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

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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), BioMediTech, Turun Yliopisto/Turun Biomateriaalikeskus
Authors: Suominen, M., Lehtimäki, S., Yewale, R., Damlin, P., Tuukkanen, S., Kvarnström, C.
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Scopus rating (2015): SJR 1.945 SNIP 1.686 CiteScore 6.34
Scopus rating (2014): SJR 1.983 SNIP 2.071 CiteScore 6.3
Scopus rating (2013): SJR 1.985 SNIP 2.138 CiteScore 5.63
Scopus rating (2012): SJR 2.293 SNIP 2.016 CiteScore 5.04
Scopus rating (2011): SJR 2.247 SNIP 2.181 CiteScore 5.13
Scopus rating (2010): SJR 2.297 SNIP 1.981
Scopus rating (2009): SJR 2.117 SNIP 1.793
Scopus rating (2008): SJR 1.968 SNIP 1.726
Scopus rating (2007): SJR 1.597 SNIP 1.489
Scopus rating (2006): SJR 1.8 SNIP 2.224
Scopus rating (2005): SJR 1.65 SNIP 1.825
Scopus rating (2004): SJR 1.852 SNIP 1.818
Scopus rating (2003): SJR 1.66 SNIP 1.583
Scopus rating (2002): SJR 1.959 SNIP 1.4
Scopus rating (2001): SJR 1.115 SNIP 1.492
Scopus rating (2000): SJR 1.106 SNIP 0.914
Scopus rating (1999): SJR 0.854 SNIP 0.998
Original language: English
Keywords: Choline, Electropolymerization, Flexible supercapacitor, Ionic liquid, Polyazulene
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http://www.scopus.com/inward/record.url?scp=85019024216&partnerID=8YFLogxK (Link to publication in Scopus)
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The role of inorganics in modelling of biomass gasification

In this work, a summary of the research carried out about the role of inorganic elements in biomass gasification is presented. The research work has focused on the catalytic effects of alkali and alkaline earth metals in char gasification. The work has included gasification experiments using thermogravimetric analysis (TGA) and fluidized beds as well as modeling techniques. The results of the research presented in this paper indicate that the laboratory measured TGA reactivity numbers and correlations (including the effect of fuel ash inorganics) are possible to be converted to numbers predicting carbon conversion in a large scale fluidized bed gasification reactor. The model, called Carbon Conversion Predictor, is a relatively simple and transparent tool for the comparison of the gasification reactivity of different fuels in fluidized bed gasification.

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Ministry of Education publication type: A4 Article in a conference publication
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Univ Seville, University of Sevilla, Chem & Environrn Engr Dept, Bioenergy Grp, Escuela Super Ingenieros
Authors: Konttinen, J., Kramb, J., DeMartini, N., Gomez-Barea, A.
Number of pages: 5
Pages: 443-447
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Host publication information
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Publisher: ETA-Florence Renewable Energies
Editors: Ek, L., Ernrooth, H., Scarlat, N., Grassi, A., Helm, P.

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Name: European biomass conference and exhibition proceedings
Publisher: ETA Florence renewable energies
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Research output: Scientific - peer-review > Conference contribution

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
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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
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
Event: Paper presented at 30 Years of Drug Delivery Research, Kuopio, Finland.
ASJC Scopus subject areas: Chemistry(all), Pharmaceutical Science
Research output: Scientific › Paper, poster or abstract

**Synthesis of new acylsilanes**

**General information**
State: Published
Authors: Rafael Candeias, N., Campos Do Vale, J.
Publication date: 2017
Peer-reviewed: Unknown
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 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**
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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
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**Publication information**
Journal: Anti-Cancer Agents in Medicinal Chemistry
Volume: 17
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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 lixiviant.
Benzen-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.
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.
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 perylenedimidoimide-based dyes (1–4) both as free and adsorbed on the NiO (100) semiconductor surface have been investigated to gain better understanding of the p-type devices. In particular, the electronic transitions relevant to charge transfer between the dye and the surface have been identified. Excitations have been evaluated by using the time dependent DFT calculations and the roles of frontier orbitals and band edges in transitions have been assessed. The adsorbed dyes can take either upright or slightly tilted geometries depending on the structure of the anchoring group and the binding mode of the dye. The adsorption slightly lowers the NiO band gap, from 4.06 eV to 3.90–3.96 eV depending on the surface–adsorbate system, and the band gaps of the dye molecules by 0.1–0.2 eV. Additionally, the adsorption mode of dye 1 moves the LUMO+1 level down by 0.5 eV. The effective mass of the charge carrier holes is significantly smaller at the NiO surface than in the bulk indicating the importance of the surface conductivity. We also found that the potential drop, i.e. the driving force for charge transfer from NiO to dye molecule depends on the adsorption mode of 1.

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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
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Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
Scopus rating (2010): SJR 1.802 SNIP 1.196
Scopus rating (2009): SJR 2.127 SNIP 1.369
Scopus rating (2008): SJR 2.158 SNIP 1.211
Scopus rating (2007): SJR 1.84 SNIP 1.138
Scopus rating (2006): SJR 1.467 SNIP 1.128
Scopus rating (2005): SJR 1.389 SNIP 1.104
Scopus rating (2004): SJR 1.173 SNIP 1.007
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.

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Department of Physics, Research area: Computational Physics
Authors: Kastinen, T., Niskanen, M., Risko, C., Cramariuc, O., Hukka, T. I.
Number of pages: 14
Pages: 1051-1064
Publication date: 3 Feb 2016
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Publication Information
Journal: Journal of Physical Chemistry A
Volume: 120
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Scopus rating (2015): SJR 1.179 SNIP 1.106 CiteScore 2.78
Scopus rating (2014): SJR 1.154 SNIP 1.071 CiteScore 2.65
Scopus rating (2013): SJR 1.194 SNIP 1.102 CiteScore 2.84
Scopus rating (2012): SJR 1.494 SNIP 1.124 CiteScore 2.78
Scopus rating (2011): SJR 1.402 SNIP 1.135 CiteScore 2.87
Scopus rating (2010): SJR 1.466 SNIP 1.102
Scopus rating (2009): SJR 1.562 SNIP 1.132
Scopus rating (2008): SJR 1.787 SNIP 1.093
Scopus rating (2007): SJR 1.907 SNIP 1.136
Scopus rating (2006): SJR 1.728 SNIP 1.195
Scopus rating (2005): SJR 1.789 SNIP 1.215
Scopus rating (2004): SJR 1.669 SNIP 1.224
Scopus rating (2003): SJR 1.75 SNIP 1.241
Scopus rating (2002): SJR 1.81 SNIP 1.196
Scopus rating (2001): SJR 1.732 SNIP 1.224
Scopus rating (2000): SJR 1.953 SNIP 1.272
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.
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
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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Authors: Carraro, G., Maccato, C., Gasparotto, A., Kaunisto, K., Sada, C., Barreca, D.
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Publication date: 1 Jan 2016
Peer-reviewed: Yes
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Volume: 13
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ISSN (Print): 1612-8869
Ratings:
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Scopus rating (2014): SJR 0.894 SNIP 1.16 CiteScore 2.67
Scopus rating (2013): SJR 1.113 SNIP 1.404 CiteScore 3.39
Scopus rating (2012): SJR 1.222 SNIP 1.205 CiteScore 2.59
Scopus rating (2011): SJR 1.342 SNIP 1.295 CiteScore 2.71
Scopus rating (2010): SJR 0.87 SNIP 0.776
Scopus rating (2009): SJR 0.798 SNIP 0.993
Scopus rating (2008): SJR 0.609 SNIP 0.594
Scopus rating (2007): SJR 0.732 SNIP 1.194
Scopus rating (2006): SJR 0.618 SNIP 1.629
Scopus rating (2005): SJR 0.722 SNIP 2.959
Original language: English
Keywords: Co3O4, Fe2O3, plasma-enhanced chemical vapor deposition (PE-CVD), sputtering, water splitting
DOIs: 10.1002/ppap.201500106
Source: Bibtex
Source-ID: urn:fea2caf64465a2349fed5a21683d16de
Research output: Scientific › peer-review › Article

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
A study on raw, torrefied, and steam-exploded wood: Fine grinding, drop-tube reactor combustion tests in N₂/O₂ and CO₂/O₂ atmospheres, particle geometry analysis, and numerical kinetics modeling

The purpose of this study was to compare the fine grinding properties and combustion behavior of three wood pellet products: raw, torrefied, and steam-exploded wood. The energy required to fine grind the pellets was tested, and so was the geometry and size distribution of the resulting ground products. Out of all the samples the steam-exploded wood pellet required the most energy for grinding. However, it also produced more sphere-like particles compared to the other two types of samples. The combustion behavior of the samples was tested in a laminar drop-tube reactor (DTR). The samples were predried and the particles were sieved with vibration sieves with an opening of 112–125 μm. The pyrolysis process was examined separately at a temperature range of 973–1173 K. The combined pyrolysis and combustion tests were carried out at a reactor temperature of 1123 K. The O₂ concentrations used in the measurements were 3–21 vol-% in either N₂ or CO₂ atmospheres. The initial size distribution of the sample particles as well as their diameter evolution during pyrolysis and combustion was studied by using optical techniques. The surface temperature of the combusting particles was measured with a two-color pyrometer from within the DTR. The density, specific surface area, and pore diameter were measured from the ground samples with a mercury porosimeter. The chemical kinetic parameters, which describe the pyrolysis and char oxidation rates of the samples, were determined by using the data from the measurements.
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 quin-1,5-lactone that is supported by experimental and computational calculation data.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Supramolecular photochemistry
Authors: Assoah, B., Veiros, L. F., Afonso, C. A. M., R. Candeias, N.
Number of pages: 6
Pages: 3856-3861
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Scopus rating (2015): SJR 1.198 SNIP 0.758 CiteScore 2.88
Scopus rating (2014): SJR 1.181 SNIP 0.767 CiteScore 2.96
Scopus rating (2013): SJR 1.292 SNIP 0.796 CiteScore 2.96
Scopus rating (2012): SJR 1.471 SNIP 0.811 CiteScore 2.93
Scopus rating (2011): SJR 1.536 SNIP 0.857 CiteScore 3.2
Scopus rating (2010): SJR 1.572 SNIP 0.785
Scopus rating (2009): SJR 1.497 SNIP 0.778
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.

General information

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, CSIRO Land and Water Flagship, Boliden Harjavalta Oy, Department of Microbiology, Ohio State University
Authors: Kaksonen, A. H., Särkijärvi, S., Puhakka, J. A., Peuruniemi, E., Junnikkala, S., Tuovinen, O. H.
Pages: 46-53
Publication date: 2016
Peer-reviewed: Yes
Early online date: 1 Jan 2015

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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.

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.

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Authors: Neto, I., Andrade, J., Pinto Reis, C., Salunke, J. K., Primagi, A., R. Candeias, N., Rijo, P.
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**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.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Kyoto Women's University, Tokushima University, Kobe University, Japan Science and Technology Agency, University of Tokyo
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 (Ferrosiphite, 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.
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 cellullosic 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.

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Organisations: Department of Materials Science, Research group: Fibre Materials, Department of Forest Products Technology, VTT Technical Research Centre of Finland, Aalto University
Authors: Grönqvist, S., Kamppuri, T., Maloney, T., Vehviläinen, M., Liliä, T., Suurnäkki, A.
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Graphene-intercalated Fe$_2$O$_3$/TiO$_2$ heterojunctions for efficient photoelectrolysis of water

Interfacial modification of α-Fe$_2$O$_3$/TiO$_2$ 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-Fe$_2$O$_3$ films (1 V vs. RHE), the α-Fe$_2$O$_3$/TiO$_2$ 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/m² 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/m², 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.

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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.
Cultivation of Nannochloropsis for eicosapentaenoic acid production in wastewaters of pulp and paper industry

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

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Authors: Polishchuk, A., Valev, D., Tarvainen, M., Mishra, S., Kinnunen, V., Antal, T., Yang, B., Rintala, J., Tyystjärvi, E.
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Publication information
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)₂HPO₄). The deactivation was studied by inductively coupled plasma optical emission spectroscopy, electron microscopy, X-ray diffractometry, X-ray photoelectron spectroscopy and Fourier-transform infrared reflectance, N₂-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 μm), and phosphorus was found as phosphate, although it can also form compounds like AlPO₄ 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 °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.

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Authors: Kärkkäinen, M., Kolli, T., Honkanen, M., Heikkinen, O., Huuhtanen, M., Kallinen, K., Lepistö, T., Lahtinen, J., Vippola, M., Keiski, R. L.
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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.
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 CrO2(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.
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 Desulfitobacterium 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.
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%.

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Authors: Frankberg, E. J., George, L., Efimov, A., Honkanen, M., Pessi, J., Levänen, E.
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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.
Fe2O3-TiO2 nanosystems by a hybrid PE-CVD/ALD approach: controllable synthesis, growth mechanism, and photocatalytic properties

Supported Fe2O3-TiO2 nanocomposites are fabricated by an original vapor phase synthetic strategy, consisting of the initial growth of Fe2O3 nanosystems on fluorine-doped tin oxide substrates by plasma enhanced-chemical vapor deposition, followed by atomic layer deposition of TiO2 overlayers with variable thickness, and final thermal treatment in air. A thorough characterization of the target systems is carried out by X-ray diffraction, atomic force microscopy, field emission-scanning electron microscopy, energy dispersive X-ray spectroscopy, transmission electron microscopy, and X-ray photoelectron spectroscopy. High purity nanomaterials characterized by the co-presence of Fe2O3 (hematite) and TiO2 (anatase), with an intimate Fe2O3-TiO2 contact, are successfully obtained. In addition, photocatalytic tests demonstrate that, whereas both single-phase oxides do not show appreciable activity, the composite systems are able to degrade methyl orange aqueous solutions under simulated solar light, and even visible light, with an efficiency directly dependent on TiO2 overlayer thickness. This finding opens attractive perspectives for eventual applications in wastewater treatment.

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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.
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).

General information

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Authors: George Abraham, B., Sarkisyan, K. S., Mishin, A. S., Santala, V., Tkachenko, N. V., Karp, M.
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Photoinduced Electron Transfer in CdSe/ZnS Quantum Dot-Fullerene Hybrids

Photoinduced electron transfer (ET) in CdSe/ZnS core-shell quantum dot (QD) - fullerene (COOH-C<sub>60</sub>) hybrids was studied by the means of time-resolved emission and absorption spectroscopy techniques. A series of four QDs with emission in the range 540-630 nm was employed to investigate the dependence of the electron transfer rate on the QD size. Emission of the QDs is quenched upon hybrid formation, and the quenching mechanism is identified as photoinduced electron transfer from the QD to the fullerene moiety due to the fullerene anion signature observed in transient absorption. In order to obtain quantitative information on the ET reaction, several kinetic data analysis techniques were used, including a conventional multiexponential fitting and a maximum entropy method for emission decay analysis, as well as a distributed decay model based on the Poisson distribution of fullerenes in the hybrids. The latter gradually simplifies the interpretation of the transient absorption spectra and indicates that the spectra of QD cations are essentially similar to those of neutral QDs, differing only by a minor decrease in the intensity and broadening. Furthermore, only a minor decrease in the ET rate with the increasing QD size was observed, the time constants being in the range 100-200 ps for all studied QDs. The charge recombination is extended to 10 ns or longer for all hybrids.
Subpicosecond to Second Time-Scale Charge Carrier Kinetics in Hematite-Titania Nanocomposite Photoanodes

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

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology, Department of Materials Engineering, Frontier Photonics, ETH Zürich, Laboratory for Multifunctional Materials
Authors: Ruoko, T. P., Kaunisto, K., Bärtsch, M., Pohjola, J., Hiltunen, A., Niederberger, M., Tkachenko, N. V., Lemmetyinen, H.
Number of pages: 6
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Peer-reviewed: Yes

Publication information
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Scopus rating (2014): SJR 3.722 SNIP 1.724 CiteScore 7
Scopus rating (2013): SJR 3.515 SNIP 1.61 CiteScore 6.61
Scopus rating (2012): SJR 3.943 SNIP 1.751 CiteScore 6.3
Scopus rating (2011): SJR 3.244 SNIP 1.602 CiteScore 5.95
Original language: English
Keywords: FILM ELECTRODES, IRON-OXIDE, SEMICONDUCTOR ELECTRODES, WATER OXIDATION, VISIBLE-LIGHT, ALPHA-FE2O3, PHOTOELECTRODES, TIO2, RECOMBINATION, ELECTROLYSIS
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Source: Scopus
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Research output: Scientific - peer-review › Article

Synthesis and study of electrochemical and optical properties of substituted perylenemonoimides in solutions and on solid surfaces
A new and efficient methodology towards the synthesis of 7-pyrrolidinyl and 7,12-bispyrrolidinyl perylenemonoimide monoanhydrides (PMI monoanhydrides) and their corresponding dicarboxylic acids is devised. The high yields (70-96%) and facile synthesis of PMI monoanhydrides, as compared to traditional methodologies, make the method attractive and versatile. The reported 7,12-bispyrrolidinyl PMI monoanhydrides are a new family of peryleneimides, where both the bay-substituents are located towards the anhydride cycle. The electrochemical and optical properties of target molecules and their precursors were investigated using UV-Vis spectroscopy and differential pulse voltammetry. Atomic charges and electronic properties were calculated using density functional theory (DFT). In addition, self-assembling monolayers of the PMI monoanhydrides and their corresponding diacids were successfully formed over ZnO and TiO$_2$ films. The results of the current study indicate that these molecules are potentially good candidates for various applications in the fields of organic electronics and solar cells.

**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: Ahmed, Z., George, L., Hiltunen, A., Lemmetyinen, H., Hukka, T., Efimov, A.
Number of pages: 8
Pages: 13332-13339
Publication date: 7 Jul 2015
Peer-reviewed: Yes

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Volume: 3
Issue number: 25
ISSN (Print): 2050-7488
Ratings:
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Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
Original language: English
ASJC Scopus subject areas: Chemistry(all), Renewable Energy, Sustainability and the Environment, Materials Science(all)
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http://www.scopus.com/inward/record.url?scp=84934958229&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source-ID: 84934958229
Research output: Scientific - peer-review › Article

**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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Ministry of Education publication type: A1 Journal article-refereed
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.
Number of pages: 3
Pages: 54-56
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**Publication Information**
Journal: Journal of Microbiological Methods
Volume: 114
ISSN (Print): 0167-7012
Ratings:
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 π- 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 π- 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.
potential measurements and density functional theory calculations supported the proposed mechanism.

Catalytic effect of Ca and K on CO2 gasification of spruce wood char
Gasification is one route to produce chemicals and liquid fuels from biomass. The gasification of the char is catalyzed by alkali and alkaline earth metals in the biomass. In this work the catalytic effect of calcium (Ca) and potassium (K) on CO2 gasification of spruce wood was studied using a thermo gravimetric analyzer (TGA). The ash-forming elements were first removed from the wood using an acid leaching method. Then, various concentrations of K and Ca were absorbed to the wood by ion-exchange to carboxylic and phenolic groups, impregnation of K2CO3 or physically mixing of CaC2O4. The prepared spruce samples were placed in a mesh holder and gasified in the TGA at 850°C in 100% CO2. The results demonstrate that the gasification rate of the char increased linearly with an increase in the concentration of Ca or K. Crystalline CaC2O4 distributed only at the surface of the wood particles resulted in low catalytic activity. The catalytic activity of Ca was higher than K in the beginning of char gasification but the catalytic effect of Ca decreased earlier than the catalytic effect of potassium. Further, the char structure was investigated by SEM-EDX. The SEM analysis from interrupted gasification experiments showed the formation of CaCO3 and K2CO3 layer on the char surface. By adding
corresponding levels of Ca and K as the original spruce to the acid washed sample, a similar gasification reactivity was obtained at 850 °C.

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), 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.
Number of pages: 9
Pages: 464-472
Publication date: 15 Jun 2015
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Publication information
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ISSN (Print): 0016-2361
Ratings:
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Scopus rating (2015): SJR 1.809 SNIP 2.125 CiteScore 4.46
Scopus rating (2014): SJR 1.667 SNIP 2.331 CiteScore 4.14
Scopus rating (2013): SJR 1.811 SNIP 2.595 CiteScore 4.31
Scopus rating (2012): SJR 1.852 SNIP 2.465 CiteScore 3.99
Scopus rating (2011): SJR 2.093 SNIP 2.427 CiteScore 4.1
Scopus rating (2010): SJR 1.984 SNIP 2.319
Scopus rating (2009): SJR 2.012 SNIP 2.277
Scopus rating (2008): SJR 1.635 SNIP 2.184
Scopus rating (2007): SJR 1.383 SNIP 1.86
Scopus rating (2006): SJR 1.278 SNIP 1.64
Scopus rating (2005): SJR 1.623 SNIP 1.73
Scopus rating (2004): SJR 1.273 SNIP 1.883
Scopus rating (2003): SJR 1.103 SNIP 1.481
Scopus rating (2002): SJR 1.13 SNIP 1.301
Scopus rating (2001): SJR 1.136 SNIP 1.264
Scopus rating (2000): SJR 1.047 SNIP 1.272
Scopus rating (1999): SJR 1.117 SNIP 1.157
Original language: English
ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry
Keywords: Biomass, Calcium, Char reactivity, CO, Gasification, Potassium
DOI:
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http://www.scopus.com/inward/record.url?scp=84924100908&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source-ID: 84924100908
Research output: Scientific - peer-review › Article

Polymorph crystal packing effects on charge transfer emission in the solid state
Condensation of 1,8-naphthalic anhydride with N,N-(dimethylamino)aniline produced the donor-acceptor compound DMIM, which crystallised from a chloroform-diethyl ether mixture to afford two different coloured crystal polymorphs. Crystals for one polymorph are small and green, whereas the other crystals are orange and needle-like. X-ray crystal structures for both polymorphs were determined. The donor N,N-dimethylaniline and acceptor naphthalimide groups are twisted with respect to each other; the degree of twist is marginally different for the two structures. The orange crystal polymorph crystallises in the monoclinic space group C2/c and contains two slightly different molecular conformers in the unit cell (calculated density is 1.401 g cm<sup>-3</sup>). The green crystal polymorph crystallises in the triclinic space group P1 and contains only one type of molecule in the unit cell (calculated density is 1.410 g cm<sup>-3</sup>). The crystal packing motifs for the two polymorphs are subtly different, explaining the small variance in the observed densities. Very weak room temperature emission was observed for DMIM in a CHCl<sub>3</sub> solution, but crystals deposited on a
A glass slide glowed when irradiated at 488 nm using a fluorescence microscope. Disparate solid-state emission spectra and lifetimes for the two polymorphic crystal forms are observed for the dyad. The emission is assigned to charge recombination fluorescence from a charge transfer state. This journal is

**General information**

State: Published

Ministry of Education publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Molecular Photonics Laboratory, School of Chemistry, Newcastle University, United Kingdom, University of Malta

Authors: He, X., Benniston, A. C., Saarenpää, H., Lemmetyinen, H., Tkachenko, N. V., Baisch, U.

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Pages: 3525-3532

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**Publication information**

Journal: Chemical Science

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- Scopus rating (2015): SJR 4.74 SNIP 1.749 CiteScore 9.13
- Scopus rating (2014): SJR 4.991 SNIP 1.745 CiteScore 8.99
- Scopus rating (2013): SJR 4.675 SNIP 1.587 CiteScore 8.44
- Scopus rating (2012): SJR 5.146 SNIP 1.819 CiteScore 8.18
- Scopus rating (2011): SJR 4.33 SNIP 1.799 CiteScore 7.01

Original language: English

ASJC Scopus subject areas: Chemistry(all)

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Source: Scopus

Source-ID: 84929589670

Research output: Scientific - peer-review › Article

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.

**General information**

State: Published

Ministry of Education publication type: A1 Journal article-refereed


Authors: Vehviläinen, M., Kampuri, T., Gronqvist, S., Rissanen, M., Maloney, T., Honkanen, M., Nousiainen, P.

Number of pages: 22

Pages: 1653-1674

Publication date: Jun 2015

Peer-reviewed: Yes
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 crystalline 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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Ministry of Education publication type: A1 Journal article-refereed
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.
Number of pages: 12
Pages: 6216-6227
Publication date: 18 May 2015
Peer-reviewed: Yes

Publication information
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.

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, 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.
Number of pages: 7
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Publication information
Journal: Scientific Reports
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Article number: 9890
ISSN (Print): 2045-2322
Ratings:
Scopus rating (2016): CiteScore 4.63 SJR 1.625 SNIP 1.401
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.

General information
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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
Number of pages: 13
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Publication information
Journal: Biomaterials
Volume: 51
ISSN (Print): 0142-9612
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Scopus rating (2015): SJR 3.425 SNIP 2.028 CiteScore 9.35
Scopus rating (2014): SJR 3.289 SNIP 2.186 CiteScore 9.31
Scopus rating (2013): SJR 3.395 SNIP 2.185 CiteScore 9.02
Scopus rating (2012): SJR 3.545 SNIP 2.19 CiteScore 8.32
Scopus rating (2011): SJR 3.287 SNIP 2.235 CiteScore 8.1
Scopus rating (2010): SJR 3.428 SNIP 2.708
Scopus rating (2009): SJR 3.359 SNIP 2.887
Scopus rating (2008): SJR 2.986 SNIP 2.908
Scopus rating (2007): SJR 2.783 SNIP 2.782
Scopus rating (2006): SJR 2.369 SNIP 2.602
Scopus rating (2005): SJR 1.845 SNIP 2.675
Scopus rating (2004): SJR 1.231 SNIP 2.431
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.
Number of pages: 12
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Peer-reviewed: Yes

Publication information
Journal: FEMS Microbiology Ecology
Volume: 91
Issue number: 5
Article number: 035
ISSN (Print): 0168-6496
Ratings:
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Scopus rating (2015): SJR 1.682 SNIP 1.133 CiteScore 3.77
Scopus rating (2014): SJR 1.564 SNIP 1.239 CiteScore 3.8
Scopus rating (2013): SJR 1.656 SNIP 1.294 CiteScore 4.15
Scopus rating (2012): SJR 1.668 SNIP 1.21 CiteScore 3.78
Scopus rating (2011): SJR 1.638 SNIP 1.174 CiteScore 3.63
Scopus rating (2010): SJR 1.681 SNIP 1.25
Scopus rating (2009): SJR 1.7 SNIP 1.17
Scopus rating (2008): SJR 1.739 SNIP 1.281
Scopus rating (2007): SJR 1.495 SNIP 1.44
Scopus rating (2006): SJR 1.751 SNIP 1.496
Scopus rating (2005): SJR 1.54 SNIP 1.253
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.

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.

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, Qingdao Univ, Qingdao University, Cultivat Base State Key Lab, Qingdao Univ, Qingdao University, Coll Chem Sci & Engr, Qingdao Univ, Qingdao University, Coll Phys, Qingdao Univ, Qingdao University, Shandong University, Shandong Univ, Key Lab Photon Mat & Technol
Authors: Diao, F., Liang, W., Tian, F., Wang, Y., Vivo, P., Efimov, A., Lemmetyinen, H.
Number of pages: 6
Pages: 8960-8965
Publication date: 23 Apr 2015
Peer-reviewed: Yes

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Journal: Journal of Physical Chemistry C
Volume: 119
Issue number: 16
ISSN (Print): 1932-7447
Ratings:
Scopus rating (2016): SJR 1.948 SNIP 1.181 CiteScore 4.48
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
Scopus rating (2010): SJR 2.438 SNIP 1.356
Scopus rating (2009): SJR 2.128 SNIP 1.417
Scopus rating (2008): SJR 1.856 SNIP 1.033
Original language: English
Keywords: SENSITIZED SOLAR-CELLS, ANATASE, SURFACES, ADSORPTION, WATER, OXIDE
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10.1021/acs.jpcc.5b01369
Links:
http://www.scopus.com/inward/record.url?scp=84928527015&partnerID=8YFLogxK (Link to publication in Scopus)
Source: WOS
Source-ID: 000353603500062
Research output: Scientific - peer-review » Article
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.

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, Aalto Univ, Aalto University, Sch Chem Technol, Dept Forest Prod Technol, Univ Helsinki, University of Helsinki, Ctr Drug Res, Div Pharmaceut Biosci, Andalusian Ctr Nanomed & Biotechnol, Univ Eastern Finland, University of Eastern Finland, Sch Pharm, University of Helsinki
Number of pages: 14
Pages: 85-98
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Peer-reviewed: Yes

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Volume: 203
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Ratings:
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Scopus rating (2015): SJR 2.725 SNIP 2.08 CiteScore 8.11
Scopus rating (2014): SJR 2.416 SNIP 2.092 CiteScore 6.86
Scopus rating (2013): SJR 2.416 SNIP 2.044 CiteScore 6.31
Scopus rating (2012): SJR 2.417 SNIP 2.061 CiteScore 5.84
Scopus rating (2011): SJR 2.745 SNIP 2.098 CiteScore 6.33
Scopus rating (2010): SJR 3.194 SNIP 2.306
Scopus rating (2009): SJR 2.897 SNIP 2.033
Scopus rating (2008): SJR 2.25 SNIP 1.886
Scopus rating (2007): SJR 2.149 SNIP 1.82
Scopus rating (2006): SJR 1.771 SNIP 1.779
Scopus rating (2005): SJR 1.552 SNIP 1.81
Scopus rating (2004): SJR 1.475 SNIP 1.778
Scopus rating (2003): SJR 1.592 SNIP 1.682
Scopus rating (2002): SJR 1.393 SNIP 1.534
Scopus rating (2001): SJR 1.275 SNIP 1.361
Scopus rating (2000): SJR 1.067 SNIP 1.384
Scopus rating (1999): SJR 1.046 SNIP 1.298
Original language: English
Keywords: Light activation, Liposome, Gold nanoparticle, Intracellular delivery, Triggered release, Retinal pigment epithelium, RETINAL-PIGMENT EPITHELIUM, NEAR-INFRARED LIGHT, PH-SENSITIVE LIPOSOMES, GENE DELIVERY, THERMOSENSITIVE LIPOSOMES, TRIGGERED DRUG, MULTIFOCAL CHOROIDITIS, UNILAMELLAR LIPOSOMES, MACULAR DEGENERATION, CONTENTS RELEASE
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 cellulolytic 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, \( \text{H}_2, \text{CH}_4, \text{CO}_2, \) and organic acids were the main metabolites on all substrates but the metabolite profiles varied with the substrate. Similar \( \text{H}_2 \) yields of 2-3mol\( \text{mol}^{-1} \) substrate at 48h were obtained with all monosaccharides and disaccharides. The \( \text{CO}_2 \) yields were higher with disaccharides than with monosaccharides, 4.5 vs 2mol\( \text{mol}^{-1} \) 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 \( \leq 74\% \) 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 cellulolytic organisms. Most differences among the samples were attributed to small taxonomic groups represented by \( \leq 10\% \) 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.

General information

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Fibre Materials, Polymer Technology, Department of Biotechnology and Chemical Technology, Aalto University
Authors: Saarikoski, E., Rissanen, M., Seppälä, J.
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Scopus rating (2014): SJR 1.584 SNIP 1.969 CiteScore 4.69
Scopus rating (2013): SJR 1.346 SNIP 1.967 CiteScore 4.39
Scopus rating (2012): SJR 1.409 SNIP 2.045 CiteScore 3.93
Scopus rating (2011): SJR 1.287 SNIP 1.991 CiteScore 4.08
Scopus rating (2010): SJR 1.372 SNIP 1.808
Scopus rating (2009): SJR 1.43 SNIP 1.718
Scopus rating (2008): SJR 1.142 SNIP 1.515
Scopus rating (2007): SJR 0.879 SNIP 1.369
Scopus rating (2006): SJR 0.824 SNIP 1.424
Scopus rating (2005): SJR 0.816 SNIP 1.349
Scopus rating (2004): SJR 0.885 SNIP 1.538
Scopus rating (2003): SJR 0.937 SNIP 1.41
Scopus rating (2002): SJR 0.878 SNIP 1.372
Scopus rating (2001): SJR 0.828 SNIP 1.062
Scopus rating (2000): SJR 0.858 SNIP 1.086
Scopus rating (1999): SJR 0.764 SNIP 1.074
Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics
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http://www.scopus.com/inward/record.url?scp=84916613635&partnerID=8YFLogxK (Link to publication in Scopus)
Crystal structure of 2-methylpiperazine-1,4-diium bis(hydrogen maleate)

In the title salt, C₅H₁₄N₂²⁺·2C₄H₃O₄⁻, 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 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.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Russian Acad Sci, Russian Academy of Sciences, Inst Gen Phys
Authors: Alekseev, A. S., Lemmetyinen, H., Tolkki, A.
Number of pages: 9
Pages: 741-749
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Scopus rating (2014): SJR 0.171 SNIP 0.352 CiteScore 0.5
Scopus rating (2013): SJR 0.183 SNIP 0.21 CiteScore 0.36
Scopus rating (2012): SJR 0.269 SNIP 0.381 CiteScore 0.52
Scopus rating (2011): SJR 0.38 SNIP 0.548 CiteScore 0.82
Scopus rating (2010): SJR 0.578 SNIP 0.45
Scopus rating (2009): SJR 0.679 SNIP 0.786
Scopus rating (2008): SJR 0.644 SNIP 0.939
Scopus rating (2007): SJR 0.335 SNIP 0.508
Original language: English
Keywords: Photoinduced Charge Transfer, Donor-Acceptor Dyad, Solar Cell, LANGMUIR-BLODGETT-FILMS, PORPHYRIN-FULLERENE DYAD, MOLECULAR FILMS, REGIOREGULAR POLY(3-HEXYLTHIOPHENE), MONOLAYERS, COMPLEXES, EXCIPLEX, DEVICES, DESIGN, ENERGY
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Source: WOS
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Research output: Scientific - peer-review → Article

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. 1H NMR spectroscopy and electrospray ionisation mass spectrometry were utilized in analysing the complexes in solution and in the gas phase, respectively. The 1H NMR titration studies in methanol-d4 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.

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Organisations: Department of Chemistry and Bioengineering, University of Jyväskylä
Authors: Beyeh, N. K., Pan, F., Valkonen, A., Rissanen, K.
Number of pages: 7
Pages: 1182-1188
Publication date: 7 Feb 2015
Integrated in vitro-in silico screening strategy for the discovery of antibacterial compounds

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

General information

State: Published
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Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Tampere University of Technology, Urban circular bioeconomy (UrCirBio), Centre for Drug Research, Division of Pharmaceutical Biosciences, Helsinki University, Division of Pharmaceutical Chemistry and Technology
Authors: Nybond, S., Ghemtio, L., Nawrot, D. A., Karp, M., Xhaard, H., Tammela, P.
Number of pages: 9
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Peer-reviewed: Yes

Publication information
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.
Glycerol as an Efficient Medium for the Petasis Borono-Mannich Reaction

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

General information
State: Published
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.
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Scopus rating (2014): SJR 0.913 SNIP 0.775 CiteScore 2.72
Scopus rating (2013): SJR 0.111 SNIP 0
Supramolecular hierarchy among halogen and hydrogen bond donors in light-induced surface patterning

Halogen bonding, a noncovalent interaction possessing several unique features compared to the more familiar hydrogen bonding, is emerging as a powerful tool in functional materials design. Herein, we unambiguously show that one of these characteristic features, namely high directionality, renders halogen bonding the interaction of choice when developing azobenzene-containing supramolecular polymers for light-induced surface patterning. The study is conducted by using an extensive library of azobenzene molecules that differ only in terms of the bond-donor unit. We introduce a new tetrafluorophenol-containing azobenzene photoswitch capable of forming strong hydrogen bonds, and show that an iodoethynyl-containing azobenzene comes out on top of the supramolecular hierarchy to provide unprecedented photoinduced surface patterning efficiency. Specifically, the iodoethyl motif seems highly promising in future development of polymeric optical and photoactive materials driven by halogen bonding.

Photophysical Study of a Self-Assembled Donor-Acceptor Two-Layer Film on TiO2

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

Perylenedimidies (PDIs) and perylenemonomide 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.
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.
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 $^{19}$F NMR signals. However, any specific interaction cannot be assigned to this effect. In order to study the interaction in more detail, the salt derivatives 3 and 4 were prepared and studied by single crystal X-ray diffraction revealing weak anion-π interactions in the solid state.
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.
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′:5′,2″-terthiophene) vinylene, (BSTV) and octathienylene vinylene (BOTV) (E)-Bis-l,2-(5,5″-Dimethyl-(2,2':5',2″-terthiophene) 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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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Universidad de Chile
Authors: Martinez, F., Neculqueo, G., Vasquez, S. O., Lemmetyinen, H., Efimov, A., Vivo, P.
Number of pages: 7
Pages: 19-25
Publication date: 2015

Host publication information

Title of host publication: Materials Research Society Symposium Proceedings
Volume: 1737
Combination of a novel electrode material and artificial mediators to enhance power generation in an MFC

This study focuses on two main aspects: developing a novel cost-effective electrode material and power production from domestic wastewater using three different mediators. Methylene blue (MB), neutral red (NR) and 2-hydroxy-1,4-naphthoquinone (HNQ) were selected as electrode mediators with different concentrations. A tin-coated copper mesh electrode was tested as anode electrode. Maximum power density of the microbial fuel cell (MFC) with 300 μM MB was 636 mW/m². Optimal mediator concentrations with respect to the achieved maximum power output for MB, NR and HNQ were 300 μM, 200 μM and 50 μM, respectively. The results demonstrate that tin-coated copper mesh showed a higher biocompatibility and electrical conductivity.
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.
Publication date: 2015

**Host publication information**

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ISBN (Electronic): 978-90-821727-3-7
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**

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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.
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ISSN (Print): 0969-0239
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Scopus rating (2014): SJR 1.071 SNIP 1.334 CiteScore 3.58
Scopus rating (2013): SJR 1.127 SNIP 1.48 CiteScore 3.83
Scopus rating (2012): SJR 1.179 SNIP 1.71 CiteScore 3.74
Scopus rating (2011): SJR 1.354 SNIP 1.795 CiteScore 3.99
Scopus rating (2010): SJR 0.873 SNIP 1.384
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 \( \approx 2.0 \text{ mA cm}^{-2} \) 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


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Peer-reviewed: Yes

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ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials

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From partial to complete optical erasure of azobenzene-polymer gratings: effect of molecular weight

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Aalto University
Authors: Vapaavuori, J., Ras, R. H. A., Kaivola, M., Bazuin, C. G., Priimägi, A.
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ISSN (Print): 2050-7526
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Original language: English
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Research output: Scientific - peer-review › Article

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

General information
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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, VTT Technical Research Centre of Finland, Politecnico di Milano, Aalto University
Authors: Saccone, M., Cavallo, G., Metrangolo, P., Resnati, G., Priimägi, A.
Number of pages: 20
Pages: 147-166
Publication date: 2015

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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.
Number of pages: 3
Pages: 78-80
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Journal of Microbiological Methods
Volume: 118
Article number: 4723
ISSN (Print): 0167-7012
Ratings:
Scopus rating (2016): SJR 0.723 SNIP 0.8 CiteScore 2.05
Scopus rating (2015): SJR 0.816 SNIP 0.873 CiteScore 2.04
Scopus rating (2014): SJR 0.903 SNIP 1.037 CiteScore 2.28
Scopus rating (2013): SJR 0.917 SNIP 1.019 CiteScore 2.5
Scopus rating (2012): SJR 0.87 SNIP 1.004 CiteScore 2.32
Scopus rating (2011): SJR 0.9 SNIP 0.972 CiteScore 2.29
Scopus rating (2010): SJR 0.945 SNIP 1.05
Scopus rating (2009): SJR 0.993 SNIP 1.156
Scopus rating (2008): SJR 0.926 SNIP 1.031
Scopus rating (2007): SJR 0.942 SNIP 1.111
Scopus rating (2006): SJR 1.138 SNIP 1.251
Scopus rating (2005): SJR 0.964 SNIP 1.141
Scopus rating (2004): SJR 0.921 SNIP 1.037
Scopus rating (2003): SJR 0.933 SNIP 1.217
Scopus rating (2002): SJR 0.821 SNIP 1.002
Scopus rating (2001): SJR 0.867 SNIP 0.894
Scopus rating (2000): SJR 0.721 SNIP 0.864
Scopus rating (1999): SJR 0.724 SNIP 0.729
Original language: English
Keywords: Antioxidative activity, Bacterial biosensor, Bioscreening, Microplate technique
ASJC Scopus subject areas: Microbiology, Molecular Biology, Microbiology (medical)
DOIs:
10.1016/j.jmimet.2015.08.018
Source: Scopus
Source-ID: 84941101607
Research output: Scientific - peer-review › Article
Microvesicle- and exosome-mediated drug delivery enhances the cytotoxicity of Paclitaxel in autologous prostate cancer cells

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

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:

Scopus rating (2016): SJR 2.33 SNIP 0.835 CiteScore 4.72

Scopus rating (2015): SJR 2.34 SNIP 0.886 CiteScore 4.51

Original language: English

Keywords: ELECTRON DONOR SOLVENTS, RECOGNITION, ANALOGS, SHIFTS

DOI:

10.1039/c4qo00326h

Source: WOS

Source-ID: 000364444500006

Research output: Scientific - peer-review › Article

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**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 › Conference contribution

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

The role of π-conjugated molecular bridges in through-space and through-bond electron transfer is studied by comparing two porphyrin-fullerene donor-acceptor (D-A) dyads. One dyad, ZnP-Ph-C60 (ZnP=zinc porphyrin), incorporates a phenyl bridge between D and A and behaves very similarly to analogous dyads studied previously. The second dyad, ZnP-EDOTV-C60, introduces an additional 3,4-ethylenedioxythiophenylvinylene (EDOTV) unit into the conjugated bridge, which increases the distance between D and A, but, at the same time, provides increased electronic communication between them. Two essential outcomes that result from the introduction of the EDOTV unit in the bridge are as follows: 1) faster charge recombination, which indicates enhanced electronic coupling between the charge-separated and ground electronic states; and 2) the disappearance of the intramolecular exciplex, which mediates photoinduced charge separation in the ZnP-Ph-C60 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 determinate 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.]
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
Number of pages: 6
Pages: 553-558
Publication date: 2015
Peer-reviewed: Yes

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Journal: Chemistry - An Asian Journal
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ISSN (Print): 1861-4728
Ratings:
Scopus rating (2016): SJR 1.584 SNIP 0.773 CiteScore 3.92
Scopus rating (2015): SJR 1.766 SNIP 0.911 CiteScore 4.41
Scopus rating (2014): SJR 1.762 SNIP 0.974 CiteScore 4.38
Scopus rating (2013): SJR 1.767 SNIP 0.872 CiteScore 4.12
Scopus rating (2012): SJR 2.267 SNIP 1.026 CiteScore 4.36
Scopus rating (2011): SJR 2.31 SNIP 1.017 CiteScore 4.43
Scopus rating (2010): SJR 2.259 SNIP 1.014
Scopus rating (2009): SJR 2.372 SNIP 1.019
Scopus rating (2008): SJR 2.57 SNIP 1.153
Scopus rating (2007): SJR 1.566 SNIP 0.669
Original language: English
ASJC Scopus subject areas: Chemistry(all)
Keywords: Cyclization, Fluorescence, Heterocycles, Pyrenes, Quinolines
DOIs:
10.1002/asia.201403339
The effect of physical adhesion promotion treatments on interfacial adhesion in cellulose-epoxy composite

General information
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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.
Number of pages: 11
Pages: 3955-3965
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Cellulose
Volume: 22
Issue number: 6
ISSN (Print): 0969-0239
Ratings:
Scopus rating (2016): CiteScore 3.68 SJR 1.126 SNIP 1.144
Scopus rating (2015): SJR 1.153 SNIP 1.24 CiteScore 3.55
Scopus rating (2014): SJR 1.071 SNIP 1.334 CiteScore 3.58
Scopus rating (2013): SJR 1.127 SNIP 1.48 CiteScore 3.83
Scopus rating (2012): SJR 1.179 SNIP 1.71 CiteScore 3.74
Scopus rating (2011): SJR 1.354 SNIP 1.795 CiteScore 3.99
Scopus rating (2010): SJR 0.873 SNIP 1.384
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.
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 & Bioeng
Authors: Ranta, J., Niskanen, M., Kaunisto, K., Manninen, V., Mundy, M. E., Virkki, K., Hakola, H., Hukka, T. I., Lemmetyinen, H.
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:
Scopus rating (2016): SJR 0.354 SNIP 0.379 CiteScore 1.05
Scopus rating (2015): SJR 0.419 SNIP 0.467 CiteScore 1.17
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
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

Publication information
Journal: RSC Advances
Issue number: xx
ISSN (Print): 2046-2069
Ratings:
Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
Original language: English
DOIs:
10.1039/C4RA10662H

Bibliographical note
Contribution: organisation=mol,FACT1=1<br/>Portfolio EDEND: 2014-11-27<br/>Publisher name: The Royal Society of Chemistry
Source: researchoutputwizard
Source-ID: 1845
Research output: Scientific - peer-review › Review Article

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

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

Journal: Chemistry of Materials  
Volume: 26  
Issue number: 17  
ISSN (Print): 0897-4756  
Ratings:  
Scopus rating (2016): SJR 4.114 SNIP 1.905 CiteScore 8.89  
Scopus rating (2015): SJR 4.038 SNIP 2.102 CiteScore 9.38  
Scopus rating (2014): SJR 3.603 SNIP 2.253 CiteScore 8.89  
Scopus rating (2013): SJR 3.658 SNIP 2.277 CiteScore 8.94  
Scopus rating (2012): SJR 4.169 SNIP 2.264 CiteScore 8.1  
Scopus rating (2011): SJR 3.484 SNIP 2.145 CiteScore 7.38  
Scopus rating (2010): SJR 3.267 SNIP 1.849  
Scopus rating (2009): SJR 2.894 SNIP 1.763  
Scopus rating (2008): SJR 2.882 SNIP 1.844  
Scopus rating (2007): SJR 3.111 SNIP 1.863  
Scopus rating (2006): SJR 3.168 SNIP 1.943  
Scopus rating (2005): SJR 2.746 SNIP 1.937  
Scopus rating (2004): SJR 2.5 SNIP 1.976  
Scopus rating (2003): SJR 2.56 SNIP 1.938  
Scopus rating (2002): SJR 2.499 SNIP 1.894  
Scopus rating (2001): SJR 2.321 SNIP 1.911  
Scopus rating (2000): SJR 2.201 SNIP 1.686  
Scopus rating (1999): SJR 2.23 SNIP 1.796  
Original language: English  
DOIs:  
10.1021/cm5023129

**Bibliographical note**

Contribution: organisation=keb,FACT1=1  
Portfolio EDEND: 2014-09-30  
Publisher name: American Chemical Society  
Source: researchoutputwizard  
Source-ID: 1702  
Research output: Scientific - peer-review › Article

**Charge-Transfer Dynamics In Poly(3-hexylthiophene):Perylenedilimide-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:  
Scopus rating (2016): SJR 1.948 SNIP 1.181 CiteScore 4.48  
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68  
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08  
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14  
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
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:
Scopus rating (2016): SJR 1.043 SNIP 0.904 CiteScore 3.37
Scopus rating (2015): SJR 1.063 SNIP 0.999 CiteScore 3.83
Scopus rating (2014): SJR 1.131 SNIP 1.11 CiteScore 3.97
Scopus rating (2013): SJR 1.079 SNIP 1.11 CiteScore 3.81
Scopus rating (2012): SJR 1.253 SNIP 1.142 CiteScore 3.83
Scopus rating (2011): SJR 1.174 SNIP 1.191 CiteScore 3.87
Scopus rating (2010): SJR 1.233 SNIP 1.229
Scopus rating (2009): SJR 1.227 SNIP 1.257
Scopus rating (2008): SJR 1.297 SNIP 1.183
Scopus rating (2007): SJR 1.42 SNIP 1.704
Scopus rating (2006): SJR 1.296 SNIP 1.406
Scopus rating (2005): SJR 1.419 SNIP 1.051
Scopus rating (2004): SJR 1 SNIP 0.951
Scopus rating (2003): SJR 0.73 SNIP 0.751
Scopus rating (2002): SJR 0.228 SNIP 0.509
Scopus rating (2001): SJR 0.138 SNIP 0.153
Scopus rating (2000): SJR 0.102 SNIP 0
Original language: English
DOIs:
10.1039/c3ce42291g

Bibliographical note
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-11-12
Publisher name: Royal Society of Chemistry
Source: researchoutputwizard
Source-ID: 167
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 demonstrators 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 cellulosic raw materials.

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
Volume: 118
Issue number: 8
ISSN (Print): 1089-5639
Ratings:
Scopus rating (2016): SJR 1.258 SNIP 0.98 CiteScore 2.64
Scopus rating (2015): SJR 1.179 SNIP 1.106 CiteScore 2.78
Scopus rating (2014): SJR 1.154 SNIP 1.071 CiteScore 2.65
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:
Scopus rating (2016): SJR 0.733 SNIP 0.951 CiteScore 2.32
Scopus rating (2015): SJR 0.71 SNIP 0.909 CiteScore 2.13
Scopus rating (2014): SJR 0.742 SNIP 0.933 CiteScore 2.05
Scopus rating (2013): SJR 0.734 SNIP 0.947 CiteScore 2.17
Scopus rating (2012): SJR 0.732 SNIP 0.957 CiteScore 1.95
Scopus rating (2011): SJR 0.726 SNIP 0.926 CiteScore 1.97
Scopus rating (2010): SJR 0.747 SNIP 0.992
Scopus rating (2009): SJR 0.788 SNIP 0.984
Scopus rating (2008): SJR 0.839 SNIP 1.159
Scopus rating (2007): SJR 0.662 SNIP 0.823
Scopus rating (2006): SJR 0.592 SNIP 0.775
Scopus rating (2005): SJR 0.474 SNIP 0.693
Scopus rating (2004): SJR 0.549 SNIP 0.664
Scopus rating (2003): SJR 0.498 SNIP 0.709
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:
Scopus rating (2016): SJR 1.258 SNIP 0.98 CiteScore 2.64
Scopus rating (2015): SJR 1.179 SNIP 1.106 CiteScore 2.78
Scopus rating (2014): SJR 1.154 SNIP 1.071 CiteScore 2.65
Scopus rating (2013): SJR 1.194 SNIP 1.102 CiteScore 2.84
Scopus rating (2012): SJR 1.494 SNIP 1.124 CiteScore 2.78
Scopus rating (2011): SJR 1.402 SNIP 1.135 CiteScore 2.87
Scopus rating (2010): SJR 1.466 SNIP 1.102
Scopus rating (2009): SJR 1.562 SNIP 1.132
Scopus rating (2008): SJR 1.787 SNIP 1.093
Scopus rating (2007): SJR 1.907 SNIP 1.136
Scopus rating (2006): SJR 1.728 SNIP 1.195
Scopus rating (2005): SJR 1.789 SNIP 1.215
Scopus rating (2004): SJR 1.669 SNIP 1.224
Scopus rating (2003): SJR 1.75 SNIP 1.241
Scopus rating (2002): SJR 1.81 SNIP 1.196
Scopus rating (2001): SJR 1.732 SNIP 1.224
Scopus rating (2000): SJR 1.953 SNIP 1.272
Scopus rating (1999): SJR 1.507 SNIP 1.592
Original language: English
DOI: 10.1021/jp411395c
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:
Scopus rating (2016): SJR 1.243 SNIP 0.931 CiteScore 3.85
Scopus rating (2015): SJR 1.351 SNIP 1.026 CiteScore 4.1
Scopus rating (2014): SJR 1.413 SNIP 1.085 CiteScore 4.06
Scopus rating (2013): SJR 1.436 SNIP 1.083 CiteScore 4.07
Scopus rating (2012): SJR 1.554 SNIP 1.001 CiteScore 3.79
Scopus rating (2011): SJR 1.505 SNIP 1.013 CiteScore 3.68
Scopus rating (2010): SJR 1.399 SNIP 0.875
Scopus rating (2009): SJR 0.928 SNIP 0.783
Scopus rating (2008): SJR 0.629 SNIP 0.572
Scopus rating (2007): SJR 0.669 SNIP 0.539
Scopus rating (2006): SJR 1.084 SNIP 0.907
Scopus rating (2005): SJR 1.128 SNIP 0.815
Scopus rating (2004): SJR 1.045 SNIP 0.933
Scopus rating (2003): SJR 1.1 SNIP 1.051
Scopus rating (2002): SJR 0.973 SNIP 0.827
Scopus rating (2001): SJR 0.626 SNIP 0.488
Scopus rating (2000): SJR 0.318 SNIP 0.183
Scopus rating (1999): SJR 0.29 SNIP 0.188
Original language: English
DOIs:
10.1039/C4DT01407C

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2015-01-12<br/>Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 1281
Research output: Scientific - peer-review › Article

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.
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:
Scopus rating (2016): SJR 1.948 SNIP 1.181 CiteScore 4.48
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
Scopus rating (2010): SJR 2.438 SNIP 1.356
Scopus rating (2009): SJR 2.128 SNIP 1.417
Scopus rating (2008): SJR 1.856 SNIP 1.033
Original language: English
DOIs:
10.1021/jp507486x
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.

Light-driven surface patterning of supramolecular polymers with extremely low concentration of photoactive molecules

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Authors: Koskela, J. E., Vapaavuori, J., Ras, R. H. A., Priimagi, A.
Number of pages: 5
Pages: 1196-1200
Publication date: 2014
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

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

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 16
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
Scopus rating (2010): SJR 1.802 SNIP 1.196
Scopus rating (2009): SJR 2.127 SNIP 1.369
Scopus rating (2008): SJR 2.158 SNIP 1.211
Scopus rating (2007): SJR 1.84 SNIP 1.138
Scopus rating (2006): SJR 1.467 SNIP 1.128
Scopus rating (2005): SJR 1.389 SNIP 1.104
Scopus rating (2004): SJR 1.173 SNIP 1.007
Scopus rating (2003): SJR 1.093 SNIP 0.925
Scopus rating (2002): SJR 1.122 SNIP 0.973
Scopus rating (2001): SJR 1.09 SNIP 0.914
Scopus rating (2000): SJR 0.948 SNIP 1.068
Scopus rating (1999): SJR 0.121 SNIP 0
Original language: English
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:
Scopus rating (2016): SJR 1.948 SNIP 1.181 CiteScore 4.48
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
Scopus rating (2010): SJR 2.438 SNIP 1.356
Scopus rating (2009): SJR 2.128 SNIP 1.417
Scopus rating (2008): SJR 1.856 SNIP 1.033
Original language: English
DOIs:
10.1021/jp4096002

Bibliographical note
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-06-27
Publisher: American Chemical Society
Source: researchoutputwizard
Source-ID: 1344
Research output: Scientific - peer-review » Article

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
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., Tagmatachris, N.
Number of pages: 7
Pages: 14729-14735
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Chemistry: A European Journal
Volume: 20
Issue number: 45
ISSN (Print): 0947-6539
Ratings:
Scopus rating (2016): CiteScore 5.03 SJR 2.247 SNIP 1.046
Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Scopus rating (2014): SJR 2.487 SNIP 1.219 CiteScore 5.51
Scopus rating (2013): SJR 2.604 SNIP 1.239 CiteScore 5.68
Scopus rating (2012): SJR 2.884 SNIP 1.294 CiteScore 5.55
Scopus rating (2011): SJR 2.726 SNIP 1.336 CiteScore 5.46
Scopus rating (2010): SJR 2.527 SNIP 1.292
Scopus rating (2009): SJR 2.499 SNIP 1.365
Scopus rating (2008): SJR 2.887 SNIP 1.407
Scopus rating (2007): SJR 3.233 SNIP 1.532
Scopus rating (2006): SJR 2.911 SNIP 1.505
Scopus rating (2005): SJR 2.62 SNIP 1.454
Scopus rating (2004): SJR 2.32 SNIP 1.472
Scopus rating (2003): SJR 2.156 SNIP 1.45
Scopus rating (2002): SJR 2.554 SNIP 1.472
Scopus rating (2001): SJR 2.834 SNIP 1.612
Scopus rating (2000): SJR 2.956 SNIP 1.652
Scopus rating (1999): SJR 3.013 SNIP 1.73
Original language: English
DOIs:
10.1002/chem.201403517

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-11-20<br/>Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA
Source: researchoutputwizard
Source-ID: 1407
Research output: Scientific - peer-review  Article
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:
Scopus rating (2016): SJR 1.264 SNIP 0.771 CiteScore 2.81
Scopus rating (2015): SJR 1.334 SNIP 0.912 CiteScore 3.21
Scopus rating (2014): SJR 1.362 SNIP 0.905 CiteScore 3.12
Scopus rating (2013): SJR 1.442 SNIP 0.948 CiteScore 3.22
Scopus rating (2012): SJR 1.763 SNIP 0.955 CiteScore 3.24
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:
Scopus rating (2016): SJR 1.948 SNIP 1.181 CiteScore 4.48
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
Scopus rating (2010): SJR 2.438 SNIP 1.356
Scopus rating (2009): SJR 2.128 SNIP 1.417
Scopus rating (2008): SJR 1.856 SNIP 1.033
Original language: English
DOIs: 10.1021/jp410436f

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
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:
Scopus rating (2016): SJR 1.243 SNIP 0.931 CiteScore 3.85
Scopus rating (2015): SJR 1.351 SNIP 1.026 CiteScore 4.1
Scopus rating (2014): SJR 1.413 SNIP 1.085 CiteScore 4.06
Scopus rating (2013): SJR 1.436 SNIP 1.083 CiteScore 4.07
Scopus rating (2012): SJR 1.554 SNIP 1.001 CiteScore 3.79
Scopus rating (2011): SJR 1.505 SNIP 1.013 CiteScore 3.68
Scopus rating (2010): SJR 1.399 SNIP 0.875
Scopus rating (2009): SJR 0.928 SNIP 0.783
Scopus rating (2008): SJR 0.629 SNIP 0.572
Scopus rating (2007): SJR 0.669 SNIP 0.539
Scopus rating (2006): SJR 1.084 SNIP 0.907
Scopus rating (2005): SJR 1.128 SNIP 0.815
Scopus rating (2004): SJR 1.045 SNIP 0.933
Scopus rating (2003): SJR 1.1 SNIP 1.051
Scopus rating (2002): SJR 0.973 SNIP 0.827
Scopus rating (2001): SJR 0.626 SNIP 0.488
Scopus rating (2000): SJR 0.318 SNIP 0.183
Scopus rating (1999): SJR 0.29 SNIP 0.188
Original language: English
DOIs: 10.1039/c3dt52960f

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2015-01-13<br/>Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 346
Research output: Scientific - peer-review › Article

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
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:
Scopus rating (2016): SJR 1.179 SNIP 0.915 CiteScore 2.55
Scopus rating (2015): SJR 1.257 SNIP 0.915 CiteScore 2.56
Scopus rating (2014): SJR 1.213 SNIP 0.933 CiteScore 2.63
Scopus rating (2013): SJR 1.293 SNIP 1.113 CiteScore 2.94
Scopus rating (2012): SJR 1.202 SNIP 1.059 CiteScore 2.9
Scopus rating (2011): SJR 1.265 SNIP 1.216 CiteScore 3.04
Scopus rating (2010): SJR 1.217 SNIP 1.075
Scopus rating (2009): SJR 1.292 SNIP 1.038
Scopus rating (2008): SJR 1.178 SNIP 1.015
Scopus rating (2007): SJR 1.399 SNIP 1.076
Scopus rating (2006): SJR 1.321 SNIP 1.067
Scopus rating (2005): SJR 1.13 SNIP 0.997
Scopus rating (2004): SJR 0.895 SNIP 0.841
Scopus rating (2003): SJR 0.768 SNIP 0.821
Scopus rating (2002): SJR 0.696 SNIP 0.738
Scopus rating (2001): SJR 0.812 SNIP 0.809
Scopus rating (2000): SJR 0.708 SNIP 0.764
Scopus rating (1999): SJR 0.763 SNIP 0.832
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:
Scopus rating (2016): SJR 2.506 SNIP 1.159 CiteScore 6.06
Scopus rating (2015): SJR 2.664 SNIP 1.314 CiteScore 6.7
Scopus rating (2014): SJR 2.701 SNIP 1.446 CiteScore 6.83
Scopus rating (2013): SJR 2.755 SNIP 1.38 CiteScore 6.73
Scopus rating (2012): SJR 3.09 SNIP 1.347 CiteScore 6.21
Scopus rating (2011): SJR 2.857 SNIP 1.322 CiteScore 5.96
Scopus rating (2010): SJR 2.709 SNIP 1.232
Scopus rating (2009): SJR 2.588 SNIP 1.252
Scopus rating (2008): SJR 2.791 SNIP 1.236
Scopus rating (2007): SJR 2.851 SNIP 1.237
Scopus rating (2006): SJR 2.366 SNIP 1.183
Scopus rating (2005): SJR 2.129 SNIP 1.15
Scopus rating (2004): SJR 1.954 SNIP 1.158
Scopus rating (2003): SJR 1.644 SNIP 1.098
Scopus rating (2002): SJR 1.956 SNIP 1.19
Scopus rating (2001): SJR 1.817 SNIP 1.098
Scopus rating (2000): SJR 1.649 SNIP 1.028
Scopus rating (1999): SJR 1.454 SNIP 0.947
Original language: English
DOIs:
10.1039/c4ra03105a

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
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
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:
Scopus rating (2016): SJR 0.722 SNIP 0.799 CiteScore 2.37
Scopus rating (2015): SJR 0.805 SNIP 0.811 CiteScore 2.4
Scopus rating (2014): SJR 0.874 SNIP 0.946 CiteScore 2.55
Scopus rating (2013): SJR 0.989 SNIP 1.006 CiteScore 3
Scopus rating (2012): SJR 1.049 SNIP 0.919 CiteScore 2.73
Scopus rating (2011): SJR 1.013 SNIP 0.962 CiteScore 2.63
Scopus rating (2010): SJR 1.082 SNIP 0.927
Scopus rating (2009): SJR 0.983 SNIP 1.115
Scopus rating (2008): SJR 0.936 SNIP 0.872
Scopus rating (2007): SJR 1.09 SNIP 0.957
Scopus rating (2006): SJR 0.838 SNIP 0.914
Scopus rating (2005): SJR 0.938 SNIP 1.061
Scopus rating (2004): SJR 0.667 SNIP 1.098
Scopus rating (2003): SJR 0.492 SNIP 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
Number of pages: 8
Pages: 193-200
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Synthetic Metals
Volume: 195
ISSN (Print): 0379-6779
Ratings:
Scopus rating (2016): SJR 0.675 SNIP 0.764 CiteScore 2.45
Scopus rating (2015): SJR 0.643 SNIP 0.75 CiteScore 2.27
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 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.
Ultrafast photophysical processes for Fe(III)-carboxylates
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 \( \pi \)-interactions of the porphyrin ring with ZnO. Because porphyrins are closely packed and near the surface, emerging van der Waals (vdW) interactions are examined using Grimme's D2 method. While the orientation affects the initial excitation of porphyrin only slightly, the coupling between the LUMO and LUMO + 1 of porphyrin and the conduction band of ZnO increases considerably if porphyrin is close to the surface, especially if the \( \pi \)-electrons are interacting with the surface. Based on the results of coupling studies, not only the distance between porphyrin and the
ZnO surface but also the orientation of porphyrin can greatly affect the electron transfer. © 2013 the Owner Societies.

**General information**

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

**Publication information**

Journal: Physical Chemistry Chemical Physics

Volume: 15

Issue number: 40

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
Scopus rating (2010): SJR 1.802 SNIP 1.196
Scopus rating (2009): SJR 2.127 SNIP 1.369
Scopus rating (2008): SJR 2.158 SNIP 1.211
Scopus rating (2007): SJR 1.84 SNIP 1.138
Scopus rating (2006): SJR 1.467 SNIP 1.128
Scopus rating (2005): SJR 1.389 SNIP 1.104
Scopus rating (2004): SJR 1.173 SNIP 1.007
Scopus rating (2003): SJR 1.093 SNIP 0.925
Scopus rating (2002): SJR 1.122 SNIP 0.973
Scopus rating (2001): SJR 1.09 SNIP 0.914
Scopus rating (2000): SJR 0.948 SNIP 1.068
Scopus rating (1999): SJR 0.121 SNIP 0

Original language: English

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

DOIs:

10.1039/c3cp51685g

Links:

http://www.scopus.com/inward/record.url?scp=84886933383&partnerID=8YFLogxK (Link to publication in Scopus)

**Bibliographical note**
opostettu tuplat r=2454 ja r=3218<br/>Contribution: organisation=keb,FACT1=0.5<br/>Contribution: organisation=fys,FACT2=0.5<br/>Portfolio EDEND: 2013-10-29<br/>Publisher name: R S C Publications

Source: researchoutputwizard

Source-ID: 2999

Research output: Scientific - peer-review › Article

**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 (VSₐdd), 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/kgVSₐdd) were detected than in grass silage or maize assays (from 14.7 to 20.4 and from 7.4 to 12.1 μg/kgVSₐdd, 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. ©
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., Lemmetinen, H.
Number of pages: 9
Pages: 1540-1548
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Russian Chemical Bulletin
Volume: 62
Issue number: 7
ISSN (Print): 1066-5285
Ratings:
Scopus rating (2016): SJR 0.241 SNIP 0.45 CiteScore 0.6
Scopus rating (2015): SJR 0.251 SNIP 0.428 CiteScore 0.62
Charge transfer properties of a donor-acceptor dyad based on an expanded acridinium cation

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

Publication information
Journal: RSC Advances
Volume: 3
Issue number: 15
ISSN (Print): 2046-2069
Ratings:
Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
Original language: English
DOIs: 10.1039/c3ra22813d

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-04-29<br/>Publisher name: Springer New York LLC
Source: researchoutputwizard
Source-ID: 2177
Research output: Scientific - peer-review › Article

Charge transfer properties of a donor-acceptor dyad based on an expanded acridinium cation

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

Publication information
Journal: RSC Advances
Volume: 3
Issue number: 15
ISSN (Print): 2046-2069
Ratings:
Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
Original language: English
DOIs: 10.1039/c3ra22813d

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-10-29<br/>Publisher name: RSC Publishing
Source: researchoutputwizard
Source-ID: 1988
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:
Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
Original language: English
DOI:
10.1039/c3ra41741g

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

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:
Scopus rating (2016): CiteScore 2.74 SJR 1.133 SNIP 0.653
Scopus rating (2015): SJR 1.198 SNIP 0.758 CiteScore 2.88
Scopus rating (2014): SJR 1.181 SNIP 0.767 CiteScore 2.96
Scopus rating (2013): SJR 1.292 SNIP 0.796 CiteScore 2.96
Scopus rating (2012): SJR 1.471 SNIP 0.811 CiteScore 2.93
Scopus rating (2011): SJR 1.536 SNIP 0.857 CiteScore 3.2
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:
Scopus rating (2016): SJR 3.037 SNIP 1.468 CiteScore 8.46
Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
Original language: English
DOI: 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 › Article

Demonstrating the mechanism and efficacy of water-induced shape memory and the influence of water on the thermal properties of oriented poly(d,l-lactide)

General information
Determination of preferential molecular orientation in porphyrin-fullerene dyad ZnDHD6ee monolayers by the X-ray standing-wave method and X-ray reflectometry

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

Publication information
Journal: Journal of Applied Polymer Science
Volume: 130
Issue number: 6
ISSN (Print): 0021-8995
Ratings:
Scopus rating (2016): SJR 0.532 SNIP 0.724 CiteScore 1.73
Scopus rating (2015): SJR 0.574 SNIP 0.827 CiteScore 1.74
Scopus rating (2014): SJR 0.658 SNIP 0.964 CiteScore 1.76
Scopus rating (2013): SJR 0.628 SNIP 1.085 CiteScore 1.71
Scopus rating (2012): SJR 0.658 SNIP 1.081 CiteScore 1.57
Scopus rating (2011): SJR 0.601 SNIP 0.965 CiteScore 1.45
Scopus rating (2010): SJR 0.679 SNIP 0.909
Scopus rating (2009): SJR 0.697 SNIP 0.825
Scopus rating (2008): SJR 0.647 SNIP 0.822
Scopus rating (2007): SJR 0.678 SNIP 0.931
Scopus rating (2006): SJR 0.782 SNIP 1.145
Scopus rating (2005): SJR 0.779 SNIP 0.912
Scopus rating (2004): SJR 0.774 SNIP 0.962
Scopus rating (2003): SJR 0.816 SNIP 1.067
Scopus rating (2002): SJR 0.866 SNIP 1.084
Scopus rating (2001): SJR 0.964 SNIP 1.157
Scopus rating (2000): SJR 0.864 SNIP 1.157
Scopus rating (1999): SJR 0.978 SNIP 1.277
Original language: English
DOIs:
10.1002/app.39513

Bibliographical note
Contribution: organisation=keb,FACT1=0.5<br/>Contribution: organisation=elt,FACT2=0.5<br/>Portfolio EDEND: 2013-10-29<br/>Publisher name: John Wiley & Sons, Inc
Source: researchoutputwizard
Source-ID: 3071
Research output: Scientific - peer-review › Article

Determination of preferential molecular orientation in porphyrin-fullerene dyad ZnDHD6ee monolayers by the X-ray standing-wave method and X-ray reflectometry

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Research group: Supramolecular photochemistry, Frontier Photonics
Authors: Seregin, A., Dyakova, Y., Yakunin, S., Makhotkin, I., Alekseev, A., Klechkovskaya, V., Terechenko, E., Tkachenko, N., Lemmetyinen, H., Feigin, L., Kovalchuk, M.
Number of pages: 5
Pages: 934-938
Publication date: 2013
Peer-reviewed: Yes
Dipyrrolidinyl-substituted perylene diimide as additive for poly(3-hexylthiophene): [6,6]-Phenyl C61 butyric acid methyl ester bulk-heterojunction blends

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

Publication information
Journal: Thin Solid Films
Volume: 548
ISSN (Print): 0040-6090
Ratings:
Scopus rating (2016): CiteScore 1.83 SJR 0.64 SNIP 0.897
Scopus rating (2015): SJR 0.705 SNIP 0.98 CiteScore 1.84
Scopus rating (2014): SJR 0.73 SNIP 1.115 CiteScore 1.94
Scopus rating (2013): SJR 0.818 SNIP 1.215 CiteScore 2
Scopus rating (2012): SJR 0.899 SNIP 1.162 CiteScore 1.86
Direct evidence of significantly different chemical behavior and excited-state dynamics of 1,7- and 1,6-regioisomers of pyrrolidinyl-substituted perylene dilmide

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:
Scopus rating (2016): CiteScore 5.03 SJR 2.247 SNIP 1.046
Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Scopus rating (2014): SJR 2.487 SNIP 1.219 CiteScore 5.51
Scopus rating (2013): SJR 2.604 SNIP 1.239 CiteScore 5.68
Scopus rating (2012): SJR 2.884 SNIP 1.294 CiteScore 5.55
Scopus rating (2011): SJR 2.726 SNIP 1.336 CiteScore 5.46
Scopus rating (2010): SJR 2.527 SNIP 1.292
Scopus rating (2009): SJR 2.499 SNIP 1.365
Scopus rating (2008): SJR 2.887 SNIP 1.407
Scopus rating (2007): SJR 3.233 SNIP 1.532
Scopus rating (2006): SJR 2.911 SNIP 1.505
Scopus rating (2005): SJR 2.62 SNIP 1.454
Scopus rating (2004): SJR 2.32 SNIP 1.472
Scopus rating (2003): SJR 2.156 SNIP 1.45
Scopus rating (2002): SJR 2.554 SNIP 1.472
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:
Scopus rating (2016): SJR 0.726 SNIP 0.721 CiteScore 1.71
Scopus rating (2015): SJR 0.733 SNIP 0.747 CiteScore 1.83
Scopus rating (2014): SJR 0.757 SNIP 0.773 CiteScore 1.83
Scopus rating (2013): SJR 0.856 SNIP 0.844 CiteScore 2.07
Scopus rating (2012): SJR 1.101 SNIP 0.916 CiteScore 2.2
Scopus rating (2011): SJR 1.156 SNIP 1.013 CiteScore 2.38
Scopus rating (2010): SJR 1.207 SNIP 0.94
Scopus rating (2009): SJR 1.234 SNIP 0.972
Scopus rating (2008): SJR 1.296 SNIP 0.937
Scopus rating (2007): SJR 1.43 SNIP 1.001
Scopus rating (2006): SJR 1.483 SNIP 1.107
Scopus rating (2005): SJR 1.503 SNIP 1.086
Scopus rating (2004): SJR 1.512 SNIP 1.129
Scopus rating (2003): SJR 1.556 SNIP 1.156
Scopus rating (2002): SJR 1.694 SNIP 1.095
Scopus rating (2001): SJR 1.706 SNIP 1.102
Scopus rating (2000): SJR 1.774 SNIP 1.07
Scopus rating (1999): SJR 1.4 SNIP 1

Original language: English
DOIs: 10.1016/j.cplett.2013.04.035

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-10-29<br/>Publisher name: Elsevier
Source: researchoutputwizard
Source-ID: 1896
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:
Scopus rating (2016): SJR 1.774 SNIP 1.198 CiteScore 4.64
Scopus rating (2015): SJR 1.805 SNIP 1.239 CiteScore 4.7
Scopus rating (2014): SJR 1.869 SNIP 1.314 CiteScore 4.69
Scopus rating (2013): SJR 1.819 SNIP 1.379 CiteScore 4.9
Scopus rating (2012): SJR 2.08 SNIP 1.35 CiteScore 4.72
Scopus rating (2011): SJR 1.952 SNIP 1.373 CiteScore 4.64
Scopus rating (2010): SJR 1.98 SNIP 1.323
Scopus rating (2009): SJR 1.982 SNIP 1.47
Scopus rating (2008): SJR 2.025 SNIP 1.412
Scopus rating (2007): SJR 2.136 SNIP 1.544
Scopus rating (2006): SJR 1.828 SNIP 1.508
Scopus rating (2005): SJR 2.012 SNIP 1.46
Scopus rating (2004): SJR 1.672 SNIP 1.382
Scopus rating (2003): SJR 1.498 SNIP 1.465
Scopus rating (2002): SJR 1.616 SNIP 1.398
Scopus rating (2001): SJR 1.749 SNIP 1.511
Scopus rating (2000): SJR 1.667 SNIP 1.511
Scopus rating (1999): SJR 1.704 SNIP 1.497
Original language: English
DOIs:
10.1021/ic400474b

**Bibliographical note**
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-10-29<br/>Publisher name: American Chemical Society
Source: researchoutputwizard
Source-ID: 2088
Research output: Scientific - peer-review › Article

**Homoleptic Bis(aryl)acenaphthenequinonediimine-Cul 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
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-Laukkonen, 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:
Scopus rating (2016): SJR 1.348 SNIP 1.02 CiteScore 3.03
Scopus rating (2015): SJR 1.367 SNIP 1.096 CiteScore 3.25
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:
Scopus rating (2016): SJR 0.447 SNIP 0.482 CiteScore 1.23
Scopus rating (2015): SJR 0.454 SNIP 0.589 CiteScore 1.35
Scopus rating (2014): SJR 0.51 SNIP 0.727 CiteScore 1.69
Scopus rating (2013): SJR 0.523 SNIP 0.734 CiteScore 1.94
Scopus rating (2012): SJR 0.571 SNIP 0.679 CiteScore 1.66
Scopus rating (2011): SJR 0.52 SNIP 0.773 CiteScore 1.7
Scopus rating (2010): SJR 0.919 SNIP 1.148
Scopus rating (2009): SJR 0.752 SNIP 1.025
Scopus rating (2008): SJR 0.75 SNIP 0.719
Scopus rating (2007): SJR 0.637 SNIP 0.75
Scopus rating (2006): SJR 0.466 SNIP 0.532
Scopus rating (2005): SJR 0.542 SNIP 0.668
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:
Scopus rating (2016): SJR 0.732 SNIP 0.841 CiteScore 2.6
Scopus rating (2015): SJR 0.72 SNIP 0.86 CiteScore 2.47
Scopus rating (2014): SJR 0.782 SNIP 0.97 CiteScore 2.39
Scopus rating (2013): SJR 0.818 SNIP 1.006 CiteScore 2.5
Scopus rating (2012): SJR 0.919 SNIP 1.116 CiteScore 2.51
Scopus rating (2011): SJR 0.97 SNIP 1.342 CiteScore 2.84
Scopus rating (2010): SJR 1.021 SNIP 1.05
Scopus rating (2009): SJR 1.163 SNIP 1.191
Scopus rating (2008): SJR 1.04 SNIP 1.137
Scopus rating (2007): SJR 1.175 SNIP 1.364
Scopus rating (2006): SJR 0.996 SNIP 1.263
Scopus rating (2005): SJR 1.102 SNIP 1.436
Scopus rating (2004): SJR 0.952 SNIP 1.213
Scopus rating (2003): SJR 0.76 SNIP 0.987
Scopus rating (2002): SJR 0.646 SNIP 0.864
Scopus rating (2001): SJR 0.572 SNIP 0.934
Scopus rating (2000): SJR 0.782 SNIP 0.945
Scopus rating (1999): SJR 0.666 SNIP 1.047
Original language: English
DOIs:
10.1016/j.jphotochem.2012.08.005

Bibliographical note
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
Publication date: 2013
Peer-reviewed: Yes

Publication Information
Journal: Physical Chemistry Chemical Physics
Volume: 15
Issue number: 31
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
Scopus rating (2010): SJR 1.802 SNIP 1.196
Scopus rating (2009): SJR 2.127 SNIP 1.369
Scopus rating (2008): SJR 2.158 SNIP 1.211
Scopus rating (2007): SJR 1.84 SNIP 1.138
Scopus rating (2006): SJR 1.467 SNIP 1.128
Scopus rating (2005): SJR 1.389 SNIP 1.104
Scopus rating (2004): SJR 1.173 SNIP 1.007
Scopus rating (2003): SJR 1.093 SNIP 0.925
Scopus rating (2002): SJR 1.122 SNIP 0.973
Scopus rating (2001): SJR 1.09 SNIP 0.914
Scopus rating (2000): SJR 0.948 SNIP 1.068
Scopus rating (1999): SJR 0.121 SNIP 0
Original language: English
DOIs: 10.1039/c3cp50838b

Bibliographical note
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher: R S C Publications
Source: researchoutputwizard
Source-ID: 3093
Research output: Scientific - peer-review » Article

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)
Sequential photoinduced energy and electron transfer directed improved performance of the supramolecular solar cell of a zinc porphyrin - zinc phthalocyanine conjugate modified TiO2 surface
Short synthesis of the natural product 3β-hydroxy-labd-8(17)-en-15-oic acid via microbial transformation of labdanolic acid

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

Publication information
Journal: Phytochemistry Letters
Volume: 6
Issue number: 2
ISSN (Print): 1874-3900
Ratings:
Scopus rating (2016): SJR 0.543 SNIP 0.81 CiteScore 1.49
Scopus rating (2015): SJR 0.524 SNIP 0.852 CiteScore 1.51
Scopus rating (2014): SJR 0.592 SNIP 1.072 CiteScore 1.53
Scopus rating (2013): SJR 0.647 SNIP 1.014 CiteScore 1.57
Scopus rating (2012): SJR 0.545 SNIP 0.944 CiteScore 1.37
Scopus rating (2011): SJR 0.544 SNIP 0.776 CiteScore 1.42
Scopus rating (2010): SJR 0.468 SNIP 1.038
Scopus rating (2009): SJR 0.375 SNIP 0.87
Original language: English

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-06-29
Source: researchoutputwizard
Source-ID: 2147
Research output: Scientific - peer-review › Article

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

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Authors: Wondraczek, H., Kotiaho, A., Niemi, M., Fardim, P., Heinze, T.
Number of pages: 7
Study of structural order in porphyrin-fullerene dyad ZnDHD6ee monolayers by electron diffraction and atomic force microscopy

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

Publication information
Journal: Crystallography Reports
Volume: 58
Issue number: 6
ISSN (Print): 1063-7745
Ratings:
Scopus rating (2016): SJR 0.313 SNIP 0.644 CiteScore 0.55
Supramolecular assemblies of bay-substituted perylene diimides in solution and on a solid substrate

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

Publication information
Journal: Organic and Biomolecular Chemistry
Volume: 11
ISSN (Print): 1477-0520
Ratings:
Scopus rating (2016): SJR 1.363 SNIP 0.803 CiteScore 3.39
Scopus rating (2015): SJR 1.41 SNIP 0.858 CiteScore 3.47
Scopus rating (2014): SJR 1.387 SNIP 0.903 CiteScore 3.5
Scopus rating (2013): SJR 1.481 SNIP 0.897 CiteScore 3.55
Scopus rating (2012): SJR 1.635 SNIP 0.934 CiteScore 3.47
Scopus rating (2011): SJR 1.73 SNIP 0.974 CiteScore 3.71
Scopus rating (2010): SJR 1.775 SNIP 0.951
Scopus rating (2009): SJR 1.831 SNIP 1.073
Scopus rating (2008): SJR 1.936 SNIP 1.042
Scopus rating (2007): SJR 1.843 SNIP 0.984
Scopus rating (2006): SJR 1.557 SNIP 0.957
Scopus rating (2005): SJR 1.245 SNIP 1.098
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:
Scopus rating (2016): SJR 7.368 SNIP 2.584 CiteScore 13.18
Scopus rating (2015): SJR 6.826 SNIP 2.632 CiteScore 12.81
Scopus rating (2014): SJR 6.273 SNIP 2.578 CiteScore 11.92
Scopus rating (2013): SJR 5.953 SNIP 2.455 CiteScore 11.38
Scopus rating (2012): SJR 6.141 SNIP 2.379 CiteScore 10.37
Scopus rating (2011): SJR 5.447 SNIP 2.336 CiteScore 9.94
Scopus rating (2010): SJR 5.076 SNIP 2.132
Scopus rating (2009): SJR 4.883 SNIP 2.176
Scopus rating (2008): SJR 4.936 SNIP 2.116
Scopus rating (2007): SJR 5.023 SNIP 2.126
Scopus rating (2006): SJR 4.546 SNIP 2.22
Scopus rating (2005): SJR 4.284 SNIP 2.207
Scopus rating (2004): SJR 3.754 SNIP 2.178
Scopus rating (2003): SJR 3.267 SNIP 2.215
Scopus rating (2002): SJR 3.527 SNIP 2.346
Scopus rating (2001): SJR 3.449 SNIP 2.199
Scopus rating (2000): SJR 3.573 SNIP 2.224
Scopus rating (1999): SJR 3.56 SNIP 2.182
Original language: English
DOIs:
10.1021/ja4002376

Bibliographical note
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-06-29
Publisher name: American Chemical Society; ACS Publications
Source: researchoutputwizard
Source-ID: 1998
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:
Scopus rating (2016): SJR 2.385 SNIP 1.276 CiteScore 6.7
Scopus rating (2015): SJR 2.494 SNIP 1.411 CiteScore 7.33
Scopus rating (2014): SJR 2.863 SNIP 1.663 CiteScore 7.97
Scopus rating (2013): SJR 2.548 SNIP 1.452 CiteScore 6.79
Scopus rating (2012): SJR 3.046 SNIP 1.563 CiteScore 6.72
Scopus rating (2011): SJR 2.767 SNIP 1.504 CiteScore 5.53
Scopus rating (2010): SJR 1.945 SNIP 1.134
Scopus rating (2009): SJR 0.973 SNIP 0.72
Scopus rating (2008): SJR 0.291 SNIP 0.48
Scopus rating (2007): SJR 0.273 SNIP 0.495
Scopus rating (2006): SJR 0.243 SNIP 0.372
Scopus rating (2005): SJR 0.195 SNIP 0.285
Scopus rating (2004): SJR 0.214 SNIP 0.276
Scopus rating (2003): SJR 0.276 SNIP 0.419
Scopus rating (2002): SJR 0.312 SNIP 0.586
Scopus rating (2001): SJR 0.292 SNIP 0.496
Scopus rating (2000): SJR 0.422 SNIP 0.556
Scopus rating (1999): SJR 0.511 SNIP 0.708
Original language: English
DOIs:
10.1002/cssc.201200869

Bibliographical note
Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2013-11-29<br/>Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA
Source: researchoutputwizard
Source-ID: 2255
Research output: Scientific - peer-review › Article

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.
In this work, the intramolecular C-H insertion of diazoacetamides catalyzed by dirhodium(II) complexes and using CO2 as solvent is disclosed. The expected lactams were obtained in yields over 97%. The asymmetric intramolecular C-H insertion was also achieved and the beta-lactam 14 was obtained in > 97% yield and 65% ee using the chiral dirhodium(II) catalyst Rh-2(S-PTTL)(4). Finally, the dirhodium(II) complex Rh-2(OAc)(4) was used in two consecutive cycles in which complete conversion to the lactam was observed.
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.
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.
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.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: Tan, B., Candeias, N. R., Barbas, C. F.
Number of pages: 4
Pages: 4672-4675
Publication date: 6 Apr 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of the American Chemical Society
Volume: 133
Issue number: 13
ISSN (Print): 0002-7863
Ratings:
Scopus rating (2016): SJR 7.368 SNIP 2.584 CiteScore 13.18
Scopus rating (2015): SJR 6.826 SNIP 2.632 CiteScore 12.81
Scopus rating (2014): SJR 6.273 SNIP 2.578 CiteScore 11.92
Scopus rating (2013): SJR 5.953 SNIP 2.455 CiteScore 11.38
Scopus rating (2012): SJR 6.141 SNIP 2.379 CiteScore 10.37
Scopus rating (2011): SJR 5.447 SNIP 2.336 CiteScore 9.94
Scopus rating (2010): SJR 5.076 SNIP 2.132
Scopus rating (2009): SJR 4.883 SNIP 2.176
Scopus rating (2008): SJR 4.936 SNIP 2.116
Scopus rating (2007): SJR 5.023 SNIP 2.126
Scopus rating (2006): SJR 4.546 SNIP 2.22
Scopus rating (2005): SJR 4.284 SNIP 2.207
Scopus rating (2004): SJR 3.754 SNIP 2.178
Scopus rating (2003): SJR 3.267 SNIP 2.215
Scopus rating (2002): SJR 3.527 SNIP 2.346
Scopus rating (2001): SJR 3.449 SNIP 2.199
Scopus rating (2000): SJR 3.573 SNIP 2.224
Scopus rating (1999): SJR 3.56 SNIP 2.182
Original language: English
Keywords: ASYMMETRIC ASSEMBLY REACTIONS, MODIFIED ALLYLIC COMPOUNDS, PHOSPHORUS YLIDE REACTION, MICHAEL-HENRY REACTIONS, BAYLIS-HILLMAN REACTION, DIELS-ALDER REACTIONS, ANNULATION REACTION, DOMINO REACTIONS, 4 STEREOCENTERS, MULTISUBSTITUTED CYCLOPENTANES
DOIs:
10.1021/ja110147w
Source: WOS
Source-ID: 000289492700004
Research output: Scientific - peer-review › Article

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

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: Candeias, N. R., Montalbano, F., Cal, P. M. S. D., Gois, P. M. P.
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:
Scopus rating (2016): SJR 19.282 SNIP 10.369 CiteScore 42.79
Scopus rating (2015): SJR 18.373 SNIP 11.51 CiteScore 45.92
Scopus rating (2014): SJR 18.369 SNIP 11.47 CiteScore 44.56
Scopus rating (2013): SJR 22.176 SNIP 12.915 CiteScore 49.12
Scopus rating (2012): SJR 20.511 SNIP 11.43 CiteScore 39.08
NHC-Iron-Catalyzed Aerobic Oxidative Aromatic Esterification of Aldehydes using Boronic Acids

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

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Lisbon, Universidade de Lisboa, Fac Farm, iMed UL
Authors: Rosa, J. N., Reddy, R. S., Candeias, N. R., Cal, P. M. S. D., Gois, P. M. P.
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:
Scopus rating (2016): SJR 2.964 SNIP 1.218 CiteScore 6.32
Scopus rating (2015): SJR 3.055 SNIP 1.336 CiteScore 6.38
Scopus rating (2014): SJR 2.958 SNIP 1.324 CiteScore 6.18
Scopus rating (2013): SJR 3.144 SNIP 1.329 CiteScore 6.12
Scopus rating (2012): SJR 3.312 SNIP 1.355 CiteScore 5.7
Scopus rating (2011): SJR 3.271 SNIP 1.377 CiteScore 5.81
Scopus rating (2010): SJR 2.985 SNIP 1.307
Scopus rating (2009): SJR 3.048 SNIP 1.37
Scopus rating (2008): SJR 3.263 SNIP 1.295
Scopus rating (2007): SJR 3.185 SNIP 1.296
Scopus rating (2006): SJR 2.936 SNIP 1.352
Scopus rating (2005): SJR 2.552 SNIP 1.329
Scopus rating (2004): SJR 2.515 SNIP 1.262
Scopus rating (2003): SJR 2.451 SNIP 1.325
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
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.
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:
Scopus rating (2016): SJR 0.843 SNIP 0.846 CiteScore 2.52
Scopus rating (2015): SJR 0.932 SNIP 0.884 CiteScore 2.55
Scopus rating (2014): SJR 0.94 SNIP 0.89 CiteScore 2.43
Scopus rating (2013): SJR 0.931 SNIP 0.911 CiteScore 2.47
Scopus rating (2012): SJR 1.087 SNIP 0.936 CiteScore 2.49
Scopus rating (2011): SJR 1.127 SNIP 0.991 CiteScore 2.7
Scopus rating (2010): SJR 1.065 SNIP 0.987
Scopus rating (2009): SJR 1.114 SNIP 1.022
Scopus rating (2008): SJR 1.111 SNIP 0.984
Scopus rating (2007): SJR 1.111 SNIP 0.962
Scopus rating (2006): SJR 0.971 SNIP 0.955
Scopus rating (2005): SJR 0.961 SNIP 0.81
Scopus rating (2004): SJR 0.921 SNIP 0.952
Scopus rating (2003): SJR 0.849 SNIP 0.845
Scopus rating (2002): SJR 0.876 SNIP 0.832
Scopus rating (2001): SJR 0.808 SNIP 0.728
Scopus rating (2000): SJR 0.924 SNIP 0.677
Scopus rating (1999): SJR 0.875 SNIP 0.691
Original language: English
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
DOIs:
10.1016/j.bmcl.2010.04.002
Dimeric Quinidine-Catalyzed Enantioselective Aminooxygenation of Oxindoles: An Organocatalytic Approach to 3-Hydroxyoxindole Derivatives

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

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Authors: Bui, T., Candeias, N. R., Barbas, C. F.
Number of pages: 2
Pages: 5574-5575
Publication date: 28 Apr 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of the American Chemical Society
Volume: 132
Issue number: 16
ISSN (Print): 0002-7863
Ratings:
Scopus rating (2016): SJR 7.368 SNIP 2.584 CiteScore 13.18
Scopus rating (2015): SJR 6.826 SNIP 2.632 CiteScore 12.81
Scopus rating (2014): SJR 6.273 SNIP 2.578 CiteScore 11.92
Scopus rating (2013): SJR 5.953 SNIP 2.455 CiteScore 11.38
Scopus rating (2012): SJR 6.141 SNIP 2.379 CiteScore 10.37
Scopus rating (2011): SJR 5.447 SNIP 2.336 CiteScore 9.94
Scopus rating (2010): SJR 5.076 SNIP 2.132
Scopus rating (2009): SJR 4.883 SNIP 2.176
Scopus rating (2008): SJR 4.936 SNIP 2.116
Scopus rating (2007): SJR 5.023 SNIP 2.126
Scopus rating (2006): SJR 4.546 SNIP 2.22
Scopus rating (2005): SJR 4.284 SNIP 2.207
Scopus rating (2004): SJR 3.754 SNIP 2.178
Scopus rating (2003): SJR 3.267 SNIP 2.215
Scopus rating (2002): SJR 3.527 SNIP 2.346
Scopus rating (2001): SJR 3.449 SNIP 2.199
Scopus rating (2000): SJR 3.573 SNIP 2.224
Scopus rating (1999): SJR 3.56 SNIP 2.182
Original language: English
Keywords: ASYMMETRIC ADDITION, ARYLBORONIC ACIDS, ISATINS, HYDROXYLATION, NITROALKENES, 2-OXINDOLES, ALKALOIDS, ACCESS
DOI: 10.1021/ja101032j
Source: WOS
Source-ID: 000277788900047
Research output: Scientific - peer-review » Article

Water as the reaction medium for multicomponent reactions based on boronic acids
Water is a suitable medium for the Petasis-borono-Mannich multicomponent reaction Salicylaldehyde, glyoxalic acid, glycoaldehyde and glyoxal were reacted with several boronic acids and different amines affording alkylaminophenols, 2H-
chromenes, alpha-amino acids, alpha-amino alcohols and 2-hydroxylmorpholines 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.
Number of pages: 10
Pages: 2736-2745
Publication date: 3 Apr 2010
Peer-reviewed: Yes

Publication information
Journal: Tetrahedron
Volume: 66
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ISSN (Print): 0040-4020
Ratings:
Scopus rating (2016): SJR 0.907 SNIP 0.742 CiteScore 2.54
Scopus rating (2015): SJR 0.954 SNIP 0.84 CiteScore 2.72
Scopus rating (2014): SJR 0.971 SNIP 0.905 CiteScore 2.79
Scopus rating (2013): SJR 1.101 SNIP 0.92 CiteScore 2.85
Scopus rating (2012): SJR 1.32 SNIP 0.999 CiteScore 2.89
Scopus rating (2011): SJR 1.476 SNIP 1.094 CiteScore 3.22
Scopus rating (2010): SJR 1.508 SNIP 1.065
Scopus rating (2009): SJR 1.534 SNIP 1.124
Scopus rating (2008): SJR 1.579 SNIP 1.078
Scopus rating (2007): SJR 1.639 SNIP 1.116
Scopus rating (2006): SJR 1.507 SNIP 1.142
Scopus rating (2005): SJR 1.354 SNIP 1.138
Scopus rating (2004): SJR 1.459 SNIP 1.261
Scopus rating (2003): SJR 1.448 SNIP 1.265
Scopus rating (2002): SJR 1.677 SNIP 1.177
Scopus rating (2001): SJR 1.46 SNIP 1.178
Scopus rating (2000): SJR 1.536 SNIP 1.165
Scopus rating (1999): SJR 1.37 SNIP 1.172
Original language: English
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
DOIs: 10.1016/j.tet.2010.01.084
Source: WOS
Source-ID: 000276371000026
Research output: Scientific - peer-review › Article

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
Cyclization of Diazoacetamides Catalyzed by N-Heterocyclic Carbene Dirhodium(II) Complexes

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

**General information**

State: Published

Ministry of Education publication type: A1 Journal article-refereed


Authors: Candeias, N. R., Branco, L. C., Gois, P. M. P., Afonso, C. A. M., Trindade, A. F.

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:

Scopus rating (2016): SJR 19.282 SNIP 10.369 CiteScore 42.79
Scopus rating (2015): SJR 18.373 SNIP 11.51 CiteScore 45.92
Scopus rating (2014): SJR 18.369 SNIP 11.47 CiteScore 44.56
Scopus rating (2013): SJR 22.176 SNIP 12.915 CiteScore 49.12
Scopus rating (2012): SJR 20.511 SNIP 11.43 CiteScore 39.08
Scopus rating (2011): SJR 19.538 SNIP 11.534 CiteScore 39.19
Scopus rating (2010): SJR 18.393 SNIP 11.114
Scopus rating (2008): SJR 16.038 SNIP 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.

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Tecn Lisboa, Instituto Superior Tecnico, Universidade de Lisboa, Inst Nanosci & Nanotechnol, Ctr Quim Fis Mol & IN, Inst Super Tecn
Authors: Candeias, N. R., Afonso, C. A. M.
Number of pages: 25
Pages: 763-787
Publication date: May 2009
Peer-reviewed: Yes
Water: A Suitable Medium for the Petasis Borono-Mannich Reaction

Water was used as the solvent in the Petasis borono-Mannich reaction. With the use of salicylaldehyde, secondary amines and boronic acids, several alkylaminophenols were obtained in considerably high yields in water. By using the same methodology, 2H-chromenes were prepared with the use of vinyl boronic acids. The reaction mechanism was studied by DFT calculations, and the results obtained corroborate the solvent effect experimentally observed. (© Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, Germany, 2009)

General information

State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Lisbon, Universidade de Lisboa, Fac Farm, iMed UL, Univ Tecn Lisboa, Instituto Superior Tecnico, Universidade de Lisboa, Inst Nanosci & Nanotechnol, Ctr Quim Fis Mol & IN, Inst Super Tecn, Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, Dept Engn Quim & Biol, Ctr Quim Estrutural
Authors: Candeias, N. R., Veiros, L. F., Afonso, C. A. M., Gois, P. M. P.
Number of pages: 5
Pages: 1859-1863
Publication date: Apr 2009
Peer-reviewed: Yes

Electronic versions:
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DOIs:
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Source: WOS
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Research output: Scientific - peer-review » Literature review

Publication information
Issue number: 12
ISSN (Print): 1434-193X
Ratings:
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Scopus rating (2015): SJR 1.198 SNIP 0.758 CiteScore 2.88
Scopus rating (2014): SJR 1.181 SNIP 0.767 CiteScore 2.96
Scopus rating (2013): SJR 1.292 SNIP 0.796 CiteScore 2.96
Scopus rating (2012): SJR 1.471 SNIP 0.811 CiteScore 2.93
Scopus rating (2011): SJR 1.536 SNIP 0.857 CiteScore 3.2
Scopus rating (2010): SJR 1.572 SNIP 0.785
Scopus rating (2009): SJR 1.497 SNIP 0.778
Scopus rating (2008): SJR 1.652 SNIP 0.759
Scopus rating (2007): SJR 1.711 SNIP 0.84
Scopus rating (2006): SJR 1.505 SNIP 0.849
Scopus rating (2005): SJR 1.246 SNIP 0.763
Scopus rating (2004): SJR 1.2 SNIP 0.81
Scopus rating (2003): SJR 1.19 SNIP 0.802
Scopus rating (2002): SJR 1.382 SNIP 0.829
Scopus rating (2001): SJR 1.159 SNIP 0.816
Scopus rating (2000): SJR 1.192 SNIP 1.048
Intramolecular C-H insertion using NHC-di-rhodium(II) complexes the influence of axial coordination

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.

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, Inst Nanosci & Nanotechnol, CQFM
Authors: Gomes, L. F. R., Trindade, A. F., Candeias, N. R., Gois, P. M. P., Afonso, C. A. M.
Number of pages: 4
Pages: 7372-7375
Publication date: 22 Dec 2008
Peer-reviewed: Yes

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Journal: Tetrahedron Letters
Volume: 49
Issue number: 52
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Scopus rating (2016): SJR 0.754 SNIP 0.635 CiteScore 2.13
Scopus rating (2015): SJR 0.757 SNIP 0.747 CiteScore 2.3
Scopus rating (2014): SJR 0.794 SNIP 0.796 CiteScore 2.41
Scopus rating (2013): SJR 0.904 SNIP 0.802 CiteScore 2.4
Scopus rating (2012): SJR 1.084 SNIP 0.844 CiteScore 2.45
Scopus rating (2011): SJR 1.216 SNIP 0.949 CiteScore 2.76
Scopus rating (2010): SJR 1.232 SNIP 0.916
Scopus rating (2009): SJR 1.289 SNIP 0.937
Scopus rating (2008): SJR 1.325 SNIP 0.881
Scopus rating (2007): SJR 1.443 SNIP 0.956
Scopus rating (2006): SJR 1.301 SNIP 0.925
Scopus rating (2005): SJR 1.243 SNIP 0.949
Scopus rating (2004): SJR 1.294 SNIP 0.963
Scopus rating (2003): SJR 1.28 SNIP 0.994
Scopus rating (2002): SJR 1.684 SNIP 1.025
Scopus rating (2001): SJR 1.477 SNIP 1.009
Scopus rating (2000): SJR 1.621 SNIP 1.007
Scopus rating (1999): SJR 1.5 SNIP 1.015

Original language: English
Keywords: C-H insertion, Di-rhodium(II) complexes, N-heterocyclic carbenes (NHC), Axial coordination, Decarbonylation, CHIRAL LEWIS-ACID, DIRHODIUM(II,III) CAPROLACTAMATE, CATALYSIS, AMINATION, STEREOCONTROL, ALDEHYDES
DOIs:
10.1016/j.tetlet.2008.10.054
Source: WOS
C-H carbene insertion of alpha-diazo acetamides by photolysis in non-conventional media

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

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Tecn Lisboa, Instituto Superior Tecnico, Universidade de Lisboa, Inst Nanosci & Nanotechnol, Ctr Quim Fis Mol & IN, Inst Super Tecn, Inst Superior Tecnico, Universidade de Lisboa, Dept Engn Quim & Biol, Ctr Quim Estrutural, Univ Lisbon, Universidade de Lisboa, Fac Farm, iMed UL
Authors: Candeias, N. R., Gois, P. M. P., Veiros, L. F., Afonso, C. A. M.
Number of pages: 7
Pages: 5926-5932
Publication date: 1 Aug 2008
Peer-reviewed: Yes

Publication information
Journal: Journal of Organic Chemistry
Volume: 73
Issue number: 15
ISSN (Print): 0022-3263
Ratings:
Scopus rating (2016): CiteScore 4.59 SJR 1.976 SNIP 1.03
Scopus rating (2015): SJR 2.018 SNIP 1.174 CiteScore 4.69
Scopus rating (2014): SJR 2.003 SNIP 1.222 CiteScore 4.69
Scopus rating (2013): SJR 2.078 SNIP 1.176 CiteScore 4.51
Scopus rating (2012): SJR 2.272 SNIP 1.23 CiteScore 4.31
Scopus rating (2011): SJR 2.27 SNIP 1.261 CiteScore 4.43
Scopus rating (2010): SJR 2.112 SNIP 1.173
Scopus rating (2009): SJR 2.186 SNIP 1.254
Scopus rating (2008): SJR 2.309 SNIP 1.208
Scopus rating (2007): SJR 2.37 SNIP 1.309
Scopus rating (2006): SJR 2.222 SNIP 1.31
Scopus rating (2005): SJR 1.995 SNIP 1.3
Scopus rating (2004): SJR 1.945 SNIP 1.315
Scopus rating (2003): SJR 1.865 SNIP 1.355
Scopus rating (2002): SJR 2.319 SNIP 1.441
Scopus rating (2001): SJR 2.064 SNIP 1.406
Scopus rating (2000): SJR 2.172 SNIP 1.403
Scopus rating (1999): SJR 2.013 SNIP 1.402
Original language: English
Keywords: CARBON-HYDROGEN INSERTION, ORGANIC-REACTIONS, AQUEOUS-MEDIA, WOLFF REARRANGEMENT, DIAZOCARBONYL COMPOUNDS, WATER, DECOMPOSITION, ESTERS, DIAZOAETAMIDES, STEROEOCHEMISTRY
DOI: 10.1021/jo800980c
Source: WOS
Source-ID: 000257953600027
Research output: Scientific - peer-review › Article

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.
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.
Rh(II)-catalyzed intramolecular C-H insertion of diazo substrates in water: Scope and limitations

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

General information

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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, CQFM
Authors: Candeias, N. R., Gois, P. M. P., Afonso, C. A. M.
Number of pages: 9
Pages: 5489-5497
Publication date: 21 Jul 2006
Peer-reviewed: Yes

Publication information

Journal: Journal of Organic Chemistry
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Ratings:

Scopus rating (2016): CiteScore 4.59 SJR 1.976 SNIP 1.03
Scopus rating (2015): SJR 2.018 SNIP 1.174 CiteScore 4.69
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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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Universidade de Lisboa
Authors: Candeias, N., Afonso, C.
Number of pages: 23
Pages: 195-217
Publication date: 1 Dec 2005
Peer-reviewed: Yes

Publication information
Journal: Journal of Molecular Catalysis A: Chemical
Volume: 242
Issue number: 1-2
ISSN (Print): 1381-1169
Ratings:
Scopus rating (2016): SJR 1.006 SNIP 1.095 CiteScore 3.96
Scopus rating (2015): SJR 1.052 SNIP 1.262 CiteScore 3.93
Scopus rating (2014): SJR 1.092 SNIP 1.431 CiteScore 3.93
Scopus rating (2013): SJR 1.155 SNIP 1.315 CiteScore 3.56
Scopus rating (2012): SJR 1.257 SNIP 1.363 CiteScore 3.25
Scopus rating (2011): SJR 1.242 SNIP 1.252 CiteScore 3.14
Scopus rating (2010): SJR 1.248 SNIP 1.342
Scopus rating (2009): SJR 1.321 SNIP 1.425
Scopus rating (2008): SJR 1.259 SNIP 1.232
Scopus rating (2007): SJR 1.316 SNIP 1.206
Preparation of enantioselective enriched alpha-(dialkoxyphosphoryl) lactams via intramolecular C-H insertion with chiral dirhodium(II) catalysts

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

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Nova Lisboa, Universidade Nova de Lisboa, REQUIMTE, Dept Quim, Fac Ciencias & Tecnol
Authors: Gois, P. M. P., Candeias, N. R., Afonso, C. A. M.
Number of pages: 8
Pages: 17-24
Publication date: 1 Mar 2005
Peer-reviewed: Yes

Publication information
Journal: Journal of Molecular Catalysis A: Chemical
Volume: 227
Issue number: 1-2
ISSN (Print): 1381-1169
Ratings:
Scopus rating (2016): SJR 1.006 SNIP 1.095 CiteScore 3.96
Scopus rating (2015): SJR 1.052 SNIP 1.262 CiteScore 3.93
Scopus rating (2014): SJR 1.092 SNIP 1.431 CiteScore 3.93
Scopus rating (2013): SJR 1.155 SNIP 1.315 CiteScore 3.56
Scopus rating (2012): SJR 1.257 SNIP 1.363 CiteScore 3.25
Scopus rating (2011): SJR 1.242 SNIP 1.252 CiteScore 3.14
Scopus rating (2010): SJR 1.248 SNIP 1.342
Scopus rating (2009): SJR 1.321 SNIP 1.425
Scopus rating (2008): SJR 1.259 SNIP 1.232
Scopus rating (2007): SJR 1.316 SNIP 1.206
Scopus rating (2006): SJR 1.118 SNIP 1.076
Scopus rating (2005): SJR 1.269 SNIP 1.117
Scopus rating (2004): SJR 1.125 SNIP 1.291
Scopus rating (2003): SJR 1.061 SNIP 1.236
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 mug/ml; piperacillin, 0.0025-25 mug/ml; imipenem, 0.0025-0.25 mug/ml; cephalirin, 0.025-2.5 mug/ml; cefoxitin, 0.0025-1.5 mug/ml; and oxacillin, 25-500 mug/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.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Univ Turku, University of Turku, Dept Biotechnol, Innotrac Diagnost Oy
Authors: Valtonen, S. J., Kurittu, J. S., Karp, M. T.
Number of pages: 8
Pages: 127-134
Publication date: Apr 2002
Peer-reviewed: Yes

Publication information
Journal: Journal of Biomolecular Screening
Volume: 7
Issue number: 2
ISSN (Print): 1087-0571
Ratings:
Scopus rating (2016): SJR 1.312 SNIP 0.681 CiteScore 2.48
Scopus rating (2015): SJR 1.075 SNIP 0.653 CiteScore 2.22
Scopus rating (2014): SJR 1.146 SNIP 0.65 CiteScore 2.22
Scopus rating (2013): SJR 0.966 SNIP 0.661 CiteScore 1.97
Scopus rating (2012): SJR 0.941 SNIP 0.706 CiteScore 2.06
Scopus rating (2011): SJR 0.962 SNIP 0.644 CiteScore 2.11
Scopus rating (2010): SJR 0.998 SNIP 0.676
Scopus rating (2009): SJR 1.058 SNIP 0.728
Scopus rating (2008): SJR 0.984 SNIP 0.653
Scopus rating (2007): SJR 0.988 SNIP 0.725
Scopus rating (2006): SJR 1.122 SNIP 0.881
Scopus rating (2005): SJR 0.972 SNIP 0.899
Scopus rating (2004): SJR 0.883 SNIP 0.694
Scopus rating (2003): SJR 0.788 SNIP 0.901
Scopus rating (2002): SJR 0.762 SNIP 0.891
Scopus rating (2001): SJR 0.5 SNIP 0.897
Scopus rating (2000): SJR 0.699 SNIP 0.779
Scopus rating (1999): SJR 0.862 SNIP 0.731
Original language: English
Keywords: MICROBIAL BIOSENSORS, GENE-EXPRESSION, INDUCTION, BACTERIA, BIOLUMINESCEENCE, ARSENITE, SENSOR, ASSAY, MILK, ANTIBIOTICS
Source: WOS
Source-ID: 000175404800004
Research output: Scientific - peer-review › Article
Comparison of the total mercury content in sediment samples with a mercury sensor bacteria test and Vibrio fischeri toxicity test

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

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: University of Turku
Authors: Lappalainen, J. O., Karp, M. T., Juvonen, R., Virta, M. P. J., Nurmi, J.
Number of pages: 6
Pages: 443-448
Publication date: Dec 2000
Peer-reviewed: Yes

Publication Information
Journal: Environmental Toxicology
Volume: 15
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ISSN (Print): 1520-4081
Ratings:
Scopus rating (2016): SJR 0.688 SNIP 0.829 CiteScore 2.2
Scopus rating (2015): SJR 0.804 SNIP 0.848 CiteScore 2.26
Scopus rating (2014): SJR 0.748 SNIP 0.98 CiteScore 2.16
Scopus rating (2013): SJR 0.767 SNIP 0.897 CiteScore 1.97
Scopus rating (2012): SJR 0.828 SNIP 0.94 CiteScore 2.16
Scopus rating (2011): SJR 0.765 SNIP 0.807 CiteScore 1.98
Scopus rating (2010): SJR 0.762 SNIP 0.795
Scopus rating (2009): SJR 0.683 SNIP 0.868
Scopus rating (2008): SJR 0.784 SNIP 1.021
Scopus rating (2007): SJR 0.766 SNIP 0.963
Scopus rating (2006): SJR 0.847 SNIP 0.837
Scopus rating (2005): SJR 0.574 SNIP 0.722
Scopus rating (2004): SJR 0.584 SNIP 0.836
Scopus rating (2003): SJR 0.612 SNIP 0.783
Scopus rating (2002): SJR 0.638 SNIP 0.772
Scopus rating (2001): SJR 0.564 SNIP 0.764
Scopus rating (2000): SJR 0.619 SNIP 1.135
Scopus rating (1999): SJR 0.658 SNIP 0.823
Original language: English
Keywords: heavy metal, biosensor, mercury, sediment, REPORTER, ARSENITE, ENVIRONMENT, ANTIMONITE, BIOSENSOR, STRAIN
DOIs:
Source: WOS
Source-ID: 000165446600012
Research output: Scientific - peer-review > Article

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

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

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Simultaneous extraction and combined bioluminescent assay of oxidized and reduced nicotinamide adenine dinucleotide
Bioluminescent assay of lactate dehydrogenase and its isoenzyme-1 activity

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

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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%.

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

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