of Toronto, Dept Mech & Ind Engn
Authors: Puranen, J., Laakso, J., Honkanen, M., Heinonen, S., Kylmälahti, M., Lugowski, S., Coyle, T. W., Kesler, O., Vuoristo, P.
Keywords: (High velocity solution precursor flame spray, SOFC interconnect, Protective coating, FUEL-CELLS, ELECTRICAL-CONDUCTIVITY, SOLID-SOLUTION, MN)
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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
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.
Keywords: (ORIENTATIONAL OPTICAL NONLINEARITY, GENERATION, STORAGE, LIGHT)
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Volume: 5
Article number: 9890
ISSN (Print): 2045-2322
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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 0.722 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
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.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology, BioMediTech, Frontier Photonics, Integrated Technologies for Tissue Engineering Research (ITTE), Aalto University, BioMediTech, Univ Tampere, University of Tampere, BioMediTech, BMT FM5, Centre for Drug Research, Faculty of Pharmacy, Helsinki University, Department of Forest Products Technology, School of Chemical Technology, Division of Biopharmaceutical Sciences
Keywords: (Biomimetic material, Collagen structure, Human embryonic stem cell, Langmuir Blodgett film, Retina, Retinal pigment epithelial cell)
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ASJC Scopus subject areas: Biomaterials, Bioengineering, Ceramics and Composites, Mechanics of Materials, Biophysics

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Publication Forum (2015): 2
Scopus rating (2014): 3.289 2.186
Web of Science (2014): 8.557 9.305 6.3 1.711 0.14867 2.005
Publication Forum (2014): 3
Scopus rating (2013): 3.395 2.185
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.
Keywords: (Vibrio parahaemolyticus, whole genome gene expression, microarray, viable but not culturable state, VBNC, exponential phase, early stationary phase, ESCHERICHIA-COLI O157-H7, REAL-TIME PCR, NONCULTURABLE STATE, BIOFILM FORMATION, ADAPTIVE MUTAGENESIS, MESSENGER-RNA, CHOLEREA O1, IN-SITU, BACTERIA, VULNIFICUS)
Number of pages: 12
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Peer-reviewed: Yes

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Ratings:
Publication Forum (2017): 1
Preferential Attachments of Organic Dyes onto {101} Facets of TiO2 Nanoparticles

Hybrid nanostructures of organic dyes/TiO2 nanoparticles were successfully fabricated by self-assembly method. Compared with pure organic dyes, these hybrid nanostructures showed enhanced performance of belt absorption. Extensive high-resolution transmission electron microscopy observations demonstrated that the organic dyes are preferentially attached onto the {101} facets of anatase TiO2 nanoparticles. Density functional theory calculations further confirmed that the; preferential attachments are reasonable. These discoveries are very important.
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.
Fermentative metabolism of an anaerobic, thermophilic consortium on plant polymers and commercial paper samples
The purpose of the study was to examine the feasibility and capacity of a thermophilic microbial consortium to produce fermentative metabolites from plant polymers. The consortium comprised of cellulytic anaerobes that were originally enriched from a compost pile using cellulose as the substrate. Fermentative metabolism was examined with monosaccharides, disaccharides, hemicellulose, starch, pectin, chitin, and eight commercial paper samples without further enrichment of the culture to each specific substrate. In general, H\textsubscript{2}, CH\textsubscript{4}, CO\textsubscript{2}, and organic acids were the main metabolites on all substrates but the metabolite profiles varied with the substrate. Similar H\textsubscript{2} yields of 2-3 mol mol\textsuperscript{-1} substrate at 48h were obtained with all monosaccharides and disaccharides. The CO\textsubscript{2} yields were higher with disaccharides than with monosaccharides, 4.5 vs 2 mol mol\textsuperscript{-1} substrate. Metabolite yields were relatively low with glyceraldehyde, glycerol, and arabinose. Paper samples containing high amounts of chemical pulp produced the highest metabolite yields, and biodegradation accounted for ≤74% of total dry weight loss. The fermentative metabolism of the paper samples varied with the pulp composition and the amount of inorganic material. Bacterial community analysis using pyrosequencing analysis of 16S rRNA gene showed a predominance of members of the order Clostridiales, including members of genera Clostridium and Lutispora, which contain known cellulytic organisms. Most differences among the samples were attributed to small taxonomic groups represented by ≤10% of total sequences.
Effect of rheological properties of dissolved cellulose/microfibrillated cellulose blend suspensions on film forming

Enzymatically treated cellulose was dissolved in a NaOH/ZnO solvent system and mixed together with microfibrillated cellulose (MFC) in order to find the threshold in which MFC fibers form a percolation network within the dissolved cellulose solution and in order to improve the properties of regenerated cellulose films. In the aqueous state, correlations between the rheological properties of dissolved cellulose/MFC blend suspensions and MFC fiber concentrations were investigated and rationalized. In addition, rheological properties of diluted MFC suspensions were characterized and a correlation with NaOH concentration was found, thus partly explaining the flow properties of dissolved cellulose/MFC blend suspensions. Finally, based on results from Dynamic Mechanical Analysis (DMA), MFC addition had strengthening/plasticizing effect on regenerated cellulose films if low concentrations of MFC, below the percolation threshold (5.5-6 wt%, corresponding to 0.16-0.18 wt% of MFC in the blend suspensions), were used.
Crystal structure of 2-methylpiperazine-1,4-dilium bis(hydrogen maleate)

In the title salt, \(\text{C}_5\text{H}_{14}\text{N}_2^{2+}\cdot2\text{C}_4\text{H}_3\text{O}_4^{-}\), 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 O-H⋯O hydrogen bonds generate \(S(7)\) rings. In the crystal, the four independent anions are linked to the 2-methylpiperazinium cations through N-H⋯O hydrogen bonds, forming two-dimensional layered structures lying parallel to (001).
Photocurrent Generation and Charge Recombination in Multilayer Stacks of Hole Transporting Layer, Electron Donor-Acceptor Dyad and Electron Transporting Layer

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 (perylenediimide, 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 and D-A vertical bar E), compared to the reference structures, H-(D-A) or (DA)-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.
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.
Sulfonated polyetheretherketone/polypropylene polymer blends for the production of photoactive materials

Sulfonated polyetheretherketone (SPEEK) was synthesized via a mono-substitution reaction of PEEK in concentrated sulphuric acid and was blended with polypropylene (PP) in 2-10%w/w concentration to be used for the production of photoactive thermoplastic products. SPEEK and SPEEK/PP blends were characterized using FTIR, DSC, TGA, NMR, rheology, SEM, and EPR. Under UV-Vis irradiation, stable benzophenone ketyl (BPK) radicals were generated by hydrogen extraction from PP. By increasing the amount of SPEEK in the polymer blend a linear increase in the BPK radicals was achieved according to the EPR data. DSC and TGA tests indicated weaknesses in the thermal stability of SPEEK but according to the rheological tests this should not have a major effect on processability. The optimal amount of SPEEK in the blend was obtained at 5%w/w. This concentration provided a good compromise between radical...
concentration, material processability, and cost.

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Materials Science
Authors: Fatarelle, E., Mylläri, V., Ruzzante, M., Pogni, R., Baratto, M. C., Skrifvars, M., Syrjälä, S., Järvelä, P.
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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
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
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Research output: Scientific - peer-review › Article
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 arylation migration from the boronate species to the iminium were determined for both mechanisms.

General information

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Organisations: Research group: Industrial Bioengineering and Applied Organic Chemistry, Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), Univ Lisbon, Fac Farm, Inst Invest Medicamento iMed ULisboa
Authors: Rosholm, T., Gois, P. M. P., Franzen, R., R. Candeias, N.
Keywords: (amines, boron, glycerol, multicomponent reactions, sustainable chemistry, CROSS-COUPLING REACTIONS, ALPHA-AMINO-ACIDS, ONE-POT, ORGANOBORONIC ACIDS, SOLVENT, DERIVATIVES, ALDEHYDES, HYDROGEN, SALICYLALDEHYDES, 2H-CHROMENES)
Number of pages: 8
Pages: 39-46
Publication date: Feb 2015
Peer-reviewed: Yes

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 iodoethyl-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.

General information
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 (
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.

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, Frontier Photonics
Authors: George, L., Ahmed, Z., Lemmetyinen, H., Efimov, A.
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-hexylthiophene) 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.

**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, Frontier Photonics, University of Oulu, Department of Chemistry and Mathematics, Faculty of Petroleum and Mining Engineering, Suez University


**Keywords:** (Anode interfacial layer, Bulk heterojunction, Computational research, Inverted organic solar cell, Oligothiophene, Spectroscopy, Suzuki-Miyaura)

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**ASJC Scopus subject areas:** Electronic, Optical and Magnetic Materials, Materials Chemistry, Metals and Alloys, Surfaces, Coatings and Films, Surfaces and Interfaces

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- 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

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http://www.scopus.com/inward/record.url?scp=84921286591&partnerID=8YFLogxK (Link to publication in Scopus)

**Source:** Scopus

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**Research output:** Scientific - peer-review > Article
Perfluoro-1,1′-biphenyl and perfluoronaphthalene and their derivatives as π-acceptors for anions

Addition of anions to perfluorinated 1,1′-biphenyl 1 or naphthalene 2 results in a shift of the 19F NMR signals. However, any specific interaction cannot be assigned to this effect. In order to study the interaction in more detail, the salt derivatives 3 and 4 were prepared and studied by single crystal X-ray diffraction revealing weak anion-π interactions in the solid state.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, University of Jyväskylä, Institut für Organische Chemie, RWTH Aachen
Authors: Yi, H., Albrecht, M., Valkonen, A., Rissanen, K.
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ASJC Scopus subject areas: Chemistry(all), Catalysis, Materials Chemistry

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Scopus rating (2016): 0.869 0.766
Publication Forum (2016): 1
Scopus rating (2015): 0.954 0.836
Web of Science (2015): 3.277 3.247 4.8 0.761 0.0224 0.626
Publication Forum (2015): 1
Scopus rating (2014): 1.01 0.872
Web of Science (2014): 3.086 2.986 5.7 0.769 0.01887 0.623
Publication Forum (2014): 2
Scopus rating (2013): 1.047 0.838
Publication Forum (2013): 2
Scopus rating (2012): 1.209 0.825
Publication Forum (2012): 2
Scopus rating (2011): 1.148 0.81
Scopus rating (2010): 1.282 0.852
Scopus rating (2009): 1.366 0.899
Scopus rating (2008): 1.549 0.936
Scopus rating (2007): 1.394 1.084
Scopus rating (2006): 1.25 1.024
Scopus rating (2005): 1.221 0.977
Scopus rating (2004): 1.17 0.952
Scopus rating (2003): 0.956 0.869
Scopus rating (2002): 1.039 0.895
Scopus rating (2001): 1.227 0.948
Scopus rating (2000): 1.153 0.816
Scopus rating (1999): 0.91 0.848
Original language: English
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http://www.scopus.com/inward/record.url?scp=84919782132&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source-ID: 84919782132
Research output: Scientific - peer-review › Article
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

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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)
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Peer-reviewed: Yes
ASJC Scopus subject areas: Chemistry(all)

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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
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′-tetrathiophene) 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
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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.
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ASJC Scopus subject areas: Materials Science(all), Condensed Matter Physics, Mechanical Engineering, Mechanics of Materials
DOIs: 10.1557/opl.2015.529
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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 (HNOQ) 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 HNOQ 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
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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
Diffusion of acidic solution through rubber at high temperature and its effect on metal-rubber interface degradation

General information
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Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Teknikum Oy, Outotec Research Center
Authors: Sarlin, E., Rosling, A., Mustakangas, M., Laihonen, P., Lindgren, M., Vuorinen, J.
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Research output: Scientific › Conference contribution
Effect of alkali and silane surface treatments on regenerated cellulose fibre type (Lyocell) intended for composites

Cellulose fibres have significant importance and potential for polymer reinforcement. It is essential to modify the surface of the fibre to obtain good fibre-matrix interface. Surface treatments can increase surface roughness of the fibre, change its chemical composition and introduce new moieties that can effectively interlock with the matrix, resulting in good mechanical properties in the composites. This is mainly due to improved fibre-matrix adhesion. The treatments may also reduce the water absorption rate by converting part of the hydroxyl groups on the fibre surface into other functional groups. Chemical modification of the surface of a regenerated cellulose fibre of the Lyocell type was carried out by alkali and silane treatments, which significantly changed the properties of the Lyocell fibres. Three parameters were considered when the fibre surface treatment was done: concentration (2–15 wt%), temperature (25 and 50 °C) and time (30 min–72 h). Fourier transform infrared spectroscopy and Raman spectroscopy were used for chemical analysis and qualitative analysis of the cellulose crystallinity due to the surface treatments; subsequently, mechanical strength of the fibres was tested by tensile testing. Weight loss, moisture regain and swelling measurements were taken before and after treatments, which showed the obvious changes in fibre properties on treatment. Heat capacity of the fibres was measured for untreated and treated fibres, and thermal degradation of fibres was examined to see the stability of fibres at elevated temperatures. Wettability and surface energies were measured using dynamic contact angle method in three wetting mediums. Scanning electron microscopy was used to study the morphological properties of the fibres.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Fibre Materials, University College of Borås, Högskolan i Borås, Swedish Centre for Resource Recovery
Authors: Ramamoorthy, S. K., Skrifvars, M., Rissanen, M.
Keywords: (Alkali, Cellulose, Fibre, Lyocell, Silane, Surface modification)
Number of pages: 18
Pages: 637-654
Publication date: 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Polymers and Plastics

Publication information
Journal: Cellulose
Volume: 22
Issue number: 1
ISSN (Print): 0969-0239
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.126 1.144
Publication Forum (2016): 2
Web of Science (2015): 3.195 3.741 4.6 0.521 0.01196 0.722
Publication Forum (2015): 2
Scopus rating (2014): 1.071 1.334
Web of Science (2014): 3.573 4.285 4.6 0.655 0.00994 0.773
Publication Forum (2014): 2
Scopus rating (2013): 1.127 1.48
Publication Forum (2013): 2
Scopus rating (2012): 1.179 1.71
Publication Forum (2012): 2
Scopus rating (2011): 1.354 1.795
Scopus rating (2010): 0.873 1.384
Scopus rating (2009): 1.038 1.219
Scopus rating (2008): 0.926 1.123
Scopus rating (2007): 0.754 1.034
Scopus rating (2006): 0.699 1.15
Scopus rating (2005): 1.112 1.318
Scopus rating (2004): 0.855 1.072
Scopus rating (2003): 0.81 1.02
Scopus rating (2002): 0.649 0.689
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.

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, Universita degli Studi di Padova, Italy, Universiteit Antwerpen, Universitat zu Koln, Universita degli Studi di Brescia
Keywords: (FeO, Nano-heterostructures, Photoelectrochemistry, TiO, Water splitting)
Publication date: 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials

Publication information
Journal: Advanced Materials Interfaces
Volume: 2
Issue number: 17
ISSN (Print): 2196-7350
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.451 0.819
Publication Forum (2016): 1
Scopus rating (2015): 1.131 0.63
Web of Science (2015): 3.365 3.365 1.4 0.758 0.00261 1.013
Publication Forum (2015): 1
Publication Forum (2014): 1
Original language: English
Electronic versions:
Fe₂O₃-TiO₂_post-print
DOIs:
10.1002/admi.201500313
Links:
http://urn.fi/URN:NBN:fi:ttty-201612024841
Source: Scopus
Source-ID: 84944534544
From partial to complete optical erasure of azobenzene-polymer gratings: effect of molecular weight

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.
High-temperature slurry erosion of vinylester matrix composites – The effect of test parameters

Glass fibre (GF) reinforced vinylester composites (VE-FRP) are commonly used materials in hydrometallurgical reactors, the pulp and paper industry and waste water treatment plants, due to their excellent chemical resistance combined with good mechanical performance. In these applications, materials can be subjected to erosion, elevated temperatures (as high as 95 °C) and various chemical environments. However, studies on the slurry erosion of vinylester-based composites at high temperatures have not yet been reported. In this study, the erosion resistance of GF reinforced VE-FRP was investigated with a pilot-scale reactor. The effect of slurry concentration, erodent particle kinetic energy and slurry temperature was studied. The dominating wear mechanism was found to be abrasive wear. The VE-FRP structure was found to be prone to erosive turbulent flow and cavitation. Moreover, an increase in the erodent concentration of the slurry (10-20 wt%) or in the total kinetic energy of the erodent particles (30-770 kJ) increased the wear rate of the material markedly (up to 6 times higher weight loss). However, the total effect of different interrelated parameters was found to be complex. Consequently, it is recommended that predictions of the erosion rate of VE-FRP components are based on tests carried out in conditions that simulate the actual service environment.
Method with high-throughput screening potential for antioxidative substances using Escherichia coli biosensor katG::lux

A new method is described for the rapid real-time screening of antioxidative properties using a recombinant Escherichia coli DPD2511 biosensor. This microplate technique, without time-consuming pre-incubations and handling, has potential for a high-throughput search of bioactive compounds. Special emphasis was given to obtaining highly reliable and repeatable results.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research group: Industrial Bioengineering and Applied Organic Chemistry, Department of Chemistry and Bioengineering, Tampere University of Technology, Urban circular bioeconomy (UrCirBio), Natural Resources Institute Finland (Luke), Parkano Research Unit
Authors: Tienaho, J., Sarjala, T., Franzén, R., Karp, M.
Keywords: (Antioxidative activity, Bacterial biosensor, Bioscreening, Microplate technique)
Number of pages: 3
Pages: 78-80
Publication date: 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Microbiology, Molecular Biology, Microbiology (medical)

Publication information

Journal: Journal of Microbiological Methods
Volume: 118
Article number: 4723
ISSN (Print): 0167-7012
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.723 0.8
Publication Forum (2016): 1
Scopus rating (2015): 0.816 0.873
Web of Science (2015): 1.857 2.247 9.1 0.333 0.01149 0.625
Publication Forum (2015): 1
Scopus rating (2014): 0.903 1.037
Web of Science (2014): 2.026 2.338 8.4 0.237 0.01275 0.672
Publication Forum (2014): 1
Scopus rating (2013): 0.917 1.019
Publication Forum (2013): 1
Scopus rating (2012): 0.87 1.004
Publication Forum (2012): 1
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.
N-Alkyl ammonium resorcinarene salts: multivalent halogen-bonded deep-cavity cavitands

N-Cyclohexyl ammonium resorcinarene halides, stabilized by an intricate array of hydrogen bonds in a cavitand-like assembly, form multivalent halogen-bonded deep-cavity cavitands with perfluoriodobenzenes. As observed from the macromolar to infinite concentration range through crystal growth and single crystal X-ray analyses, four 1,4-diiodotetrafluorobenzenes form moderate halogen bonds with the bromides of the N-cyclohexyl ammonium resorcinarene bromides leading to a deep-cavity cavitand-like structure. In this assembly, the N-cyclohexyl ammonium resorcinarene bromide also acts as a guest and sits in the upper cavity of the assembly interacting with the 1,4-diiodotetrafluorobenzene through strong pi center dot center dot center dot pi interactions. Solvent molecules act as guests and are located deep in the cavity of the resorcinarene skeleton. In the millimolar range, H-1 and F-19 NMR spectroscopic analyses confirm halogen bonding in solution. Fast exchange binding of electron rich fluorophores (naphthalene, anthracene and pyrene) in the upper layer of these assemblies was also observed in the millimolar range while in the micromolar range, using fluorescence analysis, no binding of the fluorophores was observed.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Univ Jyvaskyla, University of Jyvaskyla, Dept Chem, Nanosci Ctr
Authors: Beyeh, N. K., Valkonen, A., Bhowmik, S., Pan, F., Rissanen, K.
Keywords: (ELECTRON DONOR SOLVENTS, RECOGNITION, ANALOGS, SHIFTS)
Number of pages: 6
Pages: 340-345
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Organic chemistry frontiers
Volume: 2
Issue number: 4
ISSN (Print): 2052-4129
Ratings:
Publication Forum (2017): 1
New routes from cellulose to textile fiber and ready products

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Materials Science, Research group: Fibre Materials, Aalto University, VTT Tech Res Ctr Finland, VTT Technical Research Center Finland
Authors: Nousiainen, P., Rissanen, M., Michud, A., Sixta, H., Hummel, M., Setälä, H.
Publication date: 2015

Host publication information
Title of host publication: Proceedings of 15th AUTEX World Textile Conference, June 10-12, 2015, Bucharest, Romania
ISBN (Print): 9786066852760
Research output: Scientific - peer-review » Article

Research on icing behavior and ice adhesion testing of icephobic surfaces

Surface engineering shows potential to provide sustainable approach to icing problems. Currently several passive anti-ice mechanisms adoptable to coatings are known but further research is required to proceed for practical applications. Icing wind tunnel and centrifugal ice adhesion test equipment enable the evaluation and development of anti-ice and icephobic coatings for e.g., wind turbine applications but also other growing players in arctic environment e.g. oil, extractive and logistic industries. This research is focused on the evaluation of icing properties of various surfaces.

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Department of Materials Science, Research group: Surface Engineering
Authors: Koivuluoto, H., Stenroos, C., Ruohomaa, R., Bolelli, G., Lusvarghi, L., Vuoristo, P.
Number of pages: 6
Pages: 183-188
Publication date: 2015

Host publication information
Title of host publication: 16th International Workshop on Atmospheric Icing of Structures, IWAIS 2015, June 28-July 3, 2015, Uppsala, Sweden
Links: http://iwais.org/
Research output: Scientific » Conference contribution

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-C_{60} (ZnP=zinc porphyrin), incorporates a phenyl bridge between D and A and behaves very similarly to analogous dyads studied previously. The second dyad, ZnP-EDOTV-C_{60}, 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; 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.
Synthesis, crystal structure, spectral, dielectric characteristics and conduction mechanism of two novel carboxylates of 1-benzhydrylpiperazine

Two new 1-benzhydrylpiperazinium carboxylates with tartrate and maleate, (C17H21N2)(C4H5O6) and (C17H22N2)(C4H3O4)2, have been synthesized and characterized. Crystal structure determinations show that the compounds crystallize in the P21 and the P21/c space groups of the monoclinic system, respectively. Only in the maleate...
the organic group is protonated on both nitrogen atoms of piperazine ring. The infrared spectra of these compounds reported from 400 to 4000 cm$^{-1}$ confirmed the presence of the principal bands assigned to the internal modes of cations and anions of both compounds. The optical band gaps were calculated and found to be 3.46 and 4.14 eV for tartrate and maleate, respectively. Different molecular motions were determined via dielectric relaxation spectroscopy. Measurements of AC conductivity as a function of frequency at different temperatures indicated the hopping conduction mechanism. The number of 13C CP-MAS NMR lines is in good agreement with the crystallographic data. Graphical abstract: [Figure not available: see fulltext.]

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Laboratory of Chemical Materials, Faculty of Sciences of Bizerte, Carthage University
Authors: Wacharine, I., Valkonen, A., Rzaigui, M., Smirani, W.
Keywords: (Carboxylic acids, Crystal structure, Hydrogen bonds, NMR spectroscopy, Solid state, X-ray structure determination)
Number of pages: 14
Pages: 2007-2020
Publication date: 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Chemistry(all)

Publication information
Journal: Monatshefte fur Chemie
Volume: 146
Issue number: 12
ISSN (Print): 0026-9247
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.338 0.536
Publication Forum (2016): 1
Scopus rating (2015): 0.331 0.559
Web of Science (2015): 1.131 1.157 8.9 0.435 0.00301 0.189
Publication Forum (2015): 1
Scopus rating (2014): 0.358 0.603
Web of Science (2014): 1.222 1.326 9.3 0.195 0.0039 0.24
Publication Forum (2014): 1
Scopus rating (2013): 0.401 0.71
Publication Forum (2013): 1
Scopus rating (2012): 0.533 0.863
Publication Forum (2012): 1
Scopus rating (2011): 0.483 0.753
Scopus rating (2010): 0.471 0.68
Scopus rating (2009): 0.47 0.64
Scopus rating (2008): 0.451 0.686
Scopus rating (2007): 0.402 0.58
Scopus rating (2006): 0.44 0.672
Scopus rating (2005): 0.405 0.673
Scopus rating (2004): 0.422 0.812
Scopus rating (2003): 0.391 0.63
Scopus rating (2002): 0.495 0.794
Scopus rating (2001): 0.46 0.734
Scopus rating (2000): 0.419 0.814
Scopus rating (1999): 0.396 0.66
Original language: English
DOIs:
10.1007/s00706-015-1553-1
Links:
http://www.scopus.com/inward/record.url?scp=84939509914&partnerID=8YFLogxK (Link to publication in Scopus)
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 eukaryotic 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=8YFLLogxK (Link to publication in Scopus)
The effect of physical adhesion promotion treatments on interfacial adhesion in cellulose-epoxy composite

General information
State: Published
Ministry of Education publication type: D3 Professional conference proceedings
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Research group: Paper Converting and Packaging
Number of pages: 10
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the 20th International Conference on Composite Materials
Links: http://iccm20.org/fullpapers/file?f=WM39KAy5r2

Bibliographical note
ISBN- tai ISSN-numeroa kysytty, ei löydy
Research output: Professional → Conference contribution

The effect of the outermost fibre layers on solubility of dissolving grade pulp
Dissolving pulps are used to manufacture various cellulose derived products through cellulose dissolution. Solubility of cellulose pulp has been claimed to be strongly dependent on the porosity development, the degree of polymerisation and the pulp viscosity. The removal of external cell walls has been proposed to have a key role in the pulp solubility. In this paper, the effect of the outermost surface layers on the solubility of a dissolving grade pulp was studied. Furthermore the effect of mechanical peeling and combined mechanical and enzymatic treatment on pulp solubility was compared. Based on the results combined mechanical and enzymatic treatment efficiently opens up the fibre structure and has a clear positive effect on the solubility of dissolving pulp. It seems that long fibre fraction is less accessible to solvent chemicals than the other pulp fractions. Mechanical peeling of outer fibre layers does not improve fibre dissolution to NaOH/ZnO. Thus, it seems that peeling alone is not a sufficient pre-treatment prior to dissolution. The results also revealed that the peeling treatment does not enhance the effects of enzymes as the studied mechanical treatment does.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Fibre Materials, Department of Forest Products Technology, VTT Technical Research Centre of Finland, Latvian State Institute of Wood Chemistry, Aalto University
Authors: Grönqvist, S., Treimanis, A., Kamppuri, T., Maloney, T., Skute, M., Grinfelds, U., Vehviläinen, M., Suurnäkki, A.
Keywords: (Cellulose dissolution, Dissolving pulp, Enzymatic hydrolysis, Hydromechanical peeling, Porosity, Solute exclusion)
Number of pages: 11
Pages: 3955-3965
Publication date: 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Polymers and Plastics

Publication information
Journal: Cellulose
Volume: 22
Issue number: 6
ISSN (Print): 0969-0239
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.126 1.144
Published Forum (2016): 2
Web of Science (2015): 3.195 3.741 4.6 0.521 0.01196 0.722
Published Forum (2015): 2
Scopus rating (2014): 1.071 1.334
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-C₆₀ 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-C₆₀ 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 C₆₀ 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 C₆₀. 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, C₆₀ 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
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-C-60) 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 C 60 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
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/S1088424614500928

**Bibliographical note**
AUX=keb,“Mundy, M. Elizabeth”
Source: WOS
Source-ID: 000349121200004
Research output: Scientific - peer-review › Article
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 pthalocyanine 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-pthalocyanine 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.

General information
State: Published
Ministry of Education publication type: G5 Doctoral dissertation (article)
Organisations: Department of Chemistry and Bioengineering
Authors: Stranius, K.
Number of pages: 147
Publication date: 26 Nov 2014

Publication information
Place of publication: Tampere
Publisher: Tampere University of Technology
Original language: English

Publication series
Name: Tampere University of Technology. Publication
Publisher: Tampere University of Technology
Volume: 1269
ISSN (Print): 1459-2045
Electronic versions:
stranius.pdf
Links:

Bibliographical note
Awarding institution:Tampere University of Technology
Source: researchoutputwizard
Source-ID: 1553
Research output: Collection of articles › Doctoral Thesis

Applications of supercritical carbon dioxide in materials processing and synthesis

General information
State: Published
Ministry of Education publication type: A2 Review article in a scientific journal
Organisations: Department of Materials Science, Engineering materials science and solutions (EMASS)
Authors: Zhang, X., Heinonen, S., Levänen, E.
Number of pages: 17
Pages: 1-16
Publication date: 2014
Peer-reviewed: Yes
Are two azo groups better than one? Investigating the photoresponse of polymer-bisazobenzene complexes
Charge-Transfer Dynamics in Poly(3-hexylthiophene):Perylenediimide-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
Scopus rating (2011): 2.32 1.457
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
Scopus rating (2000): 0.102 0.0
Design driven world of cellulose-from bulk to luxury?
Tekes-the Finnish Funding Agency for Innovation has granted funding 4.5 million funding for a project targeting on new approaches for use of wood-based cellulose. Project “Design Driven Value Chains in The World of Cellulose” (DWoC) launched by VTT Technical Research Centre of Finland, Aalto University and Tampere University of Technology integrates design and design processes into the strategic development of businesses operating in the field. The aim is to create a business ecosystem to serve both existing industry and a new, growing cellulose-based industry, and to brand Finland as a producer of refined, cellulose-based products. This manuscript summarises the future visions and background aspects and facts that have led to the initiation of the project. The presentation based on the manuscript also presents some of the first demonstrator processes and products developed during the first operational year of the project. These demonstrator include: Fibre yarn process that produces yarn from cellulose pulp fibres without traditional spinning process using novel wet extrusion technique (figure on right). Foam forming method for manufacturing well-formed foamed structures for new product applications 3D-printing technology enabling customisable on demand production of fibre structures and components using modified cellulose raw materials.

General information
State: Published
Ministry of Education publication type: A4 Article in a conference publication
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland, Aalto University
Keywords: (Cellulose, Design, Design driven research, Ecodesign, New business, New cellulose tecnologies)
Number of pages: 8
Pages: 67-74
Publication date: 2014

Host publication information
Title of host publication: Fibre Value Chain Conference and Expo 2014: Pulp and Paper Bioenergy Bioproducts
Publisher: Appita Inc.
ISBN (Print): 9780987168443
Links:
http://www.scopus.com/inward/record.url?scp=84923271599&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source-ID: 84923271599
Research output: Scientific - peer-review › Conference contribution

Effect of mutual position of electron donor and acceptor on photoinduced electron transfer in supramolecular chlorophyll-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, Frontier Photonics
Authors: Stranius, K., Iashin, V., Nikkonen, T., Muuronen, M., Helaja, J., Tkachenko, N.
Number of pages: 10
Pages: 1420-1429
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Electricity generating capacity and performance deterioration of a microbial fuel cell fed with beer brewery wastewater

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Köroğlu, E., Özkaya, B., Denktas, C., Cakmakci, M.
Number of pages: 7
Pages: 672-678
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Bioscience and Bioengineering
Volume: 118
Issue number: 6
ISSN (Print): 1389-1723
Ratings:
Excited State Intramolecular Proton Transfer in π-Expanded Phenazine-Derived Phenols

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., Virkki, K., Sadowski, B., Lemmetyinen, H., Tkachenko, N. V., Gryko, D. T.
Number of pages: 8
Pages: 144-151
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry A
Volume: 118
Issue number: 1
ISSN (Print): 1089-5639
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.258 0.98
Femtosecond spectroscopy of the dithiolate Cu(II) and Ni(II) 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: Plyusnin, V. F., Pozdnyakov, I. P., Grivin, V. P., Solovyev, A. I., Lemmetyinen, H., Tkachenko, N. V., Larionov, S. V.
Number of pages: 9
Pages: 17766-17774
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Dalton Transactions
Volume: 43
Issue number: 47
ISSN (Print): 1477-9226
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.243 0.931
Publication Forum (2016): 1
Formation of a stable polymer blue phase under UV irradiation of Langmuir-Schaefer films of diin 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
Journal: Bulletin of the Lebedev Physics Institute
Volume: 41
Issue number: 6
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
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
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:
In vitro bioluminescence used as a method for real-time inhibition zone testing for antibiotic-releasing composites

Aims: This study describes the potential of real-time bioluminescence imaging in evaluating the antibiotic efficiency of two cylinder-shaped bioabsorbable antibiotic-releasing composites by in vitro inhibition zone tests. The bacterial infections of bone tissue can cause extensive hard and soft tissue damage and decrease the efficiency of oral antibiotic therapy due to the poor blood circulation in the infected area. To overcome this problem, new, locally antibiotic-releasing biodegradable composites have been developed. Study Design & Methodology: The two composites evaluated in this study were composed of poly(L-lactide-co-ε-caprolactone) matrix, β-tricalcium phosphate ceramic and either ciprofloxacin or rifampicin antibiotic. The composites were tested with genetically modified model pathogens of osteomyelitis (Pseudomonas aeruginosa and Staphylococcus epidermidis) in vitro in inhibition zone tests using a method of real-time bioluminescence. Results: The first signs of the effect of the released ciprofloxacin or rifampicin became visible after four hours of incubation and were seen as changed bioluminescence around the composite pellet on a culture dish. Both of the composite types showed excellent effects against the sensor bacteria within the diffusion area. Bioluminescence measurements suggested that no survivor bacteria capable of evolving resistant strains were left inside the inhibition zones. The S. epidermidis bacterial strain was an inhibition sensor and P. aeruginosa was a stress sensor. Conclusion: These results highlight the potential of the composite materials against the pathogens of osteomyelitis. The approach allows continuous visual inspection of the efficacy of the antibiotics against the bacteria.

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
Authors: Männistö, N. M., Ahola, N., Karp, M. T., Veiranto, M., Kellomäki, M.
Number of pages: 20
Pages: 235-254
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: British Microbiology Research Journal
Volume: 4
Issue number: 2
ISSN (Print): 2231-0886
Ratings:
Publication Forum (2017): 0
Publication Forum (2016): 0
Publication Forum (2015): 0
Publication Forum (2014): 1
Original language: English
Electronic versions:
mannisto_in_vitro_bioluminescence_used_as_a_method.pdf
DOIs: 10.9734/BMRJ/2014/6661
Links:
http://urn.fi/URN:NBN:fi:tty-201401301069

Bibliographical note
Contribution: organisation=keb,FACT1=0.5
Contribution: organisation=elt,FACT2=0.5
Portfolio EDEND: 2014-02-15
Publisher name: Sciedomian International
Source: researchoutputwizard
Source-ID: 1026
Research output: Scientific - peer-review

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: Ranta, J., Kaunisto, K., Niskanen, M., Efimov, A., Hukka, T. I., Lemmetyinen, H.
Number of pages: 12
Pages: 2754-2765
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 118
Issue number: 5
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
Nahka-alan tuotteet esillä

General information
State: Published
Ministry of Education publication type: D1 Article in a trade journal
Organisations: Department of Materials Science
Authors: Rantasalo, S.
Number of pages: 1
Pages: 14-14
Publication date: 2014
Peer-reviewed: Unknown

Publication Information
Journal: Tekstiilehti
Issue number: 3
ISSN (Print): 0040-2370
Original language: Finnish

Bibliographical note
Contribution: organisation=mol,FACT1=1<br/>Portfolio EDEND: 2014-06-26<br/>Publisher name: Suomen tekstiiletkunning liitto
Source: researchoutputwizard
Source-ID: 1356
Research output: Professional › Article

Organic-inorganic azafullerene-gold C59N-Au nanohybrid: Synthesis, characterization, and 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: Rotas, G., Niemi, M., Tkachenko, N. V., Zhao, S., Shinohara, H., Tagmatachis, N.
Number of pages: 7
Pages: 14729-14735
Publication date: 2014
Peer-reviewed: Yes

Publication Information
Photo-induced electron transfer at nanostructured semiconductor-zinc porphyrin interface

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: Hakola, H., Pyymaki Perros, A., Myllyperkiö, P., Kurotobi, K., Lipsanen, H., Imahori, H., Lemmetyinen, H., Tkachenko, N. V.
Number of pages: 5
Pages: 47-51
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 592
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
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
Scopus rating (2014): 1.362 0.905
Web of Science (2014): 3.419 3.243 5.2 0.759 0.03731 1.046
Publication Forum (2014): 3
Scopus rating (2013): 1.442 0.948
Publication Forum (2013): 3
Scopus rating (2012): 1.763 0.955
Publication Forum (2012): 3
Scopus rating (2011): 1.719 1.05
Scopus rating (2010): 1.872 1.031
Scopus rating (2009): 1.91 1.12
Scopus rating (2008): 2.153 1.098
Scopus rating (2007): 2.215 1.129
Scopus rating (2006): 2.008 1.159
Scopus rating (2005): 2.067 1.147
Scopus rating (2004): 1.799 1.087
Scopus rating (2003): 1.666 1.128
Scopus rating (2002): 1.026 0.79
Scopus rating (2001): 0.258 0.425
Scopus rating (2000): 0.198 0.278
Scopus rating (1999): 0.386 0.495
Original language: English
DOIs:
10.1002/cphc.201402320

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-10-07<br/>Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA
Source: researchoutputwizard
Source-ID: 138
Research output: Scientific - peer-review › Article

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
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
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): 1.114 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/c3ra47367h
Subcellular localization of bacteriophage PRD1 proteins in Escherichia coli

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, Integrated Technologies for Tissue Engineering Research (ITTE)
Number of pages: 9
Pages: 44-52
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Virus Research
Volume: 179
ISSN (Print): 0168-1702
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.179 0.915
Publication Forum (2016): 1
Scopus rating (2015): 1.257 0.915
Web of Science (2015): 2.526 2.611 6.4 0.699 0.01606 0.791
Publication Forum (2015): 1
Scopus rating (2014): 1.213 0.933
Web of Science (2014): 2.324 2.733 6.3 0.632 0.01637 0.786
Publication Forum (2014): 1
Scopus rating (2013): 1.293 1.113
Publication Forum (2013): 1
Scopus rating (2012): 1.202 1.059
Publication Forum (2012): 1
Scopus rating (2011): 1.265 1.216
Scopus rating (2010): 1.217 1.075
Scopus rating (2009): 1.292 1.038
Scopus rating (2008): 1.178 1.015
Scopus rating (2007): 1.399 1.076
Scopus rating (2005): 1.13 0.997
Scopus rating (2004): 0.895 0.841
Scopus rating (2003): 0.768 0.821
Scopus rating (2002): 0.696 0.738
Scopus rating (2001): 0.812 0.809
Scopus rating (2000): 0.708 0.764
Scopus rating (1999): 0.763 0.832
Original language: English
DOIs: 10.1016/j.virusres.2013.11.015

Bibliographical note
Contribution: organisation=keb,FAC1=1<br/>Portfolio EDEND: 2014-05-28<br/>Publisher name: Elsevier BV
Source: researchoutputwizard
Source-ID: 669
Research output: Scientific - peer-review › Article

Synthesis and characterization of monoisomeric phthalocyanines, phthalocyanine-fullerene dyads, and phthalocyanine-silicon complexes
Synthesis and properties of a meso-tris-ferrocene appended zinc(II) porphyrin and a critical evaluation of its dye sensitised solar cell (DSSC) performance

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: Sirbu, D., Turta, C., Benniston, A., Abou-Chahine, F., Lemmetyinen, H., Tkachenko, N., Wood, C., Gibson, E.
Number of pages: 10
Pages: 22733-22742
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: RSC Advances
Volume: 4
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/c4ra03105a

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-06-29<br/>Publisher name: R S C Publications
Tetraiodoethynyl resorcinarene cavitands as multivalent halogen bond donors

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Turunen, L., Beyeh, N. K., Pan, F., Valkonen, A., Rissanen, K.
Number of pages: 4
Pages: 15920-15923
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Chemical Communications
Volume: 50
Issue number: 100
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/c4cc07771g

Bibliographical note
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-12-12
Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 1661
Research output: Scientific - peer-review › Article
The effect of diketopyrrolopyrrole (DPP) group inclusion in p-cyanophenyl end-capped oligothiophene used as a dopant in P3HT:PCBM BHJ 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: Manninen, V., Heiskanen, J., Pankov, D., Kastinen, T., Hukka, T., Hormi, O., Lemmetyinen, H.
Number of pages: 13
Pages: 1456-1468
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Photochemical & Photobiological Sciences
Volume: 13
Issue number: 10
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/c4pp00207e

Bibliographical note
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2015-01-12
Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 1023
Research output: Scientific - peer-review › Article

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
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: 1117
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
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.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research group: Supramolecular photochemistry, Department of Chemistry and Bioengineering, Tampere University of Technology, Department of Physics, Department of Physics, Research area: Computational Physics, Research group: Electronic Structure Theory, Computational Science X (CompX), Frontier Photonics
Authors: Niskanen, M., Kuisma, M., Cramariuc, O., Golovanov, V., Hukka, T. I., Tkachenko, N., Rantala, T. T.
Number of pages: 11
Pages: 17408-17418
Publication date: 28 Oct 2013
Peer-reviewed: Yes
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Physics and Astronomy(all)

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 15
Issue number: 40
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Organic silicon compounds in biogases produced from grass silage, grass and maize in laboratory batch assays

In the present study the occurrence of volatile organic silicon compounds in biogas produced from grass silage, grass and maize in laboratory batch assays was analyzed and methane potentials were determined. Inoculum from a mesophilic farm digester was used, and its effects were subtracted. Methane yields from grass silage, grass and maize were 0.38, 0.42 and 0.34 m³CH₄/kg volatile solids added (VSₜₐ₉₉), respectively. Trimethyl silanol, hexamethylcyclotrisiloxane (D₃), octamethylcyclotetrasiloxane (D₄) and decamethylcyclopentasiloxane (D₅) were detected from all the biogases. Higher yields of volatile organic silicon compounds in the grass (from 21.8 to 37.6 μg/kgVSₜₐ₉₉) were detected than in grass silage or maize assays (from 14.7 to 20.4 and from 7.4 to 12.1 μg/kgVSₜₐ₉₉, respectively). Overall, it is important to consider silicon-containing compounds also in biogases in energy crop digestion as the number of biogas plants using energy crops as feeding material increases and some biogas applications are sensitive to organic silicon compounds. © 2013 Elsevier Ltd.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), Jyvaskylan Yliopisto, Tampere University of Technology
Authors: Rasi, S., Seppälä, M., Rintala, J.
Keywords: (Anaerobic digestion, Biogas, Energy crops, Methane, Siloxanes)
Number of pages: 6
Pages: 137-142
Bis(aryl)acenaphthenequinonediimine substituent effect on the properties and coordination environment of ligands and their bis-chelate AgI complexes

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-06-29<br/>Publisher name: Elsevier Ltd.
Source: researchoutputwizard
Source-ID: 3235
Research output: Scientific - peer-review › Article

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: Papanikolau, P., Gdaniec, M., Wicher, B., Akrivos, P. D., Tkachenko, N.
Number of pages: 10
Pages: 5196-5205
Publication date: 2013
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., Lemmettyinen, H.
Number of pages: 9
Pages: 1540-1548
Publication date: 2013
Peer-reviewed: Yes
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
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 0.13014 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/c3ra22813d
Complexation enhanced excited-state deactivation by lithium ion coordination to a borondipyrromethene (Bodipy) donor-bridge-acceptor 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: 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
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
Number of pages: 12
Pages: 7451-7462
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Chemistry A
Volume: 1
Issue number: 25
ISSN (Print): 2050-7488
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 3.037 1.468
Publication Forum (2016): 2
Scopus rating (2015): 2.672 1.663
Web of Science (2015): 8.262 8.273 1.8 1.916 0.10917 1.633
Publication Forum (2015): 2
Scopus rating (2014): 2.343 1.526
Web of Science (2014): 7.443 7.449 1.4 1.59 0.04432 1.457
Publication Forum (2014): 3
Publication Forum (2013): 3
Original language: English
DOIs:
10.1039/c3ta10686a

Bibliographical note
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 2879
Research output: Scientific - peer-review

Demonstrating the mechanism and efficacy of water-induced shape memory and the influence of water on the thermal properties of oriented poly(ε-caprolactone)

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 (ITTE)
Authors: Paakinaho, K., Hukka, T. I., Kastinen, T., Kellomäki, M.
Number of pages: 9
Pages: 4209-4218
Publication date: 2013
Peer-reviewed: Yes
Determination of preferential molecular orientation in porphyrin-fullerene dyad ZnDHD6ee monolayers by the X-ray standing-wave method and X-ray reflectometry

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
Dipyrrolidinyl-substituted perylene diimide as additive for poly(3-hexylthiophene): [6,6]-Phenyl C61 butyric acid methylester bulk-heterojunction blends
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

10.1016/j.tsf.2013.08.106
### 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

### Bibliographical note

- **DOIs:** 10.1002/chem.201203387
- **Bibliographical note:**
  - poistettu tupla r=2208<br/>
  - Contribution: organisation=keb,FACT1=1<br/>
  - Portfolio EDEND: 2013-06-29<br/>
  - Publisher name: WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
  - Source: researchoutputwizard
  - Source-ID: 2089
  - Research output: Scientific - peer-review › Article
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
Homoleptic Bis(aryl)acenaphthenequinonediimine-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 2.93 5.8 0.654 0.03239 0.665
Publication Forum (2014): 3
Hydrolytic degradation of composites of poly(L-lactide-co-epsilon-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
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
Photophysics of bis(ethylxanthato)nickel(II) [Ni(EtOCS2)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
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
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

Bibliographical note
poistettu tupla r=2204<br/>Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-02-27<br/>Publisher name: Elsevier
Source: researchoutputwizard
Source-ID: 3159
Research output: Scientific - peer-review › Article

10.1016/j.jphotochem.2012.08.005
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
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

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-10-29<br/>Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 3093
Research output: Scientific - peer-review › Article
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
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
Short synthesis of the natural product 3β-hydroxy-labd-8(17)-en-15-oic acid via microbial transformation of labdanic 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
- Scopus rating (2015): 0.524 0.852
- Web of Science (2015): 1.353 1.451 3.2 0.338 0.00335 0.323
- Scopus rating (2014): 0.592 1.072
- Web of Science (2014): 1.45 1.549 2.8 0.313 0.00285 0.342
- Scopus rating (2013): 0.647 1.014
- Scopus rating (2012): 0.545 0.944
- 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<br/>Portfolio EDEND: 2013-10-29
Source: researchoutputwizard
Source-ID: 2538
Research output: Scientific - peer-review › Article

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

General information
State: Published
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
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
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-Laukkanen, E., Yliperttula, M., Green, J. J.
Number of pages: 7
Pages: 6951-6957
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
Volume: 135
Issue number: 18
ISSN (Print): 0002-7863
Ratings:
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
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: ChemSusChem
Volume: 6
Issue number: 3
ISSN (Print): 1864-5631
Ratings:
Publication Forum (2017): 2
Tuning the Förster overlap integral: energy transfer over 20 Ångstroms from a pyrene-based donor to borondipyrromethene (Bodipy)

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., Harrington, R.
Number of pages: 8
Pages: 9854-9861
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 15
Issue number: 24
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
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-PPTL)(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.
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.

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: Candeias, N. R., Afonso, C. A. M., Gois, P. M. P.
Keywords: (C-H INSERTION, ACTIVE PHARMACEUTICAL INGREDIENTS, ALPHA-DIAZOCARBONYL COMPOUNDS, CHIRAL LEWIS-ACID, CYCLOPROPANATION REACTIONS, ASYMMETRIC-SYNTHESIS, RHODIUM CARBENOIDS, IONIC LIQUID, HOMOGENEOUS CATALYSIS, SUPERCRITICAL FLUIDS)
Number of pages: 22
Pages: 3357-3378
Publication date: 2012
Peer-reviewed: Yes

Publication Information

Journal: Organic and Biomolecular Chemistry
Volume: 10
Issue number: 17
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
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
A novel organocatalytic asymmetric [3 + 2] cycloaddition reaction between methyleneindolinones and allylic compounds yielding complex spirocyclopentaneoxindoles 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.

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 spirocyclopentaneoxindoles 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.
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
Boronic Acids and Esters in the Petasis-Borono Mannich Multicomponent Reaction

General information
State: Published
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
NHCl-Iron-Catalyzed Aerobic Oxidative Aromatic Esterification of Aldehydes using Boronic Acids

NHCl 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, Universidad 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
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.

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, COFM, Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, Inst Nanosci & Nanotechnol, IBET, ITQB, Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, CQE
Authors: Frade, R. F. M., Candeias, N. R., Duarte, C. M. M., Andre, V., Duarte, M. T., Gois, P. M. P., Afonso, C. A. M.
Keywords: (Dirhodium complex, Human colon adenocarcinoma cells, ANTITUMOR-ACTIVITY, IN-VITRO, RHODIUM(II) CARBOXYLATES, CELL-DEATH, BIOLOGICAL-ACTIVITY, STRUCTURAL EVIDENCE, CRYSTAL-STRUCTURES, GUANINE BASES, METAL-BINDING, CISPLATIN)
Number of pages: 3
Pages: 3413-3415
Publication date: 1 Jun 2010
Peer-reviewed: Yes

Publication information
Journal: Bioorganic and Medicinal Chemistry Letters
Volume: 20
Issue number: 11
ISSN (Print): 0960-894X
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.843 0.846
Publication Forum (2016): 1
Scopus rating (2015): 0.932 0.884
Web of Science (2015): 2.486 2.303 6.6 0.474 0.05446 0.514
Publication Forum (2015): 1
Scopus rating (2014): 0.94 0.89
Web of Science (2014): 2.42 2.317 6.2 0.496 0.05964 0.508
Publication Forum (2014): 2
Scopus rating (2013): 0.931 0.911
Publication Forum (2013): 2
Scopus rating (2012): 1.087 0.936
Publication Forum (2012): 2
Scopus rating (2011): 1.127 0.991
Scopus rating (2010): 1.065 0.987
Scopus rating (2009): 1.114 1.022
Scopus rating (2008): 1.111 0.984
Scopus rating (2007): 1.111 0.962
Scopus rating (2006): 0.971 0.955
Scopus rating (2005): 0.961 0.81
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.
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 glyxoxal 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. (C) 2010 Elsevier Ltd. All rights reserved.

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
A novel biosensor for the detection of zearalenone family mycotoxins in milk

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Välimaa, A., Kivistö, A. T., Leskinen, P. I., Karp, M. T.
Pages: 44-48
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Microbiological Methods
Volume: 80
Issue number: 1
ISSN (Print): 0167-7012
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.723 0.8
Publication Forum (2016): 1
Scopus rating (2015): 0.816 0.873
Web of Science (2015): 1.857 2.247 9.1 0.333 0.01149 0.625
Publication Forum (2015): 1
Scopus rating (2014): 0.903 1.037
Web of Science (2014): 2.026 2.338 8.4 0.237 0.01275 0.672
Publication Forum (2014): 1
Scopus rating (2013): 0.917 1.019
Publication Forum (2013): 1
Scopus rating (2012): 0.87 1.004
Publication Forum (2012): 1
Scopus rating (2011): 0.9 0.972
Scopus rating (2010): 0.945 1.05
Scopus rating (2009): 0.993 1.156
Scopus rating (2008): 0.926 1.031
Scopus rating (2007): 0.942 1.111
Scopus rating (2006): 1.138 1.251
Scopus rating (2005): 0.964 1.141
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.

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, CQE, Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, Inst Nanosci & Nanotechnol, CQFM
Keywords: (carbenoids, carbene complexes, catalysis, diazo compounds, rhodium, C-H INSERTION, CHIRAL LEWIS-ACID, CAPROLACTAMATE, AMINATION, STEREOCONTROL, CARBOXYLATES, OXIDATION, ALDEHYDES, LACTAMS)
Number of pages: 8
Pages: 3519-3526
Publication date: 16 Oct 2009
Peer-reviewed: Yes

Publication information
Journal: Synthesis: Stuttgart
Issue number: 20
ISSN (Print): 0039-7881
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.046 0.575
Publication Forum (2016): 1
Scopus rating (2015): 1.088 0.669
Web of Science (2015): 2.652 2.348 9.1 0.8 0.01999 0.567
Publication Forum (2015): 1
Scopus rating (2014): 1.079 0.694
Web of Science (2014): 2.689 2.389 8.9 0.476 0.02312 0.578
Publication Forum (2014): 2
Scopus rating (2013): 1.126 0.675
Publication Forum (2013): 2
Scopus rating (2012): 1.155 0.676
Publication Forum (2012): 2
Scopus rating (2011): 1.203 0.702
Scopus rating (2010): 1.168 0.693
Scopus rating (2009): 1.201 0.766
Scopus rating (2008): 1.28 0.816
Scopus rating (2007): 1.27 0.857
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
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
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 in spite of recent studies. The few examples of diazo compounds reactions with molecular oxygen and hydrogen abstraction present in the literature are also covered.
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. ((C) 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 NHC-Rh(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.

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Authors: Candeias, N. R., Gois, P. M. P., Veiros, L. F., Afonso, C. A. M.
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Web of Science (2015): 4.785 4.538 >10.0 1.289 0.10271 1.051
Publication Forum (2015): 2
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.

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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 a alpha-diazo-alpha-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.

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Keywords: (dirhodium carbenoids, alpha-diazoacetamides, ORGANIC-SYNTHESIS, GREEN CHEMISTRY, ALPHA-DIAZOACETAMIDES, DIAZO-COMPOUNDS, ACTIVATION, TRANSFORMATIONS, DECOMPOSITION, STEREOCONTROL, SEPARATION, COMPOUND)
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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.

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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.

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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.
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.
A luminescent Escherichia coli biosensor for the high throughput detection of beta-lactams

A group-specific bioluminescent Escherichia coli strain for studying the action of beta-lactam antibiotics is described. The strain contains a plasmid, pBlaLux1, in which the luciferase genes from Photorhabdus luminescens are inserted under the control of the beta-lactam-responsive element ampR/ampC from Citrobacter freundii. In the presence of beta-lactams, the bacterial cells are induced to express the luciferase enzyme and three additional enzymes generating the substrate for the luciferase reaction. This biosensor for beta-lactams does not need any substrate or cofactor additions, and the bioluminescence can be measured very sensitively in real time by using a luminometer. Basic parameters affecting the light production and induction in the gram-negative model organism E. coli SN0301/pBlaLux1 by various beta-lactams were studied. The dose-response curves were bell shaped, indicating toxic effects for the sensor strain at high concentrations of beta-lactams. Various beta-lactams had fairly different assay ranges: ampicillin, 0.05-1.0 μg/ml; piperacillin, 0.0025-25 μg/ml; imipenem, 0.0025-0.25 μg/ml; cepapirin, 0.025-2.5 μg/ml; cefoxitin, 0.0025-1.5 μg/ml; and oxacillin, 25-500 μg/ml. Also, the induction coefficients (signal over background noninduced control) varied considerably from 3 to 158 in a 2-hour assay. Different non-beta-lactam antibiotics did not cause induction. Because the assay can be automated using microplate technologies, the approach may be suitable for higher throughput analysis of beta-lactam action.
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.
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.

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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
Real-time Measurement of Cell Permeabilization With Low-molecular-weight Membranolytic Agents

A new method for studying the action of membranolytic agents by simple measurement of light emitted from cells is described. It is based on the expression of the click beetle (Pyrophorus plagiophthalmus) luciferase gene (lucGR) in Escherichia coli, Bacillus subtilis and Spodoptera frugiperda cells in order to make them bioluminescent. The diffusion of the substrate for luciferase enzyme through the cell membranes is very slow at physiological pH, and therefore a change in membrane permeability is seen as a change of in-vivo luminescence of cells. The cells used in this study represent different membrane structures, and thus allow a comparison of the reactions of the different membranes towards membranolytic agents in a real-time measurement. The dose-response data correlated well with target cell viable count. In addition, the time course of light emission as a consequence of permeabilizing compound is dose-dependent. The action of the compounds on prokaryotic and eukaryotic cells was found to be highly dependent on the permeabilizer used.
Alterations in Growth Temperature-range and Fatty-acid Composition of Thermus as a Result of Plasmid Elimination

Elimination of plasmids from Thermus flavus, T. thermophilus and three wild Thermus strains caused alterations in growth temperature range, pigmentation and membrane fatty acids without affecting viability. Following plasmid elimination all Thermus strains lost their ability to grow above 70-degrees-C. In addition, the minimum growth temperature was lowered by 5-10-degrees-C. Fatty acids were reduced by an average of approximately 35%. In addition, the contribution of iso- and ante-isobranched fatty acids were altered in four of the five strains. The iso C-15:0/iso C-17:0 ratio approached 1.0 in all strains, whereas the anteiso C-15:0/anteiso C-17:0 was reduced to 0.2. The iso C-16:0/normal C-16:0 ratio increased in all strains due to an increase in iso C-16:0 in four strains and a reduction in normal C-16:0 relative to iso C-16:0 in one strain. However, it was evident that the plasmid-free strains were able to compensate for these alterations in membrane fluidity to a certain extent by reducing the average chain length of isobranched acids. Altered fatty acid metabolism at the level of precursors may have influenced membrane composition and consequently growth temperature range.
Simultaneous extraction and combined bioluminescent assay of oxidized and reduced nicotinamide adenine dinucleotide

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Publication date: 1986
Peer-reviewed: Yes
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%.

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 (Sepharpse 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.

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Number of pages: 7
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Publication date: Feb 1984
Peer-reviewed: Yes
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.

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Number of pages: 6
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