

Mixed carbon substrates: a necessary nuisance or a missed opportunity?

Although fermentation with single carbon sources is the preferred mode of operation in current industrial biotechnology, the use of multiple substrates has been continuously investigated throughout the years. Generally, microbial metabolism varies significantly when cells are presented with mixed carbon substrates compared to a single carbon-energy source, as different nutrients interact in complex ways within the metabolic network. By exploiting these distinct modes of interaction, researchers have identified unique opportunities to optimize metabolism using mixed carbon sources. Here we review situations where process yield and productivity are markedly improved through the judicious introduction of substrate mixtures. Our goal is to illustrate that with proper design of the choice of substrates and the way they are introduced to cultures, metabolic optimization with mixed substrates can be a unique strategy that complements genetic engineering techniques to enhance cell performance beyond what is accomplished in single substrate fermentations.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Materials Science and Environmental Engineering, Massachusetts Institute of Technology, Department of Chemical Engineering

Contributors: Liu, N., Santala, S., Stephanopoulos, G.

Number of pages: 7

Pages: 15-21

Publication date: 1 Apr 2020

Peer-reviewed: Yes

Publication information

Journal: CURRENT OPINION IN BIOTECHNOLOGY

Volume: 62

ISSN (Print): 0958-1669

Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering, Biomedical Engineering

DOIs:

10.1016/j.copbio.2019.07.003

Source: Scopus

Source ID: 85071874245

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Aisala, H., Manninen, H., Laaksonen, T., Linderborg, K. M., Myoda, T., Hopia, A., Sandell, M.

Publication date: 30 Jan 2020

Peer-reviewed: Yes

Publication information

Journal: Food Chemistry

Volume: 304

Article number: 125403

ISSN (Print): 0308-8146

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Food Science

Keywords: External preference mapping, Hedonic testing, Mushrooms, NMR, PLS

DOIs:

10.1016/j.foodchem.2019.125403

Source: Scopus

Source ID: 85071453617

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

Power production and microbial community composition in thermophilic acetate-fed up-flow and flow-through microbial fuel cells

The microbial communities developed from a mixed-species culture in up-flow and flow-through configurations of thermophilic (55 °C) microbial fuel cells (MFCs), and their power production from acetate, were investigated. The up-flow MFC was operated for 202 days, obtaining an average power density of 0.13 W/m³, and *Tepidiphilus* was the dominant transcriptionally-active microorganisms. The planktonic community developed in the up-flow MFC was used to inoculate a flow-through MFC resulting in the proliferation of *Ureibacillus*, whose relative abundance increased from 1 to 61% after 45 days. Despite the differences between the up-flow and flow-through MFCs, including the anode electrode, hydrodynamic conditions, and the predominant microorganism, similar ($p = 0.05$) volumetric power (0.11–0.13 W/m³), coulombic efficiency (16–18%) and acetate consumption rates (55–69 mg/L/d) were obtained from both. This suggests that though MFC design can shape the active component of the thermophilic microbial community, the consortia are resilient and can maintain similar performance in different MFC configurations.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Dessi, P., Chatterjee, P., Mills, S., Kokko, M., Lakaniemi, A., Collins, G., Lens, P. N.

Publication date: 1 Dec 2019

Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 294

Article number: 122115

ISSN (Print): 0960-8524

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Renewable Energy, Sustainability and the Environment, Waste Management and Disposal

Keywords: Attached community, Bioelectrochemical system, Electrogenic microorganisms, MFC, Microbial electrochemical technology, Planktonic community

DOIs:

10.1016/j.biortech.2019.122115

Source: Scopus

Source ID: 85072279751

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

Programmable responsive hydrogels inspired by classical conditioning algorithm

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Publication date: 1 Dec 2019

Peer-reviewed: Yes

Publication information

Journal: Nature Communications

Volume: 10

Issue number: 1
Article number: 3267
ISSN (Print): 2041-1723
Original language: English
ASJC Scopus subject areas: Chemistry(all), Biochemistry, Genetics and Molecular Biology(all), Physics and Astronomy(all)
Electronic versions:
s41467-019-11260-3
DOIs:
10.1038/s41467-019-11260-3
URLs:
<http://urn.fi/URN:NBN:fi:tty-201909092080>
Source: Scopus
Source ID: 85070331406
Research output: Contribution to journal › Article › Scientific › peer-review

Anaerobic treatment of LCFA-containing synthetic dairy wastewater at 20°C: Process performance and microbial community dynamics

Facilitating anaerobic degradation of long-chain fatty acids (LCFA) is key for tapping the high methane production potential of the fats, oil and grease (FOG) content of dairy wastewaters. In this study, the feasibility of using high-rate granular sludge reactors for the treatment of mixed LCFA-containing synthetic dairy wastewater (SDW) was assessed at 20 °C. The effects of the LCFA concentration (33–45% of COD) and organic loading rates (2–3 gCOD/L·d) were determined using three parallel expanded granular sludge bed reactors. For the first time, long term anaerobic treatment of LCFA-containing feed at 20 °C was shown to be feasible and was linked to the microbial community dynamics in high-rate reactors. During a two-month operation, a soluble COD removal of 84–91% and COD to methane conversion of 44–51% was obtained. However, granular sludge flotation and washout occurred after two months in all reactors without volatile fatty acids (VFA) accumulation, emphasizing the need for sludge retention for long-term granular sludge reactor operation with LCFA-containing feed at low ambient temperatures. The temporal shifts in microbial community structure were studied in the high-rate treatment of SDW, and the process disturbances (elevated LCFA loading, LCFA accumulation, and batch operation) were found to decrease the microbial community diversity. The relative abundance of Methanosaeta increased with higher LCFA accumulation in the settled and flotation layer granules in the three reactors, therefore, acetoclastic methanogenesis was found to be crucial for the high-rate treatment of SDW at 20 °C. This study provides an initial understanding of the continuous anaerobic treatment of LCFA-containing industrial wastewaters at low ambient temperatures.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Tampere Water, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education, Natl. University of Ireland, Galway
Contributors: Singh, S., Rinta-Kanto, J. M., Kettunen, R., Tolvanen, H., Lens, P., Collins, G., Kokko, M., Rintala, J.
Number of pages: 9
Pages: 960-968
Publication date: 15 Nov 2019
Peer-reviewed: Yes

Publication information

Journal: Science of the Total Environment
Volume: 691
ISSN (Print): 0048-9697
Original language: English
ASJC Scopus subject areas: Environmental Engineering, Environmental Chemistry, Waste Management and Disposal, Pollution
Keywords: Dairy wastewater, Expanded granular sludge bed (EGSB), Granule disintegration, Long chain fatty acids (LCFA), Methanogenesis pathway, Microbial community dynamics
DOIs:
10.1016/j.scitotenv.2019.07.136
Source: Scopus
Source ID: 85069487981
Research output: Contribution to journal › Article › Scientific › peer-review

Miniature CoCr laser welds under cyclic shear: Fatigue evolution and crack growth

Miniature laser welds with the root depth in the range of 50–300 µm represent air-tight joints between the components in medical devices, such as those in implants, growth rods, stents and various prostheses. The current work focuses on the development of a fatigue test specimen and procedure to determine fatigue lives of shear-loaded laser welds. A cobalt-

chromium (CoCr) alloy is used as a benchmark case. S–N graphs, damage process, and fracture surfaces are studied by applying x-ray analysis, atomic force microscopy, and scanning electron microscopy both before and after the crack onset. A non-linear material model is fitted for the CoCr alloy to run finite element simulations of the damage and deformation. As a result, two tensile-loaded specimen designs are established and the performance is compared to that of a traditional torque-loaded specimen. The new generation specimens show less variation in the determined fatigue lives due to well-defined crack onset point and, therefore, precise weld seam load during the experiments. The fatigue damage concentrates to the welded material and the entire weld experiences fatigue prior to the final, fracture-governed failure phase. For the studied weld seams of hardened CoCr, a regression fatigue limit of 10.8–11.8 MPa, where the stress refers to the arithmetic average shear stress computed along the region dominated by shear loading, is determined.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Orton Orthopaedic Hospital, Surface and Corrosion Science

Contributors: Kanerva, M., Besharat, Z., Pärnänen, T., Jokinen, J., Honkanen, M., Sarlin, E., Göthelid, M., Schlenzka, D.

Number of pages: 11

Pages: 93-103

Publication date: 1 Nov 2019

Peer-reviewed: Yes

Publication information

Journal: Journal of the Mechanical Behavior of Biomedical Materials

Volume: 99

ISSN (Print): 1751-6161

Original language: English

ASJC Scopus subject areas: Biomaterials, Biomedical Engineering, Mechanics of Materials

Keywords: CoCr, Crack growth, Fatigue, Implant, Laser weld

Electronic versions:

1-s2.0-S1751616118315583-main

DOIs:

10.1016/j.jmbbm.2019.07.004

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201909052065>

Bibliographical note

EXT="Pärnänen, T."

Source: Scopus

Source ID: 85069732362

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

Effects of elevated pressures on the activity of acidophilic bioleaching microorganisms

This study reports effects of elevated pressures on the oxidation of a soluble ferrous iron and low-grade sulphidic ore as little is known about biological iron and sulphur oxidation under these conditions. Pressure effects were studied in a pressurised batch-operated stirred tank reactor using acidophilic enrichment cultures. The oxidation of soluble Fe^{2+} by enrichment culture dominated by *Leptospirillum ferriphilum*, *Sulfobacillus* sp. and *Ferrimicrobium acidiphilum* increased with increasing pressure induced by technical air to up to +3 bar (0.63 bar P_{O_2}) and was inhibited at +7 bar (1.47 bar P_{O_2}). Elevated pressures induced by nitrogen (low oxygen partial pressure) were tolerated up to +40 bar. Another enrichment culture dominated by *Acidithiobacillus ferrivorans*, *Sulfobacillus* sp. and *F. acidiphilum* partially oxidised the ore at pressures up to +20 bar induced with air (4.2 bar P_{O_2}). This is the first study reporting activity of acidophiles under pressurised conditions in a stirred tank reactor.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering

Contributors: Hajdu-Rahkama, R., Ahoranta, S., Lakaniemi, A., Puhakka, J. A.

Publication date: 15 Oct 2019

Peer-reviewed: Yes

Publication information

Journal: Biochemical Engineering Journal

Volume: 150

Article number: 107286

ISSN (Print): 1369-703X

Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering, Environmental Engineering, Biomedical Engineering

Keywords: Acidophiles, Biooxidation, Iron oxidation, Pressure tolerance, Pressurised stirred tank reactor

DOIs:

10.1016/j.bej.2019.107286

Source: Scopus

Source ID: 85070494949

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

Utilizing mixed-mineralogy ferroan magnesite tailings as the source of magnesium oxide in magnesium potassium phosphate cement

A mixed-mineralogy talc mine tailing (MT) fraction consisting of 80% ferroan magnesite (MgCO_3) was studied for utilization as the source of magnesium oxide (MgO) in magnesium potassium phosphate cement (MKPC). The effects of calcination temperature of this low-grade magnesite on the composition, BET surface area and phosphate reactivity of the resulting magnesia powder were studied. The 4-point flexural strength of resulting MKPC was measured for all calcined raw material fractions that produced a solid. Based on the strength measurement results, the optimal range for calcination resided between 700 °C and 1150 °C, which is drastically lower than commonly recommended for finer magnesia sources in MKPCs. Accelerated reactivity assessment showed that phosphate reactivity behavior could not be entirely predicted by BET surface area. The presence of impurity silicates and high iron content in all the constituent minerals was posed as the reason for densification and loss of reactivity at higher calcination temperatures.

General information

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Ceramic materials, Geological Survey of Finland, VTT Technical Research Centre of Finland

Contributors: Ismailov, A., Merilaita, N., Solismaa, S., Karhu, M., Levänen, E.

Publication date: 20 Jan 2020

Peer-reviewed: Yes

Early online date: 9 Oct 2019

Publication information

Journal: Construction and building materials

Volume: 231

Article number: 117098

ISSN (Print): 0950-0618

Original language: English

ASJC Scopus subject areas: Civil and Structural Engineering, Building and Construction, Materials Science(all)

Keywords: Bending strength, Chemically bonded ceramics, MgO, Mixed-mineralogy, pH, Phosphate cement, Surface area

Electronic versions:

1-s2.0-S0950061819325401-main

DOIs:

10.1016/j.conbuildmat.2019.117098

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201910213966>

Bibliographical note

EXT="Karhu, Marjaana"

Source: Scopus

Source ID: 85072982997

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 8

Pages: 14720-14727

Publication date: 18 Sep 2019

Peer-reviewed: Yes

Publication information

Journal: Journal of the American Chemical Society

Volume: 141

Issue number: 37

ISSN (Print): 0002-7863

Original language: English

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

DOIs:

10.1021/jacs.9b06567

Source: Scopus

Source ID: 85072270985

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

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

The aim of this study was to determine an optimal anode material for electricity production and COD removal from xylose containing synthetic wastewater in an up-flow microbial fuel cell (MFC), and assess its suitability for treatment of thermomechanical pulping (TMP) wastewater with an enrichment culture at 37 °C. The anode materials tested included carbon-based electrodes (graphite plate, carbon cloth and zeolite coated carbon cloth), metal-based electrodes (tin coated copper) and a metal-carbon assembly (granular activated carbon in stainless steel cage). During continuous operation with xylose, COD removal was 77–86% of which 25–28% was recovered as electricity. The highest power density of 333 (± 15) mW/m² was obtained with the carbon cloth electrode. However, based on an overall analysis including electrode performance, surface area and scalability, the granular activated carbon in stainless steel cage (GAC in SS cage) was chosen to be used as electrode for bioelectrochemical treatment of TMP wastewater. The TMP fed MFC was operated in continuous mode with 1.8 days hydraulic retention time, resulting in 47 ($\pm 13\%$) COD removal of which 1.5% was recovered as electricity with the average power production of 10–15 mW/m². During operation with TMP wastewater, membrane fouling increased the polarization resistance causing a 50% decrease in power production within 30 days. This study shows that MFC pretreatment removes half of the TMP wastewater COD load, reducing the energy required for aerobic treatment.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 10

Pages: 141-150

Publication date: 15 Sep 2019

Peer-reviewed: Yes

Publication information

Journal: Chemical Engineering Journal

Volume: 372

ISSN (Print): 1385-8947

Original language: English

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

Keywords: Electricity production, Electrode material, Granular activated carbon, Membrane fouling, Microbial electrochemical technology, Thermomechanical pulping wastewater

DOIs:

10.1016/j.cej.2019.04.090

Source: Scopus

Effects of nanofibrillated cellulose hydrogels on adipose tissue extract and hepatocellular carcinoma cell spheroids in freeze-drying

The aim of this study was to evaluate the effects of two nanofibrillated cellulose (NFC) hydrogels on two human derivatives during freeze-drying. Native NFC hydrogel is a suitable platform to culture 3D cell spheroids and a hydrogel processed further, called anionic NFC (ANFC) hydrogel, is an excellent platform for controlled release of proteins. Moreover, it has been shown to be compatible with freeze-drying when correct lyoprotectants are implemented. Freeze-drying is a method, where substance is first frozen, and then vacuum dried through sublimation of water in order to achieve dry matter without the loss of the original three-dimensional structures. The first chosen human derivative was adipose tissue extract (ATE) which is a cell-free growth factor-rich preparation capable of promoting growth of regenerative cells. The release of growth factors from the freeze-dried mixture of ATE and ANFC was compared to that of non-freeze-dried control mixtures. The release profiles remained at the same level after freeze-drying. The second derivative was hepatocellular carcinoma (HepG2) cell spheroids which were evaluated before and after freeze-drying. The 3D structure of the HepG2 cell spheroids was preserved and the spheroids retained 18% of their metabolic activity after rehydration. However, the freeze-dried and rehydrated HepG2 cell spheroids did not proliferate and the cell membrane was damaged by fusion and formation of crystals.

General information

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, University of Helsinki, Tampere University, Università degli Studi di Padova, Italy

Contributors: Auvinen, V., Merivaara, A., Kiiskinen, J., Paukkonen, H., Laurén, P., Hakkarainen, T., Koivuniemi, R., Sarkanen, R., Ylikomi, T., Laaksonen, T., Yliperttula, M.

Publication date: 15 Sep 2019

Peer-reviewed: Yes

Publication information

Journal: Cryobiology

ISSN (Print): 0011-2240

Original language: English

ASJC Scopus subject areas: Biochemistry, Genetics and Molecular Biology(all), Agricultural and Biological Sciences(all)

Keywords: 3D cell culture, Adipose tissue extract, Cell spheroids, Freeze-drying, Nanofibrillated cellulose

DOIs:

10.1016/j.cryobiol.2019.09.005

Bibliographical note

dupl=50229030

Source: Scopus

Source ID: 85072559849

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

Critical Sensitizer Quality Attributes for Efficient Triplet–Triplet Annihilation Upconversion with Low Power Density Thresholds

Triplet-triplet annihilation upconversion (TTAUC) is a power density-dependent process where photons of low energy are transformed into high energy ones. The most important attributes of efficient TTAUC are quantum yield ϕ_{TTAUC} , power density threshold I_{th} (photon flux at which 50% of ϕ_{TTAUC} is achieved), and the upconversion shift of emitted photons (anti-Stokes shift). To date, approaches to balance these parameters have remained unclear. Herein, the cumulative effect of sensitizer triplet lifetime (τ_0 S), sensitizer-annihilator triplet energy gap (ΔE_{T}), and the total concentration of the sensitizer on the power density threshold at high TTAUC quantum yields is evaluated experimentally using Pt, Pd, and Zn tetraphenylporphyrin derivatives and a tetra-tert-butylperylene annihilator, and by kinetic rate modeling. The results suggest that a large energy gap ($\Delta E_{\text{T}} \geq 4$ kBT) and long sensitizer triplet lifetime make the triplet-triplet energy transfer (TTET) extremely efficient and allow the utilization of high sensitizer concentrations for low I_{th} . However, for large upconversion shifts, the triplet energy gap should be as small as possible. Smaller energy gap values result in slower forward TTET and faster reverse TTET, which together with high total sensitizer concentration can lead to a quenching of annihilator's triplet state and therefore elevate the I_{th} . In this regard, low concentration of a sensitizer is beneficial, making sensitizers with high molar extinction coefficients preferential. Sensitizers with a long living triplet state and a high molar extinction coefficient can work efficiently and have low I_{th} at 0 kBT or even negative ΔE_{T} . Kinetic rate modeling further helps to optimize the parameters for best possible TTAUC performance. Thus, the findings of the study pave the way for the design of TTAUC systems with superior performance, such as high ϕ_{TTAUC} at low excitation power densities with large anti-Stokes shift, for, for example, solar-driven photovoltaics, photocatalysis, bioimaging, and safe light-triggered drug-delivery systems.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Pages: 22865–22872

Publication date: 26 Aug 2019

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 123

Issue number: 37

ISSN (Print): 1932-7447

Original language: English

Electronic versions:

acs.jpcc.9b08026

DOIs:

10.1021/acs.jpcc.9b08026

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201910213972>

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

Nano-structured TiO₂ grown by low-temperature reactive sputtering for planar perovskite solar cells

Low-temperature nanostructured electron-transporting layers (ETLs) for perovskite solar cells are grown by reactive sputtering at 160 °C with thickness in the range 22–76 nm and further stabilization in air at 180 °C to improve the lattice structure and to consequently reduce charge recombination during solar cell operation. In addition, the post-deposition treatment aims at leveling differences among samples to ensure material reproducibility. Nanostructured TiO₂ has a further added value in promoting the structural coupling with the perovskite layer and establishing conformal interfaces in favor of the charge extraction from the active material. Nanostructuring of the ETLs also allows the shaping of the band gap width and position with a beneficial impact on the electrical parameters, as tested in standard architecture containing methylammonium lead iodide perovskites. A balance among parameters is achieved using a 40-nm-thick TiO₂ ETL with a maximum efficiency of ~15% reached without surface treatments or additional layers. The proposed growth methodology would be compatible with the use of flexible substrates after appropriated ETL structural adaptation. It can be likewise applied in perovskite/silicon-heterojunction tandem solar cells to fulfill the industrial demand for clean, solvent-free, reproducible, reliable, and high-throughput processes.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Alberti, A., Smecca, E., Sanzaro, S., Bongiorno, C., Giannazzo, F., Mannino, G., La Magna, A., Liu, M., Vivo, P., Listorti, A., Calabro', E., Matteocci, F., Di Carlo, A.

Number of pages: 12

Pages: 6218-6229

Publication date: 16 Aug 2019

Peer-reviewed: Yes

Publication information

Journal: ACS Applied Energy Materials

Volume: 2

Issue number: 9

ISSN (Print): 2574-0962

Original language: English

DOIs:

10.1021/acsaem.9b00708

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

Chlorine induced high-temperature corrosion mechanisms in HVOF and HVAF sprayed Cr₃C₂-based hardmetal coatings

A novel method that combines thermal analysis and traditional furnace corrosion tests was used to study the corrosion behaviour of thermally sprayed Cr₃C₂-based hardmetal coatings at 450 °C and 550 °C under a KCl deposit. This method enabled the identification of the onset temperature of chlorine-induced oxidation to be within 450–500 °C. Two corrosion mechanisms were suggested for these temperatures. At 450 °C, the corrosion rate was slow and mainly controlled by the formation of K₂CrO₄. Exposure at 550 °C caused the formation of fine interconnected secondary-carbide precipitates in the metal matrix. Their fast corrosion was identified as the major cause of degradation.

General information

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Surface Engineering, Valmet Automation Oy

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

Publication date: 14 Aug 2019

Peer-reviewed: Yes

Publication information

Journal: Corrosion Science

Article number: 108166

ISSN (Print): 0010-938X

Original language: English

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

Keywords: A. Metal matrix composites, A. Superalloys, B. SEM, B. TGA, B. XRD, C. Chlorination, C. High temperature corrosion, C. Thermodynamic diagrams

DOIs:

10.1016/j.corsci.2019.108166

Bibliographical note

EXT="Uusitalo, Mikko"

Source: Scopus

Source ID: 85072275416

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

Alkane and wax ester production from lignin-related aromatic compounds

Lignin has potential as a sustainable feedstock for microbial production of industrially relevant molecules. However, the required lignin depolymerization yields a heterogenic mixture of aromatic monomers that are challenging substrates for the microorganisms commonly used in the industry. Here, we investigated the properties of lignin-related aromatic compounds (LRAs), namely coumarate, ferulate, and caffeate, in the synthesis of biomass and products in an LRA-utilizing bacterial host *Acinetobacter baylyi* ADP1. The biosynthesis products, wax esters, and alkanes are relevant compounds for the chemical and fuel industries. Here, wax esters were produced by a native pathway of ADP1, whereas alkanes were produced by a synthetic pathway introduced to the host. Using individual LRAs as substrates, the growth and product formation were monitored with internal biosensors and off-line analytics. Of the tested LRAs, coumarate was the most propitious in terms of product synthesis. Wax esters were produced from coumarate with yield and titer of 37 mg/gcoumarate and 202 mg/L, whereas alkanes were produced with a yield of 62.3 µg /gcoumarate and titer of 152 µg/L. This study demonstrates the microbial preference for certain LRAs and highlights the potential of *A. baylyi* ADP1 as a host for LRA upgrading to value-added products.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Salmela, M., Lehtinen, T., Efimova, E., Santala, S., Santala, V.

Number of pages: 12

Pages: 1934-1945

Publication date: 1 Aug 2019

Peer-reviewed: Yes

Publication information

Journal: Biotechnology and Bioengineering

Volume: 116

Issue number: 8

ISSN (Print): 0006-3592

Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering, Applied Microbiology and Biotechnology

Keywords: *Acinetobacter baylyi* ADP1, alkane, lignin, wax ester

DOIs:

10.1002/bit.27005

Source: Scopus

Source ID: 85070728183

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

Photochemistry of dithiophosphinate $\text{Ni}(\text{S}_2\text{P}(\text{i-Bu})_2)_2$ complex in CCl_4 . Transient species and TD-DFT calculations

Femtosecond spectroscopy and nanosecond laser flash photolysis were used to study the photophysical and photochemical transformations of the bis-diisobutyl-dithiophosphinate Ni(II) complex ($\text{Ni}(\text{S}_2\text{P}(\text{i-Bu})_2)_2 = \text{Ni}(\text{dtpi})_2$, where $\text{dtpi}^- \equiv \text{S}_2\text{P}(\text{i-Bu})_2$) in CCl_4 solutions. The radiation of second harmonic (405 nm) of Ti:Sapphire laser transfers the $\text{Ni}(\text{dtpi})_2$ complex to an excited $^1\text{LMCT}$ state. Its decay in CCl_4 is described by three exponents with time constants 0.58, 2.0 and ~ 150 ps. The first process apparently involves the fast transitions from $^1\text{LMCT}$ state to $^3\text{LMCT}$ due to the intersystem crossing (ISC) and then to lower-lying "hot" ^3LF (Ligand Field) state. The second time constant, most likely, corresponds to the vibrational cooling of this "hot" ^3LF state. And the third slow process is the transition from ^3LF state to ground state (^1GS). The quantum yield of photochemical transformation under the 405 irradiation is close to zero, so the study of photochemistry was performed with a nanosecond flash photolysis at 308 nm. In this case an electron transfer from the excited $\text{Ni}(\text{dtpi})_2$ complex to a solvent molecule leads to the appearance of primary intermediate, the $[\text{CINi}(\text{dtpi})(\text{dtpi}^{\text{rad}})]$ complex, in which a dtpi^{rad} radical is coordinated with a nickel ion via one sulfur atom. In the fast reaction with $\text{Ni}(\text{dtpi})_2$, this complex forms a long-lived dimer $\text{CINi}(\text{dtpi})(\text{dtpi}^{\text{rad}})[\text{Ni}(\text{dtpi})_2]$. This intermediate for a few hundred microseconds decays in the reaction of recombination with the formation of $(\text{dtpi})_2$ disulphide and unstable $\text{CINi}(\text{dtpi})$ complex. The insoluble NiCl_2 salt failed in CCl_4 as the sediment due to the reaction of two $\text{CINi}(\text{dtpi})$ complexes. The quantum chemical calculations allowed to determine the geometry of the intermediate complexes arising in the photochemistry of $\text{Ni}(\text{S}_2\text{P}(\text{i-Bu})_2)_2$ complex.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Novosibirsk State University, Boreskov Institute of Catalysis SB RAS, Nikolaev Institute of Inorganic Chemistry SB RAS

Contributors: Solovyev, A. I., Mikheyliis, A. V., Plyusnin, V. F., Shubin, A. A., Grivin, V. P., Larionov, S. V., Tkachenko, N. V., Lemmetyinen, H.

Publication date: 1 Aug 2019

Peer-reviewed: Yes

Publication information

Journal: Journal of Photochemistry and Photobiology A: Chemistry

Volume: 381

Article number: 111857

ISSN (Print): 1010-6030

Original language: English

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

Keywords: Bis-diisobutyl-dithiophosphinate Ni(II) complex, Intermediate particles, Kinetics, Laser flash photolysis, Photolysis mechanism, Quantum-chemical calculation

DOIs:

10.1016/j.jphotochem.2019.111857

Source: Scopus

Source ID: 85067953554

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

Pyrolytic behavior of lignocellulosic-based polysaccharides

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Ghalibaf, M., Doddapaneni, T. R. K. C., Alén, R.

Pages: 121-131

Publication date: Jul 2019

Peer-reviewed: Yes

Early online date: 2018

Publication information

Journal: Journal of Thermal Analysis and Calorimetry

Volume: 137

Issue number: 1

ISSN (Print): 1388-6150

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Physical and Theoretical Chemistry

Keywords: Cellulose, Condensable products, Glucomannan, Pyrolysis–gas chromatography, Thermogravimetry, Xylan
DOIs:

10.1007/s10973-018-7919-y

Source: Scopus

Source ID: 85057074557

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

Photocontrol of Supramolecular Azo-Containing Block Copolymer Thin Films during Dip-Coating: Toward Nanoscale Patterned Coatings

Dip-coating allows nanostructured block copolymer (BCP) thin film fabrication in a fast and facile one-step process. It can also be coupled with external controls, such as illumination. Herein, we expose several design principles that enable photocontrol of the nanostructured surface pattern and thickness of supramolecular BCP thin films. This is done using a polystyrene-poly(4-vinylpyridine) (PS-P4VP) BCP and two hydroxy-functionalized small-molecule (SM) azo derivatives that have different photochemical characteristics and that hydrogen bond to the P4VP block. We show how the film preparation concept provides tunability through the chemical structure of the photoactive SM, the relative amount of SM in the dip-coating solution, and the choice of solvent. It was found that the film thickness and SM uptake in the films are increased by illumination when THF is used but are unchanged when toluene is used as solvent, which is attributed to an optical heating effect observable with volatile solvents. The photocontrol of surface patterns is a result of photoinduced changes in the effective volume fraction of the P4VP+SM phase, which is increased by a greater volume of cis isomers, by higher SM uptake (using THF), and by more trans-cis-trans cycling for systems with shorter cis lifetime. The extent of photoinduced change can also be increased by higher molecular mobility due to more flexible SMs, lower BCP molecular weight, and nonmicellar or softer micellar solutions.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, Département de Chimie, Succ. Centre-Ville

Contributors: Vapaavuori, J., Grosrenaud, J., Siiskonen, A., Priimägi, A., Pellerin, C., Bazuin, C. G.

Number of pages: 12

Pages: 3526-3537

Publication date: 28 Jun 2019

Peer-reviewed: Yes

Publication information

Journal: ACS Applied Nano Materials

Volume: 2

Issue number: 6

ISSN (Print): 2574-0970

Original language: English

ASJC Scopus subject areas: Materials Science(all)

Keywords: azo-containing, block copolymer thin films, dip-coating, nanoscale patterns, photocontrol, supramolecular
DOIs:

10.1021/acsanm.9b00496

Bibliographical note

EXT="Vapaavuori, Jaana"

Source: Scopus

Source ID: 85068593381

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

Photoreversible Soft Azo Dye Materials: Toward Optical Control of Bio-Interfaces

Photoreversible optically switchable azo dye molecules in polymer-based materials can be harnessed to control a wide range of physical, chemical, and mechanical material properties in response to light, that can be exploited for optical control over the bio-interface. As a stimulus for reversibly influencing adjacent biological cells or tissue, light is an ideal triggering mechanism, since it can be highly localized (in time and space) for precise and dynamic control over a biosystem, and low-power visible light is also an inherently gentle, benign, and nondamaging stimulus in a biological environment. Azobenzene-based dyes in particular are emerging as especially attractive candidates among

photoreversible molecules, and soft azobenzene-containing materials are promising due to their ease of incorporation, and efficient and robust photochemistry and photophysics. This review provides a current survey of the use of photoreversible azo soft materials in cell biology and tissue engineering bio-interface applications, to afford light control over molecular motion (orientation, flow), by inscribing surface morphological patterns or macroscopically photoactuating surfaces and structures, via three key photophysical and bioactive effects enabled by the azo groups' light-induced photo-orientation, topological optical patterning, and photomechanical actuation.

General information

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, McGill University, Tokyo Institute of Technology

Contributors: Chang, V. Y., Fedele, C., Priimägi, A., Shishido, A., Barrett, C. J.

Pages: 1900091

Publication date: 29 May 2019

Peer-reviewed: Yes

Publication information

Journal: Advanced Optical Materials

ISSN (Print): 2195-1071

Original language: English

DOIs:

10.1002/adom.201900091

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

Lasing in Ni Nanodisk Arrays

We report on lasing at visible wavelengths in arrays of ferromagnetic Ni nanodisks overlaid with an organic gain medium. We demonstrate that by placing an organic gain material within the mode volume of the plasmonic nanoparticles both the radiative and, in particular, the high ohmic losses of Ni nanodisk resonances can be compensated. Under increasing pump fluence, the systems exhibit a transition from lattice-modified spontaneous emission to lasing, the latter being characterized by highly directional and sub-nanometer line width emission. By breaking the symmetry of the array, we observe tunable multimode lasing at two wavelengths corresponding to the particle periodicity along the two principal directions of the lattice. Our results are relevant for loss-compensated magnetoplasmonic devices and topological photonics.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Aalto University, University of Eastern Finland, Campus de la UAB

Contributors: Pourjamal, S., Hakala, T. K., Nečada, M., Freire-Fernández, F., Kataja, M., Rekola, H., Martikainen, J. P.,

Törmä, P., Van Dijken, S.

Number of pages: 7

Pages: 5686-5692

Publication date: 28 May 2019

Peer-reviewed: Yes

Publication information

Journal: ACS Nano

Volume: 13

Issue number: 5

ISSN (Print): 1936-0851

Original language: English

ASJC Scopus subject areas: Materials Science(all), Engineering(all), Physics and Astronomy(all)

Keywords: loss-compensated magnetoplasmonics, nanolasing, Ni nanodisk array, plasmonics, surface lattice resonance

Electronic versions:

acs.nano.9b01006

DOIs:

10.1021/acs.nano.9b01006

URLs:

<http://urn.fi/URN:NBN:fi:ty-201906251911>

Source: Scopus

Source ID: 85064967811

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

Photoinduced Charge Transfer Processes at Organic-Semiconductor Interfaces

The growing energy demand of the mankind has led to the extensive use of fossil fuels. The burning of oil, coal and natural gas has increased the global temperature and atmospheric carbon dioxide percentage to a dangerously high level. Therefore, carbon-neutral energy sources such as solar cells are needed.

In order to design more effective solar cells, a deep understanding of the primary photochemical processes in the cells is needed. Ultrafast time-resolved spectroscopy, especially transient absorption methods, are a very useful tool for investigating the reaction kinetics in order to optimize the solar cell performance.

In this thesis, kinetics of the photoinduced processes at the interface of an organic monomolecular layer and a semiconductor are studied. Such structures may be used as the active material e.g. in dye-sensitized solar cells. Two different types of organic–semiconductor hybrids were prepared: fullerenes (C60) immobilized on colloidal semiconductor quantum dots (QDs), and zinc phthalocyanine (ZnPc) derivatives on nanostructured titanium dioxide (TiO2) and zinc oxide (ZnO) surfaces. The driving force of photocurrent generation in these systems is a photonic excitation leading to an electron transfer reaction across the organic–semiconductor interface. The observed electron transfer rates vary from a few picoseconds in ZnPc monolayers on TiO2 to ca. 100 ps in QD–fullerene systems.

Phthalocyanine derivatives are very attractive sensitizing dyes for solar cell applications because of their excellent stability and strong absorption in the red part of the spectrum. A drawback with these compounds is their tendency towards aggregation. It reduces the solar cell efficiencies due to intra-aggregate losses. There are two common methods for aggregation-reduction: the use of molecular co-adsorbates and substitution of the phthalocyanine core with bulky side groups. Both mechanisms were observed to lower the degree of aggregation in the ZnPc samples. The substitution method proved to be more efficient in terms of the lifetime of the charge-separated state.

To more realistically mimic a solar cell, a hole-transporting material (HTM) was used. Its effect on the primary photoinduced reactions in the phthalocyanine–semiconductor samples was studied. With the chosen HTM, spiro-MeOTAD, the charge separation was observed to occur first at the phthalocyanine–HTM interface, followed by electron injection into the semiconductor material.

Complete solar cell samples were prepared in order to link the ultrafast spectroscopy results to actual solar cell performance. A correlation between the degree of aggregation and the produced photocurrent was confirmed. The less aggregated samples produce a higher photocurrent per number of absorbed photons. This study identifies bottlenecks in modern hybrid organic–semiconductor solar cell design and suggests solutions for improving the solar cell performance.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Materials Science and Environmental Engineering

Contributors: Virkki, K.

Number of pages: 55

Publication date: 24 May 2019

Publication information

Publisher: Tampere University

ISBN (Print): 978-952-03-1101-8

ISBN (Electronic): 978-952-03-1102-5

Original language: English

Publication series

Name: Tampere University Dissertations

Volume: 67

ISSN (Print): 2489-9860

ISSN (Electronic): 2490-0028

Electronic versions:

TUNI_virkki

URLs:

<http://urn.fi/URN:ISBN:978-952-03-1102-5>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Bioinspired Light Robots from Liquid Crystal Networks

Bioinspired material research aims at learning from the sophisticated design principles of nature, in order to develop novel artificial materials with advanced functionalities. Some of the sophisticated capabilities of biological materials, such as their ability to self-heal or adapt to environmental changes, are challenging to realize in artificial systems. Nevertheless, many efforts have been recently devoted to develop artificial materials with adaptive functions, especially materials which can generate movement in response to external stimuli. One such effort is the field of soft robots, which aims towards fabrication of autonomous adaptive systems with flexibility, beyond the current capability of conventional robotics.

However, in most cases, soft robots still need to be connected to hard electronics for powering and rely on complicated algorithms to control their deformation modes. Soft robots that can be powered remotely and are capable of self-regulating function, are of great interest across the scientific community.

In order to realize such responsive and adaptive systems, researches across the globe are making constant efforts to develop new, ever-more sophisticated stimuli-responsive materials. Among the different stimuli-responsive materials, liquid crystal networks (LCNs) are the most suited ones to design smart actuating systems as they can be controlled and powered remotely with light and thereby obviate the need for external control circuitry. They enable pre-programmable shape changes, hence equipping a single material with multiple actuation modes. In addition to light, they can also be actuated by variety of stimuli such as heat, humidity, pH, electric and magnetic fields etc., or a combination of these. Based on these advantages of LCNs, we seek inspiration from natural actuator systems present in plants and animals to devise different light controllable soft robotic systems.

In this thesis, inspired from biological systems such as octopus arm movements, iris movements in eyes, object detection and capturing ability of Venus flytraps and opening and closing of certain nocturnal flowers, we demonstrate several light robots that can be programmed to show pre-determined shape changes. By employing a proper device design, these light robots can even show the characteristics of selfregulation and object recognition, which brings new advances to the field of LCNbased light robots. For instance, octopod light robot can show bidirectional bending owing to alignment programming using a commercial laser projector; artificial iris is a fully light controllable device that can self-regulate its aperture size based on intensity of incident light; the optical flytrap can not only autonomously close on an object coming into its "mouth" but it can also distinguish between different kinds of objects based on optical feedback, and finally, integration of light and humidity responsiveness in a single LCN actuator enables a nocturnal flower-mimicking actuator, which provides an opportunity to understand the delicate interplay between different simultaneously occurring stimuli in a monolithic actuator.

We believe that besides providing a deeper understanding on the photoactuation in liquid crystal networks, at fundamental level, our work opens new avenues by providing several pathways towards next-generation intelligent soft microrobots.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

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

Contributors: Wani, O.

Number of pages: 70

Publication date: 17 May 2019

Publication information

Publisher: Tampere University

ISBN (Print): 978-952-03-1095-0

ISBN (Electronic): 978-952-03-1096-7

Original language: English

Publication series

Name: Tampere University Dissertations

Volume: 64

ISSN (Print): 2489-9860

ISSN (Electronic): 2490-0028

Electronic versions:

TUNI_wani

URLs:

<http://urn.fi/URN:ISBN:978-952-03-1096-7>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Dopant-free hole-transporting materials via thionation approach towards stable and efficient perovskite solar cells

General information

Publication status: Published

MoE publication type: Not Eligible

Organisations: Materials Science and Environmental Engineering

Contributors: Liu, M., Vivo, P.

Publication date: 12 May 2019

Peer-reviewed: Unknown

Event: Paper presented at HOPV 2019, Rome, Italy.

Research output: Other conference contribution > Paper, poster or abstract > Scientific

Long-term performance evaluation of an anoxic sulfur oxidizing moving bed biofilm reactor under nitrate limited conditions

An anoxic sulfur-oxidizing moving bed biofilm reactor (MBBR) treating sulfur and nitrate-contaminated synthetic wastewater was monitored for 306 days under feed nitrogen-to-sulfur (N/S) molar ratios of 0.5, 0.3 and 0.1. Thiosulfate (S₂O₃²⁻) removal efficiencies (RE) exceeding 98% were observed at a N/S ratio of 0.5 and a S₂O₃²⁻ loading rate of 0.9 g S₂O₃²⁻-S L⁻¹ d⁻¹, whereas a RE of 82.3 (±2.6)% and 37.7 (±3.4)% were observed at N/S ratios of 0.3 and 0.1, respectively. Complete nitrate (NO₃⁻) removal was obtained at all tested N/S ratios. A comparison of the kinetic parameters of the MBBR biomass under the same stoichiometric conditions (N/S ratio of 0.5) revealed a 1.3-fold increase of the maximum specific rate of S₂O₃²⁻ oxidation (r_{max}) and a 30-fold increase of the affinity constant for S₂O₃²⁻ (K_s) compared to those observed after long-term NO₃⁻ limitation (N/S ratio of 0.1). The MBBR showed optimal resilience to NO₃⁻ limitation as the S₂O₃²⁻ RE recovered from 37.3% to 94.1% within two days after increasing the N/S ratio from 0.1 to 0.5. Based on PCR-DGGE analysis, sulfur-oxidizing nitrate-reducing bacteria, i.e. *Thiobacillus* sp. and *Sulfuritalea* sp., dominated in the MBBR biofilm during the entire study.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Bio- and Circular Economy, Materials Science and Environmental Engineering, Department of Civil and Mechanical Engineering, University of Cassino and Southern Lazio, ENEA/CREATE/Università Degli Studi Napoli Federico II, Wageningen University and the UNESCO-IHE Institute for Water Education, Delft, The Netherlands, 18.10.2013, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education

Contributors: Khanongnuch, R., Di Capua, F., Lakaniemi, A., Rene, E. R., Lens, P.

Pages: 1072-1081

Publication date: 29 Apr 2019

Peer-reviewed: Yes

Publication information

Journal: Environmental Science: Water Research & Technology

Volume: 5

Issue number: 6

ISSN (Print): 2053-1400

Original language: English

Electronic versions:

c9ew00220k

DOIs:

10.1039/C9EW00220K

URLs:

<http://urn.fi/URN:NBN:fi:ty-201905171646>

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

Halide Perovskite Nanocrystals for Next-Generation Optoelectronics

Colloidal perovskite nanocrystals (PNCs) combine the outstanding optoelectronic properties of bulk perovskites with strong quantum confinement effects at the nanoscale. Their facile and low-cost synthesis, together with superior photoluminescence quantum yields and exceptional optical versatility, make PNCs promising candidates for next-generation optoelectronics. However, this field is still in its early infancy and not yet ready for commercialization due to several open challenges to be addressed, such as toxicity and stability. Here, the key synthesis strategies and the tunable optical properties of PNCs are discussed. The photophysical underpinnings of PNCs, in correlation with recent developments of PNC-based optoelectronic devices, are especially highlighted. The final goal is to outline a theoretical scaffold for the design of high-performance devices that can at the same time address the commercialization challenges of PNC-based technology.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Materials Science and Environmental Engineering

Contributors: Liu, M., Zhang, H., Gedamu, D., Fourmont, P., Rekola, H., Hiltunen, A., Cloutier, S. G., Nechache, R., Priimägi, A., Vivo, P.

Publication date: 23 Apr 2019

Peer-reviewed: Yes

Publication information

Journal: Small

Article number: 1900801

ISSN (Print): 1613-6810

Original language: English

DOIs:

10.1002/sml.201900801

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

H₂S removal and microbial community composition in an anoxic biotrickling filter under autotrophic and mixotrophic conditions

Removal of H₂S from gas streams using NO₃⁻-containing synthetic wastewater was investigated in an anoxic biotrickling filter (BTF) at feed N/S ratios of 1.2-1.7 mol mol⁻¹ with an initial nominal empty bed residence time of 3.5 min and a hydraulic retention time of 115 min. During 108 days of operation under autotrophic conditions, the BTF showed a maximum elimination capacity (EC) of 19.2 g S m⁻³h⁻¹ and H₂S removal efficiency (RE) above 99%. Excess biofilm growth reduced the HRT from 115 to 19 min and decreased the desulfurization efficiency of the BTF. When the BTF was operated under mixotrophic conditions by adding organic carbon (43.2 g acetate m⁻³h⁻¹) to the synthetic wastewater, the H₂S EC decreased from 16.4 to 13.1 g S m⁻³h⁻¹, while the NO₃⁻ EC increased from 9.9 to 11.1 g NO₃⁻-N m⁻³h⁻¹, respectively. *Thiobacillus* sp. (98-100% similarity) was the only sulfur-oxidizing nitrate-reducing bacterium detected in the BTF biofilm, while the increased abundance of heterotrophic denitrifiers, i.e. *Brevundimonas* sp. and *Rhodocyclales*, increased the consumed N/S ratio during BTF operation. Residence time distribution tests showed that biomass accumulation during BTF operation reduced gas and liquid retention times by 17.1% and 83.5%, respectively.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, UNESCO-IHE, Department of Civil, Architectural and Environmental Engineering (DICEA), University of Naples Federico II

Contributors: Khanongnuch, R., Di Capua, F., Lakaniemi, A., Rene, E. R., Lens, P.

Pages: 397-406

Publication date: 5 Apr 2019

Peer-reviewed: Yes

Early online date: 18 Dec 2018

Publication information

Journal: Journal of Hazardous Materials

Volume: 367

ISSN (Print): 0304-3894

Original language: English

Keywords: H₂S removal, autotrophic denitrification, nitrate-containing wastewater, substrate competition, PCR-DGGE

Electronic versions:

H₂S removal and microbial community composition in an anoxic biotrickling filter under autotrophic and mixotrophic conditions_Ramita

DOIs:

10.1016/j.jhazmat.2018.12.062

URLs:

<http://urn.fi/URN:NBN:fi:ty-201901141088>

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

GIS-data related route optimization, hierarchical clustering, location optimization, and kernel density methods are useful for promoting distributed bioenergy plant planning in rural areas

Currently, geographic information system (GIS) models are popular for studying location-allocation-related questions concerning bioenergy plants. The aim of this study was to develop a model to investigate optimal locations for two different types of bioenergy plants, for farm and centralized biogas plants, and for wood terminals in rural areas based on minimizing transportation distances. The optimal locations of biogas plants were determined using location optimization tools in R software, and the optimal locations of wood terminals were determined using kernel density tools in ArcGIS. The present case study showed that the utilized GIS tools are useful for bioenergy-related decision-making to identify potential bioenergy areas and to optimize biomass transportation, and help to plan power plant sizing when candidate bioenergy plant locations have not been defined in advance. In the study area, it was possible to find logistically viable locations for 13 farm biogas plants (>100 kW) and for 8 centralized biogas plants (>300 kW) using a 10-km threshold for feedstock supply. In the case of wood terminals, the results identified the most intensive wood reserves near the highest road classes, and two potential locations were determined.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Bio- and Circular Economy, University of Jyväskylä, Seinäjoki University of Applied Sciences

Contributors: Laasasenaho, K., Lensu, A., Lauhanen, R., Rintala, J.
Number of pages: 11
Pages: 47-57
Publication date: 1 Apr 2019
Peer-reviewed: Yes

Publication information

Journal: Sustainable Energy Technologies and Assessments
Volume: 32
ISSN (Print): 2213-1388
Original language: English
ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Energy Engineering and Power Technology
Keywords: Biogas, Circular economy, Location-allocation, Network analysis, Wood terminal
DOIs:
10.1016/j.seta.2019.01.006
URLs:
<http://urn.fi/URN:NBN:fi:tuni-201910033674>. Embargo ends: 7/02/21
Source: Scopus
Source ID: 85061098980
Research output: Contribution to journal › Article › Scientific › peer-review

Impacts of short-term temperature fluctuations on biohydrogen production and resilience of thermophilic microbial communities

Anaerobic microflora enriched for dark fermentative H₂ production from a mixture of glucose and xylose was used in batch cultivations to determine the effects of sudden short-term temperature fluctuations on H₂ yield and microbial community composition. Batch cultures initially cultivated at 55 °C (control) were subjected to downward (from 55 °C to 35 °C or 45 °C) or upward (from 55 °C to 65 °C or 75 °C) temperature shifts for 48 h after which, each culture was transferred to a fresh medium and cultivated again at 55 °C for two consecutive batch cycles. The average H₂ yield obtained during the first cultivation at 55 °C was 2.1 ± 0.14 mol H₂ mol⁻¹ hexose equivalent. During the temperature shifts, the obtained H₂ yields were 1.8 ± 0.15, 1.6 ± 0.27 and 1.9 ± 0.00 mol H₂ mol⁻¹ hexose equivalent at 35 °C, 45 °C and 65 °C, respectively, while no metabolic activity was observed at 75 °C. The sugars were completely utilized during the 48 h temperature shift to 35 °C but not at 65 °C and 45 °C. At the end of the second cycle after the different temperature shifts, the H₂ yield obtained was 96.5, 91.6, 79.9 and 54.1% (second cycle after temperature shift to 35 °C, 45 °C, 65 °C and 75 °C, respectively) when compared to the average H₂ yield produced in the control at 55 °C. Characterization of the microbial communities present in the control culture at 55 °C showed the predominance of Thermoanaerobacteriales, Clostridiales and Bacilliales. The microbial community composition differed based on the fluctuation temperature with Thermoanaerobacteriales being most dominant during the upward temperature fluctuations and Clostridiales being the most dominant during the downward temperature fluctuations.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Bio- and Circular Economy, INRA
Contributors: Okonkwo, O., Escudí, R., Bernet, N., Mangayil, R., Lakaniemi, A., Trably, E.
Pages: 8028-8037
Publication date: 29 Mar 2019
Peer-reviewed: Yes

Publication information

Journal: International Journal of Hydrogen Energy
Volume: 44
Issue number: 16
ISSN (Print): 0360-3199
Original language: English
Electronic versions:
Temperature fluctuation_Okonkwo
DOIs:
10.1016/j.ijhydene.2019.01.256
URLs:
<http://urn.fi/URN:NBN:fi:tty-201905201649>
Research output: Contribution to journal › Article › Scientific › peer-review

Thiocyanate precursor impact on the formation of cobalt complexes: Synthesis and characterization

Two new thiocyanate complexes have been synthesized with two different thiocyanate anion sources using 1-(2-Pyrimidyl) piperazine and $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$. These compounds were characterized by single X-ray diffraction, FTIR, UV-Visible and TGA-DTA. The antibacterial activity was also examined. The XRD showed that compounds 1 and 2 crystallized into monoclinic and orthorhombic systems respectively. In compound 1, cobalt is surrounded by two isothiocyanate anions and two nitrogen-amides, while in compound 2 it is surrounded by four isothiocyanate ligands and a separate protonated amide. Different interactions packed the system through $\text{N-H} \cdots \text{S}$, $\text{N-H} \cdots \text{O}$ and $\text{O-H} \cdots \text{S}$ hydrogen bonds forming a ring. Gap energy determination revealed two diverse behaviors, the first being characteristic of a semiconductor and the second of an insulator. In the 10-500 °C range, the thermal behaviors were investigated and showed the decomposition of the two complexes with metal complexes residues. The antibacterial analysis presented a weak performance.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering
Contributors: Hannachi, A., Valkonen, A., Rzaigui, M., Smirani, W.
Pages: 222-230
Publication date: 15 Mar 2019
Peer-reviewed: Yes
Early online date: 30 Dec 2018

Publication information

Journal: Polyhedron
Volume: 161
ISSN (Print): 0277-5387
Original language: English
Keywords: Thiocyanate precursor, Metal complexes, Crystal structures
DOIs:
10.1016/j.poly.2018.12.039
Source: Bibtex
Source ID: urn:57e8c491b3071e3adc8ce62c0a54169f
Research output: Contribution to journal > Article > Scientific > peer-review

Synthetic metabolic pathway for the production of 1-alkenes from lignin-derived molecules

Background: Integration of synthetic metabolic pathways to catabolically diverse chassis provides new opportunities for sustainable production. One attractive scenario is the use of abundant waste material to produce a readily collectable product, which can reduce the production costs. Towards that end, we established a cellular platform for the production of semivolatile medium-chain α -olefins from lignin-derived molecules: we constructed 1-undecene synthesis pathway in *Acinetobacter baylyi* ADP1 using ferulate, a lignin-derived model compound, as the sole carbon source for both cell growth and product synthesis. Results: In order to overcome the toxicity of ferulate, we first applied adaptive laboratory evolution to *A. baylyi* ADP1, resulting in a highly ferulate-tolerant strain. The adapted strain exhibited robust growth in 100 mM ferulate while the growth of the wild type strain was completely inhibited. Next, we expressed two heterologous enzymes in the wild type strain to confer 1-undecene production from glucose: a fatty acid decarboxylase UndA from *Pseudomonas putida*, and a thioesterase TesA from *Escherichia coli*. Finally, we constructed the 1-undecene synthesis pathway in the ferulate-tolerant strain. The engineered cells were able to produce biomass and 1-undecene solely from ferulate, and excreted the product directly to the culture headspace. Conclusions: In this study, we employed a bacterium *Acinetobacter baylyi* ADP1 to integrate a natural aromatics degrading pathway to a synthetic production route, allowing the upgradation of lignin derived molecules to value-added products. We developed a highly ferulate-tolerant strain and established the biosynthesis of an industrially relevant chemical, 1-undecene, solely from the lignin-derived model compound. This study reports the production of alkenes from lignin derived molecules for the first time and demonstrates the potential of lignin as a sustainable resource in the bio-based synthesis of valuable products.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Bio- and Circular Economy
Contributors: Luo, J., Lehtinen, T., Efimova, E., Santala, V., Santala, S.
Number of pages: 13
Publication date: 11 Mar 2019
Peer-reviewed: Yes

Publication information

Journal: Microbial Cell Factories
Volume: 18
Issue number: 1
Article number: 48

ISSN (Print): 1475-2859

Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering, Applied Microbiology and Biotechnology

Keywords: 1-Alkenes, Acinetobacter baylyi, Adaptive laboratory evolution, Ferulate, Lignin

DOIs:

10.1186/s12934-019-1097-x

URLs:

<http://www.scopus.com/inward/record.url?scp=85062867820&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 85062867820

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

Vertical stratification of bacteria and archaea in sediments of a small boreal humic lake

Although sediments of small boreal humic lakes are important carbon stores and greenhouse gas sources, the composition and structuring mechanisms of their microbial communities have remained understudied. We analyzed the vertical profiles of microbial biomass indicators (PLFAs, DNA and RNA) and the bacterial and archaeal community composition (sequencing of 16S rRNA gene amplicons and qPCR of *mcrA*) in sediment cores collected from a typical small boreal lake. While microbial biomass decreased with sediment depth, viable microbes (RNA and PLFA) were present all through the profiles. The vertical stratification patterns of the bacterial and archaeal communities resembled those in marine sediments with well-characterized groups (e.g. Methanomicrobia, Proteobacteria, Cyanobacteria, Bacteroidetes) dominating in the surface sediment and being replaced by poorly-known groups (e.g. Bathyarchaeota, Aminicenantes and Caldiseica) in the deeper layers. The results also suggested that, similar to marine systems, the deep bacterial and archaeal communities were predominantly assembled by selective survival of taxa able to persist in the low energy conditions. Methanotrophs were rare, further corroborating the role of these methanogen-rich sediments as important methane emitters. Based on their taxonomy, the deep-dwelling groups were putatively organo-heterotrophic, organo-autotrophic and/or acetogenic and thus may contribute to changes in the lake sediment carbon storage.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Department of Biological and Environmental Science, Jyväskylän yliopisto, University of Eastern Finland

Contributors: Rissanen, A. J., Peura, S., Mpamah, P. A., Taipale, S., Tirola, M., Biasi, C., Mäki, A., Nykänen, H.

Publication date: 1 Mar 2019

Peer-reviewed: Yes

Publication information

Journal: FEMS Microbiology Letters

Volume: 366

Issue number: 5

ISSN (Print): 0378-1097

Original language: English

ASJC Scopus subject areas: Microbiology, Molecular Biology, Genetics

Keywords: 16S rRNA, archaea, bacteria, biomass, lake, sediment

Electronic versions:

fnz044

DOIs:

10.1093/femsle/fnz044

URLs:

<http://urn.fi/URN:NBN:fi:tty-201906201896>

Source: Scopus

Source ID: 85066419815

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

Quantitative Sequential Photoenergy Conversion Process from Singlet Fission to Intermolecular Two-Electron Transfers Utilizing Tetracene Dimer

Singlet fission (SF) theoretically enables the performance of the sequential photoenergy conversion process starting from the singlet state and leading to electron transfer (ET) with the radical ion pair quantum yield approaching 200%. Additionally, the long lifetime of the triplet state opens the possibility for an intermolecular ET process in a diffusion-limited reaction. However, the quantitative two-electron transfer process through SF has yet to be reported. Herein we demonstrate the quantitative sequential process involving SF and leading to intermolecular two-electron transfers using 2,2'-biphenyl-bridged tetracene dimer (Tet-BP-Tet: SF and electron donor) and chloranil (Ch: electron acceptor). The high-yield and long-lived individual triplet excited states of Tet-BP-Tet by SF ($\Phi_T = 175 \pm 5\%$ and $\tau_T = 0.29$ ms) resulted in the quantitative two-electron transfer process ($\Phi_{ET} = 173 \pm 5\%$) with Ch in benzonitrile.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials
Contributors: Nakamura, S., Sakai, H., Nagashima, H., Kobori, Y., Tkachenko, N. V., Hasobe, T.
Number of pages: 6
Pages: 26-31
Publication date: 11 Jan 2019
Peer-reviewed: Yes
Early online date: 20 Nov 2018

Publication information

Journal: ACS Energy Letters
Volume: 4
Issue number: 1
ISSN (Print): 2380-8195
Original language: English
DOIs:
10.1021/acsenerylett.8b01964
Source: RIS
Source ID: urn:9E96397B0FF697D1EB23606A29362AF2
Research output: Contribution to journal › Letter › Scientific › peer-review

The economics of renewable CaC_2 and C_2H_2 production from biomass and CaO

This article presents the economics of a bio-based $\text{CaC}_2/\text{C}_2\text{H}_2$ production concept plant. The aim of the research was to study if renewable $\text{CaC}_2/\text{C}_2\text{H}_2$ production could be competitive in comparison with current technologies. The starting point was to integrate a wood char production unit into a combined heat and power (CHP) plant with a bubbling fluidized bed (BFB) boiler. The wood char was reacted with CaO in an electric arc furnace (EAF). The production costs of the CaC_2 were determined based on the wood char production costs as well as the EAF electric power consumption. The results showed that the C_2H_2 yield (18%) is similar to the current fossil-based production. However, the production costs proved to be even higher than the current selling prices of CaC_2 and C_2H_2 . With the chosen basic feedstock (20 €/MWh) and electricity prices (45 €/MWh) the production costs of CaC_2 were calculated to be 725 €/t and for C_2H_2 1805 €/t. The cost effectiveness of the concept plant was determined using the payback time method including the time value of money. The break even selling prices were 747–920 €/t for the CaC_2 and 1940–3015 €/t for C_2H_2 depending on the desired payback time (4–30 years). The key factors in the production costs of CaC_2 and C_2H_2 are the price of electricity and the electrical efficiency of the EAF. The results also showed that recycling the Ca at the site could save up to 48% in fresh Ca material costs.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Test Rig Finland, Inc.
Contributors: Pääkkönen, A., Tolvanen, H., Kokko, L.
Number of pages: 9
Pages: 40-48
Publication date: 1 Jan 2019
Peer-reviewed: Yes
Early online date: 10 Nov 2018

Publication information

Journal: Biomass and Bioenergy
Volume: 120
ISSN (Print): 0961-9534
Original language: English
ASJC Scopus subject areas: Forestry, Renewable Energy, Sustainability and the Environment, Agronomy and Crop Science, Waste Management and Disposal
Keywords: /C, H, Poly-generation, Renewable CaC, Renewable chemicals, Techno-economic evaluation
DOIs:
10.1016/j.biombioe.2018.10.020
Source: Scopus
Source ID: 85056214971
Research output: Contribution to journal › Article › Scientific › peer-review

An Artificial Nocturnal Flower via Humidity-Gated Photoactuation in Liquid Crystal Networks

Beyond their colorful appearances and versatile geometries, flowers can self-shape-morph by adapting to environmental changes. Such responses are often regulated by a delicate interplay between different stimuli such as temperature, light, and humidity, giving rise to the beauty and complexity of the plant kingdom. Nature inspires scientists to realize artificial systems that mimic their natural counterparts in function, flexibility, and adaptation. Yet, many of the artificial systems demonstrated to date fail to mimic the adaptive functions, due to the lack of multi-responsivity and sophisticated control over deformation directionality. Herein, a new class of liquid-crystal-network (LCN) photoactuators whose response is controlled by delicate interplay between light and humidity is presented. Using a novel deformation mechanism in LCNs, humidity-gated photoactuation, an artificial nocturnal flower is devised that is closed under daylight conditions when the humidity level is low and/or the light level is high, while it opens in the dark when the humidity level is high. The humidity-gated photoactuators can be fueled with lower light intensities than conventional photothermal LCN actuators. This, combined with facile control over the speed, geometry, and directionality of movements, renders the "nocturnal actuator" promising for smart and adaptive bioinspired microrobotics.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Eindhoven University of Technology

Contributors: Wani, O. M., Verpaalen, R., Zeng, H., Priimagi, A., Schenning, A. P.

Publication date: Jan 2019

Peer-reviewed: Yes

Early online date: 2018

Publication information

Journal: Advanced Materials

Volume: 31

Issue number: 2

Article number: 1805985

ISSN (Print): 0935-9648

Original language: English

ASJC Scopus subject areas: Materials Science(all), Mechanics of Materials, Mechanical Engineering

Keywords: actuator, azobenzene, bioinspired, humidity, light, liquid crystal, multi-responsive

DOIs:

10.1002/adma.201805985

Source: Scopus

Source ID: 85056318113

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

A Pentacene-based Nanotube Displaying Enriched Electrochemical and Photochemical Activities

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Pages: 1115-1119

Publication date: Jan 2019

Peer-reviewed: Yes

Early online date: 2018

Publication information

Journal: Angewandte Chemie - International Edition

Volume: 58

Issue number: 4

ISSN (Print): 1433-7851

Original language: English

ASJC Scopus subject areas: Catalysis, Chemistry(all)

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

DOIs:

10.1002/anie.201812976

Source: Scopus

Source ID: 85059193866

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

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

We employ atomic layer deposition to prepare 50 nm thick hematite photoanodes followed by passivating them with a 0.5 nm thick Ta₂O₅-overlayer and compare them with samples uniformly doped with the same amount of tantalum. We observe a three-fold improvement in photocurrent with the same onset voltage using Ta-overlayer hematite photoanodes, while electrochemical impedance spectroscopy under visible light irradiation shows a decreased amount of surface states under water splitting conditions. The Ta-doped samples have an even higher increase in photocurrent along with a 0.15 V cathodic shift in the onset voltage and decreased resistivity. However, the surface state capacitance for the Ta-doped sample is twice that of the reference photoanode, which implies a larger amount of surface hole accumulation. We further utilize transient absorption spectroscopy in the sub-millisecond to second timescale under operating conditions to show that electron trapping in both Ta₂O₅-passivated and Ta-doped samples is markedly reduced. Ultrafast transient absorption spectroscopy in the sub-picosecond to nanosecond timescale shows faster charge carrier dynamics and reduced recombination in the Ta-doped hematite photoanode resulting in the increased photoelectrochemical performance when compared with the Ta₂O₅-overlayer sample. Our results show that passivation does not affect the poor charge carrier dynamics intrinsic to hematite based photoanodes. The Ta-doping strategy results in more efficient electron extraction, solving the electron trapping issue and leading to increased performance over the surface passivation strategy.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 10

Pages: 3206-3215

Publication date: Jan 2019

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry A

Volume: 7

Issue number: 7

ISSN (Print): 2050-7488

Original language: English

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

Electronic versions:

c8ta09501a

DOIs:

10.1039/C8TA09501A

URLs:

<http://urn.fi/URN:NBN:fi:tty-201905141602>

Bibliographical note

INT=phys,"Ulkuniemi, Riina"

Source: Scopus

Source ID: 85061474749

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

Acetotrophic Activity Facilitates Methanogenesis from LCFA at Low Temperatures: Screening from Mesophilic Inocula

The inoculum source plays a crucial role in the anaerobic treatment of wastewaters. Lipids are present in various wastewaters and have a high methanogenic potential, but their hydrolysis results in the production of long chain fatty acids (LCFAs) that are inhibitory to anaerobic microorganisms. Screening of inoculum for the anaerobic treatment of LCFA-containing wastewaters has been performed at mesophilic and thermophilic conditions. However, an evaluation of inocula for producing methane from LCFA-containing wastewater has not yet been conducted at low temperatures and needs to be undertaken. In this study, three inocula (one granular sludge and two municipal digester sludges) were assessed for methane production from LCFA-containing synthetic dairy wastewater (SDW) at low temperatures (10 and 20°C). A methane yield (based on mL-CH₄/g-CODadded) of 86-65% with acetate and 45-20% with SDW was achieved within 10 days using unacclimated granular sludge, whereas the municipal digester sludges produced methane only at 20°C but not

at 10°C even after 200 days of incubation. The acetotrophic activity in the inoculum was found to be crucial for methane production from LCFA at low temperatures, highlighting the role of Methanosaeta (acetoclastic archaea) at low temperatures. The presence of bacterial taxa from the family Syntrophaceae (Syntrophus and uncultured taxa) in the inoculum was found to be important for methane production from SDW at 10°C. This study suggests the evaluation of acetotrophic activity and the initial microbial community characteristics by high-throughput amplicon sequencing for selecting the inoculum for producing methane at low temperatures (up to 10°C) from lipid-containing wastewaters.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Bio- and Circular Economy, Natl. University of Ireland, Galway

Contributors: Singh, S., Rinta-Kanto, J., Kettunen, R., Lens, P., Collins, G., Kokko, M., Rintala, J.

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: ARCHAEA

Volume: 2019

Article number: 1751783

ISSN (Print): 1472-3646

Original language: English

Electronic versions:

singh et al. 2019

DOIs:

10.1155/2019/1751783

URLs:

<http://urn.fi/URN:NBN:fi:tty-201905201648>

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

Antibacterial polymer fibres by rosin compounding and melt-spinning

The antibacterial features of natural pine/spruce rosin are well established, yet the functionality in various thermoplastics has not been surveyed. This work focuses on the processing of industrial grade purified rosin mixed with polyethylene (PE), polypropylene (PP), polylactic acid (PLA), polyamide (PA) and corn starch based biopolymer (CS). Homopolymer masterbatches were extrusion-compounded and melt-spun to form fibres for a wide range of products, such as filters, reinforcements, clothing and medical textiles. Due to the versatile chemical structure of rosin, it was observed compatible with all the selected polymers. In general, the rosin-blended systems were shear-thinning in a molten condition. The doped fibres spun of PE and PP indicated adequate melt-spinning capability and proper mechanical properties in terms of ultimate strength and Young's modulus. The antibacterial response was found dependent on the selected polymer. Especially PE with a 10 wt% rosin content showed significant antibacterial effects against *Escherichia coli* DH5 α and *Staphylococcus aureus* ATCC 12598 when analysed in the Ringer's solution for 24 h.

General information

Publication status: Accepted/In press

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Plastics and Elastomer Technology, Department of Microbiology, Bundesanstalt für Materialforschung und -prüfung (BAM), Premix Oy, Aalto University, COMP Centre of Excellence, University of Helsinki

Contributors: Kanerva, M., Puolakka, A., Takala, T. M., Elert, A. M., Mylläri, V., Jönkkäri, I., Sarlin, E., Seitsonen, J., Ruokolainen, J., Saris, P., Vuorinen, J.

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Materials Today Communications

Article number: 100527

ISSN (Print): 2352-4928

Original language: English

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

Keywords: Antibacterial, Fibre, Melt spinning, Thermoplastics

Electronic versions:

1-s2.0-S2352492819301114-main

DOIs:

10.1016/j.mtcomm.2019.05.003

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201906201900>

Bibliographical note

EXT="Mylläri, V."

Source: Scopus

Source ID: 85066275027

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

Bio-hydrogen Production from Sewage Sludge: Screening for Pretreatments and Semi-continuous Reactor Operation

Abstract: The high volumes of sewage sludge produced have raised interests for simultaneous treatment and clean energy production, e.g. in the form of hydrogen. Pretreatment of sewage sludge is required to enhance microbial degradation and in turn hydrogen yield from sewage sludge. The potential of five substrate pretreatments, individually and in combinations, to increase biohydrogen production from mixed primary and secondary sewage sludge at four incubation pH (5, 7, 9, and 11) was studied in batch assays. Alkali + ultrasonication pretreatment increased the hydrogen production almost seven times (0.35 mmol H₂/g VS) compared to untreated sewage sludge at initial pH 11. In general, higher hydrogen yields and lower acetate concentrations were obtained under alkaline conditions (pH 9 and 11), being more favorable for protein degradation and not favorable for hydrogen consumption via homoacetogenesis. Subsequently, fermentation of alkali + ultrasonication pretreated sewage sludge in a semi-continuous stirred tank reactor (CSTR) produced a maximum hydrogen yield of 0.1 mmol H₂/g VS, three times higher than the yield obtained from alkali pretreated sludge. The gas produced in the CSTRs contained a low concentration of CO₂ (< 5%), and is thus easily upgradable to biohydrogen. Graphic Abstract: [Figure not available: see fulltext.].

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Water Pollution Research Department, National Research Centre, Indian Institute of Technology Hyderabad, Natl. University of Ireland, Galway, Ain Shams University

Contributors: El-Qelish, M., Chatterjee, P., Dessì, P., Kokko, M., El-Gohary, F., Abo-Aly, M., Rintala, J.

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Waste and Biomass Valorization

ISSN (Print): 1877-2641

Original language: English

ASJC Scopus subject areas: Environmental Engineering, Renewable Energy, Sustainability and the Environment, Waste Management and Disposal

Keywords: Alkali treatment, Continuously stirred tank reactor (CSTR), Dark fermentation, Pretreatment, Sewage sludge, Ultrasonication

DOIs:

10.1007/s12649-019-00743-5

Source: Scopus

Source ID: 85069208392

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

Charge transfer dynamics in CsPbBr₃ perovskite quantum dots-anthraquinone/fullerene (C₆₀) hybrids

An advantage of colloidal quantum dots, particularly perovskite quantum dots (PQDs), as photoactive components is that they easily form complexes with functional organic molecules, which results in hybrids with enriched photophysical properties. Herein, we demonstrate the formation of stable ground state complexes of CsPbBr₃ PQD with two widely used molecular electron acceptors, fullerene (C₆₀) and anthraquinone, (AQ) which contain carboxylic anchor groups. Dynamics of the photo-induced electron transfer in the hybrids were compared. The use of carboxylic groups for binding results in stable complex formation and their photophysical properties depend on the ratio of components but not the absolute concentrations (up to micromolar concentrations). Time-resolved transient absorption (TA) spectroscopy shows that in both cases, a charge separated (CS) state is formed. Data analysis was aimed to evaluate the CS time constant in ideal one-to-one complexes and was found to be in the range of 30-190 ps. The CS state of PQD-AQ complexes recombines directly to the ground state in roughly one microsecond. Recombination of the CS state of PQD-C₆₀ is more complex and points to strong inhomogeneity of these complexes. Majority of the CS states relax by first forming the C₆₀ triplet state.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering

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

Number of pages: 8
Pages: 862-869
Publication date: 2019
Peer-reviewed: Yes
Early online date: 10 Dec 2018

Publication information

Journal: *Nanoscale*
Volume: 11
Issue number: 3
ISSN (Print): 2040-3364
Original language: English
ASJC Scopus subject areas: Materials Science(all)
DOIs:
10.1039/c8nr08445a
Source: Scopus
Source ID: 85060171357
Research output: Contribution to journal > Article > Scientific > peer-review

Effect of macro- and micro-nutrients addition during anaerobic mono-digestion of grass silage in leach-bed reactors

The effect of macro- (NH_4Cl) (set I) and micro-nutrients (Fe, Ni, Co and Mo) (set II) addition on chemical oxygen demand (COD) solubilisation during anaerobic mono-digestion of grass silage was investigated in two sets of leach bed reactor experiments at 35°C. Results showed that addition of NH_4Cl and micro-nutrients improved COD solubilisation by 18% (0.56 g SCOD g^{-1} volatile solids) and 7% (0.45 g SCOD g^{-1} VS), respectively than control. About 20–50% of the added micro-nutrients were bioavailable in the produced leachates, while the rest (50–80%) were adsorbed onto the grass silage. Results of biological methane potential assays showed that, specific methane yields of grass silage were improved by 17% ($0.36 \pm 0.02 \text{ m}^3 \text{ CH}_4 \text{ kg}^{-1} \text{ VS}_{\text{added}}$) when NH_4Cl was supplemented while Fe, Ni, Co and Mo addition improved methane yields by 15% ($0.33 \pm 0.005 \text{ m}^3 \text{ CH}_4 \text{ kg}^{-1} \text{ VS}_{\text{added}}$) when compared to control.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, International Crops Research Institute for the Semi-Arid Tropics, Griffith University, Jyväskylä yliopisto
Contributors: Jagadabhi, P. S., Kaparaju, P., Väisänen, A., Rintala, J.
Number of pages: 12
Pages: 418-429
Publication date: 2019
Peer-reviewed: Yes

Publication information

Journal: *Environmental Technology*
Volume: 40
Issue number: 4
ISSN (Print): 0959-3330
Original language: English
ASJC Scopus subject areas: Environmental Chemistry, Water Science and Technology, Waste Management and Disposal
Keywords: anaerobic digestion, grass silage, Leach bed reactor, methane, micro-nutrients
DOIs:
10.1080/09593330.2017.1393462
Source: Scopus
Source ID: 85032370604
Research output: Contribution to journal > Article > Scientific > peer-review

Exclusive occurrence of photoinduced energy transfer and switching of its direction by rectangular π -extension of nanographenes

As structure defined cutouts of the graphene lattice, nanographene molecules have gained plenty of attention because of their high potential for versatile applications in organic electronics and energy conversion devices and as ideal model systems for the better understanding of intrinsic structure-property correlations of graphenes. In this study, well-defined nanographenes with sp^2 carbon networks of different sizes, hexa-peri-hexabenzocoronene (HBC) and its rectangularly π -extended version, a short graphene nanoribbon (GNR), have been covalently functionalized with photoactive porphyrin molecules. On the basis of their spectroscopic studies, the photodynamics of the porphyrin-linked nanographenes was found to be influenced substantially by the size of the nanographenes. Photoexcitation of the porphyrin-HBC linked system led to exclusive energy transfer (EnT) from the first singlet excited state (S_1) of the nanographene to the porphyrin, whereas opposite selective EnT occurred from the first and second singlet excited states (S_1 and S_2) of the porphyrin to

the nanographene in the porphyrin-GNR linked system. In particular, ultrafast efficient EnTs from both the S_2 and S_1 states of the porphyrin to GNR mimic the corresponding ultrafast EnTs from the S_2 and S_1 states of carotenoids to chlorophylls in light-harvesting systems of natural photosynthesis. Such unique photophysical properties will be useful for the rational design of carbon-based photofunctional nanomaterials for optoelectronics and solar energy conversion devices.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 9

Pages: 6642-6650

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Chemical Science

Volume: 10

Issue number: 27

ISSN (Print): 2041-6520

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Electronic versions:

c9sc01538h

DOIs:

10.1039/c9sc01538h

URLs:

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

Source: Scopus

Source ID: 85068830304

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

Influence of titanium dioxide surface activation on the performance of mesoscopic perovskite solar cells

Perovskite solar cells with record efficiencies already above 24% are a highly promising clean energy technology. However, the reproducibility in their fabrication has proven to be challenging and needs more attention. Here we demonstrate that surface activation of the mesoscopic titanium dioxide (TiO₂) scaffold, utilized in the two-step perovskite synthesis process, significantly affects the final device performance. Irradiating the mesostructured substrate with ultraviolet (UV) light prior to lead iodide (PbI₂) deposition has a positive effect on the short-circuit current density and on the overall device performance (leading to a >20% increase in efficiency in our devices). As most of the UV light is absorbed in the topmost TiO₂ layer, the interior of the scaffold remains less activated. This results in a sparsely packed PbI₂ structure that facilitates an efficient conversion to the perovskite, while the activated topmost surface improves the perovskite capping layer. On the contrary, plasma treatment of the scaffold also activates the interior parts of the scaffold, which leads to a dense PbI₂ structure that hampers the conversion and causing a >25% efficiency drop. We show that also minor changes in the surface properties of the mesoporous TiO₂ scaffold can affect the device performance, which could explain some of the large efficiency variations observed between laboratories.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Åbo Akademi, Åbo Akademi University, Aalto University

Contributors: Masood, M. T., Weinberger, C., Qudsia, S., Rosqvist, E., Sandberg, O., Nyman, M., Sänden, S., Vivo, P., Aitola, K., Lund, P. D., Österbacka, R., Smått, J.

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Thin Solid Films

Volume: 686

Article number: 137418

ISSN (Print): 0040-6090

Original language: English

DOIs:

10.1016/j.tsf.2019.137418

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

Low-dimensional formamidinium lead perovskite architectures via controllable solvent intercalation

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 7

Pages: 3945-3951

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry C

Volume: 7

Issue number: 13

ISSN (Print): 2050-7534

Original language: English

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

DOIs:

10.1039/c9tc00379g

Source: Scopus

Source ID: 85064717293

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Molecules

Volume: 24

Issue number: 12

Article number: 2330

ISSN (Print): 1420-3049

Original language: English

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

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

Electronic versions:

molecules-24-02330

DOIs:

10.3390/molecules24122330

URLs:

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

Bibliographical note

EXT="Franzén, Robert"

Source: Scopus

Source ID: 85068104207

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

Multiphoton Excitation of CsPbBr₃ Perovskite Quantum Dots (PQDs): How Many Electrons Can One PQD Donate to Multiple Molecular Acceptors?

Metastable multiexcitonic states (MESs) of semiconductor quantum dots can be involved in multielectron transfer reactions, which opens new perspectives in nanomaterials-based optoelectronic applications. Herein, we demonstrate the generation of a MES in CsPbBr₃ perovskite quantum dots (PQDs) and its dissociation dynamics through multiple electron transfers to molecular electron acceptors, anthraquinones (AQs), bound to the PQD surface by a carboxylic anchor. As many as 14 excitons are produced at an excitation density of roughly 220 $\mu\text{J cm}^{-2}$ without detectable PQD degradation. Addition of AQ results in the formation of PQD-AQ hybrids with excess of AQs (PQD:AQ \approx 1:20), which opens the possibility of multielectron transfer acts from MES to AQs. We found that the electron transfer saturates after roughly five transfer acts and that the first electron transfer (ET) time constant is as short as 1 ps. However, each ET increases the Coulomb potential barrier for the next ET, which decreases the rate of ET, resulting in a saturation after five ETs.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 7

Pages: 2775-2781

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry Letters

ISSN (Print): 1948-7185

Original language: English

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

Electronic versions:

acs.jpcllett.9b01045

DOIs:

10.1021/acs.jpcllett.9b01045

URLs:

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

Source: Scopus

Source ID: 85066897133

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

O₂-requiring molecular reporters of gene expression for anaerobic microorganisms

Many genetic reporter systems require molecular oxygen; therefore, the use of reporter genes to study molecular mechanisms in anaerobic microorganisms has been hampered by the lack of convenient reporting systems. We describe reporter gene whole cell-based biosensor systems based on luciferase genes and the associated oxygen-requiring enzymes. By using two different oxygen-dependent reporters, insect and bacterial luciferases, and two bacterial hosts,

Gram (+) *Bifidobacterium longum* and Gram (-) *Escherichia coli*, we show that the enzymes can be used in gene expression studies of anaerobic bacteria. *E. coli*, a facultative anaerobe, was grown both in aerobic and anaerobic conditions with an arabinose-inducible expression system. We show that a short treatment time of few minutes in ambient atmosphere is sufficient to detect light emission from living cells that is directly proportional to the number of cells and to the inducer concentration. The induction levels were the same in both the aerobically and anaerobically cultured cells. Similar results were obtained in the case of *B. longum* cultured in anaerobic conditions.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 6

Pages: 1-6

Publication date: 2019

Peer-reviewed: Yes

Early online date: 20 Sep 2018

Publication information

Journal: Biosensors and Bioelectronics

Volume: 123

ISSN (Print): 0956-5663

Original language: English

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

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

Electronic versions:

1-s2.0-S0956566318307632-main

DOIs:

10.1016/j.bios.2018.09.066

URLs:

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

Source: Scopus

Source ID: 85053858794

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

Photoreactions of macrocyclic dyes on (1010) wurtzite surface – Interplay between conformation and electronic effects

Macrocyclic dyes such as phthalocyanine and porphyrin molecules are modeled on (10110) wurtzite surfaces using the DFT and molecular dynamics approaches. It is found that the single dye anchored on the wurtzite surface stabilizes in an inclined geometry with its core facing the surface at a tilting angle of ca 60°. The tilting of the dye relative to the crystal surface has a dual effect on the charge transfer from a chromophore to the semiconductor. Increasing the tilting angle leads to a stronger coupling between the lowest level of the semiconductor conduction band and dye's LUMO, thus raising the tunneling probability of the electron injection. By contrast, the electrostatic interaction between units upon the tilting of macrocycles results in a lowering of the molecule LUMO level with respect to the conduction band minimum of the wurtzite crystal, which may hinder the electron transfer. The type of a linker and peripheral substituents significantly affect the mutual conformation of the moieties, and their proper choice can facilitate the photoinduced charge transfer reactions.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Materials Science and Environmental Engineering, South-Ukrainian National University, Center for Innovation Technologies

Contributors: Golovanova, V. V., Nazarchuk, B. V., Postnyi, O. V., Rantala, T. T., Tkachenko, N. V., Golovanov, V. V.

Number of pages: 9

Pages: 63-71

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Ukrainian Journal of Physics

Volume: 64

Issue number: 1

ISSN (Print): 2071-0186

Original language: English

ASJC Scopus subject areas: Physics and Astronomy(all)

Keywords: DFT, Electron transfer, Macrocyclic dyes, Wurzite

DOIs:

10.15407/ujpe64.1.63

Bibliographical note

EXT="Golovanov, V. V."

Source: Scopus

Source ID: 85062936078

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

Storing of exoelectrogenic anolyte for efficient microbial fuel cell recovery

Starting up a microbial fuel cell (MFC) requires often a long-term culture enrichment period, which is a challenge after process upsets. The purpose of this study was to develop low cost storage for microbial fuel cell enrichment culture to enable prompt process recovery after upsets. Anolyte of an operating xylose-fed MFC was stored at different temperatures and for different time periods. Storing the anolyte for one week or one month at +4 °C did not significantly affect power production, but lag time for power production was increased from 2 days to 3 or 5 days, respectively. One month storing at -20 °C increased the lag time to 7 days. The average power density in these MFCs varied between 1.2 and 1.7 W/m³. The share of dead cells (measured by live/dead staining) increased with storing time. After six-month storage the power production was insignificant. However, xylose removal remained similar in all cultures (99-100%) whilst volatile fatty acids production varied. The results indicate that fermentative organisms tolerated the long storage better than the exoelectrogens. As storing at +4 °C is less energy intensive compared to freezing, anolyte storage at +4 °C for maximum of one month is recommended as start-up seed for MFC after process failure to enable efficient process recovery.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Haavisto, J. M., Lakaniemi, A., Puhakka, J. A.

Publication date: 2019

Peer-reviewed: Yes

Early online date: 2018

Publication information

Journal: Environmental Technology

Volume: 40

Issue number: 11

ISSN (Print): 0959-3330

Original language: English

Electronic versions:

Storing of exoelectrogenic anolyte for efficient microbial fuel cell recovery

DOIs:

10.1080/09593330.2017.1423395

URLs:

<http://urn.fi/URN:NBN:fi:ty-201907151971>

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

Structure and Dynamics of Thermosensitive pDNA Polyplexes Studied by Time-Resolved Fluorescence Spectroscopy

Combining multiple stimuli-responsive functionalities into the polymer design is an attractive approach to improve nucleic acid delivery. However, more in-depth fundamental understanding how the multiple functionalities in the polymer structures are influencing polyplex formation and stability is essential for the rational development of such delivery systems. Therefore, in this study the structure and dynamics of thermosensitive polyplexes were investigated by tracking the behavior of labeled plasmid DNA (pDNA) and polymer with time-resolved fluorescence spectroscopy using fluorescence resonance energy transfer (FRET). The successful synthesis of a heterofunctional poly(ethylene glycol) (PEG) macroinitiator containing both an atom transfer radical polymerization (ATRP) and reversible addition-fragmentation chain-transfer (RAFT) initiator is reported. The use of this novel PEG macroinitiator allows for the controlled polymerization of cationic and thermosensitive linear triblock copolymers and labeling of the chain-end with a fluorescent dye by maleimide-thiol chemistry. The polymers consisted of a thermosensitive poly(N-isopropylacrylamide) (PNIPAM, N), hydrophilic PEG (P), and cationic poly(2-(dimethylamino)ethyl methacrylate) (PDMAEMA, D) block, further referred to as NPD. Polymer block D chain-ends were labeled with Cy3, while pDNA was labeled with FITC. The thermosensitive NPD polymers were used to prepare pDNA polyplexes, and the effect of the N/P charge ratio, temperature, and composition of the triblock copolymer on the polyplex properties were investigated, taking nonthermosensitive PD polymers as the control. FRET was observed both at 4 and 37 °C, indicating that the introduction of the thermosensitive PNIPAM block did not compromise the polyplex structure even above the polymer's cloud point. Furthermore, FRET results showed that the NPD- and PD-based polyplexes have a less dense core compared to polyplexes based on cationic homopolymers (such

as PEI) as reported before. The polyplexes showed to have a dynamic character meaning that the polymer chains can exchange between the polyplex core and shell. Mobility of the polymers allow their uniform redistribution within the polyplex and this feature has been reported to be favorable in the context of pDNA release and subsequent improved transfection efficiency, compared to nondynamic formulations.

General information

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

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

Contributors: Fliervoet, L. A., Lisitsyna, E. S., Durandin, N. A., Kotsis, I., Maas-Bakker, R. F., Yliperttula, M., Hennink, W. E., Vuorimaa-Laukkanen, E., Vermonden, T.

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Biomacromolecules

ISSN (Print): 1525-7797

Original language: English

ASJC Scopus subject areas: Bioengineering, Biomaterials, Polymers and Plastics, Materials Chemistry

Electronic versions:

acs.biomac.9b00896

DOIs:

10.1021/acs.biomac.9b00896

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201910244071>

Source: Scopus

Source ID: 85073002500

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

Sustainability of bioenergy in finland and globally – fact check

The sustainability of bioenergy has attracted recently a lot of debate and there has been critical arguments for and against the use of bioenergy. This presentation examines six international publications dealing with the use of bioenergy and collects systematically the allegations of bioenergy, as well as arguments for defending and restricting bioenergy use in the publications. Some of the most controversial arguments are analyzed more thoroughly and they are subjected to fact checking by comparing arguments with sources in scientific literature. At the same time, the preconditions, restrictions, and assumptions that can be used to modify the claims to favor desired arguments are identified. The study finds that there are several problems that can be criticized towards the arguments. Arguments can be justified, among others, by looking at the situation over different time periods or by emphasizing the maximization of short-term or long-term climate benefits. Different values can be selected from initial data, whereupon their own argument can be confirmed.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Materials Science and Environmental Engineering, Lappeenranta University of Technology, Tampere University

Contributors: Vakkilainen, E., Konttinen, J., Orasuo, V., Aalto, P.

Number of pages: 2

Pages: 1634-1635

Publication date: 2019

Host publication information

Title of host publication: 27th European Biomass Conference and Exhibition, EUBCE 2019

Publisher: ETA-Florence Renewable Energies

Publication series

Name: European Biomass Conference and Exhibition Proceedings

ISSN (Print): 2282-5819

ASJC Scopus subject areas: Agronomy and Crop Science, Forestry, Renewable Energy, Sustainability and the Environment, Waste Management and Disposal

Keywords: Bioenergy, Carbon neutrality, Carbon sinks, Climate change, Fact check, Forest Biomass, Sustainability

Bibliographical note

jufoid=71903

Source: Scopus

Source ID: 85071067879

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Faculdade de Farmacia da Universidade de Lisboa, University of Jyväskylä

Contributors: Assoah, B., Riihonen, V., Vale, J. R., Valkonen, A., Candeias, N. R.

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Molecules

Volume: 24

Issue number: 13

Article number: 2405

ISSN (Print): 1420-3049

Original language: English

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

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

Electronic versions:

molecules-24-02405

DOIs:

10.3390/molecules24132405

URLs:

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

Bibliographical note

EXT="Valkonen, Arto"

INT=msee,"Riihonen, Vesa"

INT=msee,"Vale, João R."

Source: Scopus

Source ID: 85068362408

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

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

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

General information

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

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

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

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Separation Science and Technology (Philadelphia)

ISSN (Print): 0149-6395

Original language: English

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

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

DOIs:

10.1080/01496395.2019.1600553

Source: Scopus

Source ID: 85065190589

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

Zinc phthalocyanine activated by conventional indoor light makes a highly efficient antimicrobial material from regular cellulose

Zn phthalocyanine with improved synthesis suitable for bulk production shows extremely high antimicrobial efficacies even under weak indoor light. The dye-impregnated cellulose material inactivates over 99.996% of drug-resistant *C. albicans*, *S. aureus* and *E. faecalis* in just one hour exposure with consumer-grade fluorescent lamps and diodes.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Grammatikova, N. E., George, L., Ahmed, Z., Candeias, N. R., Durandin, N. A., Efimov, A.

Pages: 4379-4384

Publication date: 2019

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry B

Volume: 7

Issue number: 28

ISSN (Print): 2050-750X

Original language: English

Electronic versions:

c9tb01095e

DOIs:

10.1039/C9TB01095E

URLs:

<http://urn.fi/URN:NBN:fi:tty-201909032059>

Source: ORCID

Source ID: /0000-0003-2414-9064/work/59045423

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

Reversible photodoping of TiO₂ nanoparticles

Observations on strong photochromic effect of crystalline TiO₂ quantum dots (mean size \approx 4 nm) are presented. The synthesized quantum dots consist of irregularly shaped anatase TiO₂ nanoparticles (NPs) and are dispersed in butanol (8 % by mass). Obtained NPs exhibit a dramatic photo-response to UV light, enabling effective transmittance modulation in a broad wavelength range extending from visible to near-infrared region, and even the thermal black body radiation regime beyond 10 μ m. The exceptional photo-response is attributed to hole-scavenging by butanol, TiO₂ self-reduction, injection of electrons to the conduction band, and consequent localized surface plasmon resonances in NPs. Observed optical effect is reversible and the initial high transmittance state can be restored simply by exposing the NPs to air. Applied NP synthesis route is economic and can be easily scaled for applications such as smart window technologies.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Pages: 8968-8974

Publication date: 26 Dec 2018

Peer-reviewed: Yes

Early online date: 10 Dec 2018

Publication information

Journal: Chemistry of Materials

Volume: 30

Issue number: 24

ISSN (Print): 0897-4756

Ratings:

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

Original language: English

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

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

DOIs:

10.1021/acs.chemmater.8b04813

URLs:

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

Bibliographical note

INT=fot,"Joost, Urmas"

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

Bioengineering optimization and microbial characterization of elemental sulfur-fueled denitrifying biofilms

Nowadays, the increasing human population and limited water resources create a demand for sustainable wastewater treatment technologies. Chemically synthesized elemental sulfur (S^0)-based denitrification is an effective and cost-efficient biotechnology for nitrate (NO_3^-) removal from organic-deficient wastewaters. However, the hydrophobic properties of S^0 limit its application for denitrification. Thus, the goal of this project is to optimize the performance and explore the treatment mechanisms of S^0 -fueled denitrification in biofilm systems, and the understanding of the associated microbial communities.

To address the limitation of the chemically synthesized S^0 -driven denitrification applications, S^0 solubilization prior to S^0 -driven denitrification was studied in batch bioassays. The kinetic experiments showed that the achieved denitrification and denitrification rates were 20.9 and 10.7 mg $N/L \cdot d$, respectively. Microbiological analysis detected the presence of the Helicobacteraceae family onto S^0 particles, that was likely responsible for the S^0 solubilization. A mathematical model of microbially-catalyzed S^0 hydrolysis and subsequent two-step denitrification was developed. The sensitivity analysis identified the dominance of the hydrolysis-related parameters, and suggested that microbially-catalyzed surface-based S^0 hydrolysis is the rate-limiting step during S^0 -driven denitrification.

Autotrophic denitrification with biosulfur (ADBIOS), a by-product of biological gas desulfurization, was investigated in batch bioassays as an alternative technological solution for treating NO_3^- pollution in wastewaters. Denitrification and denitrification rates of 49.4 mg $NO_3^-/N/L \cdot d$ and 73.0 mg $NO_2^-/N/L \cdot d$, respectively, were obtained. The *Thiobacillus*, *Moheibacter* and *Thermomonas* genera were dominating the ADBIOS microbial community.

Two duplicate moving-bed biofilm reactors (MBBRs) with AnoxKTM K1 (K1) and AnoxKTM Z-200 (Z-200) carriers were operated for 309 days. The effect of the nitrate loading rate on the ADBIOS performance was studied by decreasing hydraulic retention time (HRT) from 72 to 21 h. The denitrification rates of 236 and 234 mg $NO_3^-/N/L \cdot d$ were achieved at an HRT of 24 h for K1 and an HRT of 21 h for Z-200 carrier, respectively. Based on RNA analysis, the same active bacteria, belonging to *Thiobacillus*, *Truepera*, *Flavobacterium* and *Hyphomonas* genera, were dominating MBBRs with K1 and Z-200 carriers.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Chemistry and Bioengineering

Contributors: Kostrytsia, A.

Number of pages: 142

Publication date: 6 Dec 2018

Publication information

Original language: English

URLs:

<http://urn.fi/URN:NBN:fi:ty-201902211260>. Embargo ends: 31/12/19

Research output: Book/Report > Doctoral thesis > Collection of Articles

Experimental and Modeling Assessment of the Main Bio-physical-chemical mechanisms and Kinetics in High-solids Anaerobic Digestion of Organic Waste

The organic fraction of municipal solid waste (OFMSW) includes readily biodegradable wastes such as food waste, and slowly biodegradable wastes such as lignocellulosic materials. Anaerobic digestion (AD) is a mature treatment biotechnology in which OFMSW is decomposed to a mixture of methane (CH₄) and carbon dioxide (CO₂), known as biogas. Due to the elevated CH₄ content (50 - 70 %), biogas can be used as a source of renewable energy. Moreover, AD yields also a partially stabilized digestate, allowing the recycle of nutrients back to agriculture.

High-solids anaerobic digestion (HS-AD) is a well-suited strategy to enhance the overall AD efficiency for OFMSW treatment. HS-AD is operated at a total solid (TS) content $\geq 10\%$, permitting to reduce the reactor size and overall operational costs. Nonetheless, the TS increase can result into biochemical instability, and even reactor failure by acidification. Both the high organic load and the buildup of inhibitors can be responsible for the HS-AD instability. The most notable inhibitor in HS-AD of OFMSW is the free ammonia nitrogen (NH₃). Therefore, a balance is often required between enhancing the HS-AD economy and the 'undesired' instability for OFMSW treatment.

This PhD research investigated the main bio-physical-chemical mechanisms and kinetics in HS-AD of OFMSW, with the aim to optimize the industrial application and maximize the kinetic rates. Laboratory-scale batch and semi-continuous experiments highlighted the main strengths and weaknesses of HS-AD. Simultaneously, the development of a HS-AD model permitted to condense the experimental knowledge about the main bio-physical-chemical effects occurring when increasing the TS content in HS-AD.

HS-AD batch experiments required a tradeoff between the initial TS, the inoculum-to-substrate ratio (ISR), the alkalinity and the nitrogen content, to assess the effects of increasing the initial TS content upon the methane yield, TS removal and chemical oxygen demand conversion. Particularly, a low ISR led to acidification, whereas the NH₃ buildup led to volatile fatty acid (VFA) accumulation, reducing the methane yield, whether or not co-digestion of OFMSW with beech sawdust was used.

In semi-continuous experiments, HS-AD of OFMSW required a reduced effluent compared to the influent to counterbalance the organic mass removal associated to the biogas production. Nonetheless, mono-digestion of readily-biodegradable OFMSW could not sustain a TS $\geq 10\%$ without exacerbating the risk of substrate overload. Overloading was associated to the high biodegradability of OFMSW and the NH₃ buildup. Thus, adding sawdust to OFMSW permitted to operate the reactors up to 30 % TS, due to the lower biodegradability and nitrogen content of lignocellulosic substrates.

As the main novelty of this PhD research, a HS-AD model based on the Anaerobic Digestion Model No.1 (ADM1) was developed. This model simulates the reactor mass and TS in HS-AD, in contrast of models focusing on 'wet' AD simulations (TS < 10 %). Moreover, the HS-AD model considers also the TS concentration effect on soluble species. A 'non-ideal' bio-physical-chemical module, modifying predominantly the acid-base equilibrium constants, was subsequently coupled to the HS-AD model. Noteworthy, HS-AD is often characterized by a high ionic strength ($I \geq 0.2$ M), affecting the pH, NH₃ concentration and CO₂ liquid-gas transfer, as the most important triggers for HS-AD inhibition.

The HS-AD model calibration required multiple experimental datasets to circumvent parameter non-identifiability. The model calibration showed that HS-AD of OFMSW might be operated at I up to 0.9 M and NH₃ concentrations up to 2.3 g N/L, particularly at higher TS contents (25 - 30 %). Moreover, the model calibration suggested that a reversible non-competitive NH₃ inhibition should be further tested. Further HS-AD model developments (e.g. precipitation) were also recommended. All these results might aid in the optimization of HS-AD for organic waste treatment, renewable energy and nutrient recovery.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Chemistry and Bioengineering

Contributors: Pastor Poquet, V.

Number of pages: 237

Publication date: 5 Dec 2018

Publication information

Original language: English

URLs:

<http://urn.fi/URN:NBN:fi:tty-201902211259>. Embargo ends: 31/12/19

Research output: Book/Report > Doctoral thesis > Collection of Articles

Optimization of fermentative biohydrogen production by *Thermotoga neapolitana*

Hydrogen has revealed a great potential as a versatile and non-polluting energy carrier of the future providing a high energy density and an efficiently conversion to usable power. Dark fermentation is one of the most promising biological production processes, but still has to overcome major challenges, most importantly low hydrogen production rates (HPRs) and hydrogen yields (HYs), before its industrial application becomes cost- and energy-efficient.

In this work, we aimed to optimize the hydrogen production via dark fermentation by *Thermotoga neapolitana*. The main

objectives were to enhance the HPR and maintain a high HY using different approaches to counteract process limitations and prevent the most relevant inhibitions. Furthermore, a development of the industrially preferred continuous-flow process was projected.

An increase of the initial biomass concentration from 0.46 to 1.74 g cell dry weight (CDW)/L in batch bioassays resulted in a more than 2-fold enhancement of the HPR up to 654 (± 30) mL/L/h (mL of hydrogen produced per L of volume of reactor per hour of reaction or per hour of liquid retention) without negatively affecting the HY. However, while the volumetric productivity increased the specific HPR (per unit of biomass) was negatively correlated with the HPR and the biomass concentration.

Subsequently, we investigated the supersaturation of hydrogen in the liquid phase (H_{2aq}) in batch bioassays. At 100 rpm agitation H_{2aq} supersaturated up to 3 times the equilibrium concentration. Increasing the agitation speed diminished the accumulation of H_{2aq} until an equilibrium between the gas and liquid phase hydrogen was reached with 500 rpm agitation at low cell concentrations. A raise from 200 to 600 rpm gradually reduced H_{2aq} from 21.9 (± 2.2) to 8.5 (± 0.1) mL/L and approximately doubled the HPR, revealing a direct correlation between the two parameters. Similarly, the addition of K1 carrier and H_2 -rich biogas recirculation (GaR) successfully counteracted the accumulation of H_{2aq} . Accelerating the process by increasing the reactors biomass concentration up to 0.79 g CDW/L, GaR revealed to be more efficient in removing H_{2aq} than 500 rpm agitation. The application of GaR at 300 and 500 rpm enhanced the HPR by approximately 260% up to 850 (± 71) mL/L/h, compared to a sole 300 rpm agitation, reaching a HY of 3.5 mol H_2 /mol glucose. We demonstrated that an insufficient gas-liquid mass transfer leads to the accumulation of H_{2aq} which inhibits the yield but even more so the rate of dark fermentation.

In the final phase of this project we successfully maintained continuous-flow hydrogen production. Increasing the feed glucose concentration from 11.1 to 41.6 mM diminished the HY from 3.6 (± 0.1) to 1.4 (± 0.1) mol H_2 /mol glucose. The HPR increased concomitantly up to approximately 55 mL/L/h at 27.8 mM of glucose, whereas a further increase of feed glucose to 41.6 mM did not enhance the HPR and the acetic acid (AA) concentration. To investigate whether high levels of AA limited the process, the feed AA concentration was gradually increased. However, this revealed no negative effect on continuous dark fermentation up to 240 mM of feed AA and, throughout the 110 days of continuous fermentation, the HY increased by 47%. Decreasing the hydraulic retention time (HRT) from 24 to 7 h also led to a HPR enhancement from 82 (± 1) to 192 (± 4) mL/L/h, while decreasing the HY. Concomitantly, the H_{2aq} accumulated, directly correlated to the HPR reaching 15.6 mL/L at an HRT of 7 h and 500 rpm agitation. The application of GaR efficiently counteracted the supersaturation of H_{2aq} and allowed the highest HPR of 277 mL/L/h at a HRT of 5 h.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Chemistry and Bioengineering

Contributors: Dreschke, G.

Number of pages: 124

Publication date: 5 Dec 2018

Publication information

Original language: English

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201902211258>. Embargo ends: 31/12/19

Research output: Book/Report > Doctoral thesis > Collection of Articles

Highly Efficient Energy Transfer Cassettes by Assembly of Boronic Acid Derived Salicylidenehydrazone Complexes

Energy transfer cassettes that build on the platform of boronic acid derived salicylidenehydrazone (BASHY) complexes were prepared. The functional flexibility of the BASHY chromophore was underpinned by its tunable role as energy donor or acceptor, integrated in compact and non-conjugated bichromophoric dyads. The energy transfer is highly efficient ($\Phi_{ET} > 0.95$) and is assumed to proceed mainly via a through-bond mechanism. Both constituent chromophores benefit mutually from their integration in the cassettes: a) The pseudo Stokes shift is increased to 110–200 nm; b) the antenna (donor) chromophore improves the light absorption of the acceptor chromophore; and c) the emission window of the BASHY chromophore is expanded in the BASHY-Bodipy dye without using strategies that compromise the observation of high quantum yields. The application of the cassettes for the formulation of fluorescent polymeric nanoparticles, that can be internalized in cells and observed by fluorescence imaging, was demonstrated using the BASHY-Bodipy dye as an example.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Chemistry & Advanced Materials, Chemistry and Bioengineering, Univ Lisbon, Fac Farm, Inst Invest Medicamento iMed ULisboa, Faculdade de Farmacia da Universidade de Lisboa, Universidad de Huelva

Contributors: Santos, F. M. F., Dominguez, Z., Alcaide, M. M., Matos, A. I., Florindo, H. F., R. Candeias, N., Gois, P. M. P., Pischel, U.

Pages: 1038-1045
Publication date: Dec 2018
Peer-reviewed: Yes
Early online date: 3 Sep 2018

Publication information

Journal: ChemPhotoChem
Volume: 2
Issue number: 12
ISSN (Print): 2367-0932
Original language: English
DOIs:
10.1002/cptc.201800150

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 12

Pages: 16191-16202

Publication date: 29 Nov 2018

Peer-reviewed: Yes

Publication information

Journal: ACS Omega

Volume: 3

Issue number: 11

ISSN (Print): 2470-1343

Ratings:

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

Original language: English

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

Electronic versions:

acsomega.8b02381

DOIs:

10.1021/acsomega.8b02381

URLs:

<http://urn.fi/URN:NBN:fi:tty-201812212899>

Source: Scopus

Source ID: 85057603661

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

Liquid Crystal Polymer Networks and Elastomers for Light-Fueled Robotics

Summary Liquid crystal (LC) polymer networks and elastomers are synthetic cross-linked polymer systems constituting liquid crystalline building blocks, or mesogens. This chapter provides an up-to-date overview of light-fueled LC network

(LCN) robotics. It explains photoactuation and light robotics, and discusses the basic physics that a small-scale LCN robot encounters, as the forces at the microscale are very different from common everyday experience. The chapter also introduces the photoactuation mechanisms, making a comparison between photothermal and photochemical actuation strategies, which often times yield distinct actuation behavior and shape changes. Azobenzene-based photochemical actuators often times exhibit photoinduced bending as opposed to in-plane photocontraction. The chapter considers autonomous actuation, driven by dynamic light-response in the material, to adopt a significant role in the design of future LCN robots. Uniaxially aligned LCNs can undergo reversible contraction-expansion along the molecular director axis, thus presenting muscle-like motion under external stimulus.

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

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

Contributors: Zeng, H., Lahikainen, M., Wani, O. M., Berdin, A., Priimagi, A.

Number of pages: 30

Pages: 197-226

Publication date: 19 Nov 2018

Host publication information

Title of host publication: Photoactive Functional Soft Materials

Publisher: John Wiley & Sons, Ltd

Editor: Li, Q.

ISBN (Print): 978-3-527-34482-6

ISBN (Electronic): 978-3-527-81677-4

Keywords: elastomers, light-fueled robotics, liquid crystal polymer networks, photochemical actuation, photothermal actuation, small-scale robots, soft micro-robotics, uniaxial contraction, uniaxial expansion

DOIs:

10.1002/9783527816774.ch6

Source: Bibtext

Source ID: urn:66e666ef0dccb2541602941e2c2fbc04

Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific › peer-review

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 10

Pages: 17062-17071

Publication date: 16 Nov 2018

Peer-reviewed: Yes

Publication information

Journal: Chemistry - A European Journal

Volume: 24

Issue number: 64

ISSN (Print): 0947-6539

Ratings:

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

Original language: English

ASJC Scopus subject areas: Catalysis, Organic Chemistry

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

DOIs:

10.1002/chem.201803257

Source: Scopus

Source ID: 85055548433

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

Understanding Dissolution and Crystallization with Imaging: A Surface Point of View

The tendency for crystallization during storage and administration is the most considerable hurdle for poorly water-soluble drugs formulated in the amorphous form. There is a need to better detect often subtle and complex surface crystallization phenomena and understand their influence on the critical quality attribute of dissolution. In this study, the interplay between surface crystallization of the amorphous form during storage and dissolution testing, and its influence on dissolution behavior, is analyzed for the first time with multimodal nonlinear optical imaging (coherent anti-Stokes Raman scattering (CARS) and sum frequency generation (SFG)). Complementary analyses are provided with scanning electron microscopy, X-ray diffraction and infrared and Raman spectroscopies. Amorphous indomethacin tablets were prepared and subjected to two different storage conditions (30 °C/23% RH and 30 °C/75% RH) for various durations and then dissolution testing using a channel flow-through device. Trace levels of surface crystallinity previously imaged with nonlinear optics after 1 or 2 days of storage did not significantly decrease dissolution and supersaturation compared to the freshly prepared amorphous tablets while more extensive crystallization after longer storage times did. Multimodal nonlinear optical imaging of the tablet surfaces after 15 min of dissolution revealed complex crystallization behavior that was affected by both storage condition and time, with up to four crystalline polymorphs simultaneously observed. In addition to the well-known α - and β -forms, the less reported metastable γ - and δ -forms were also observed, with the γ -form being widely observed in samples that had retained significant surface amorphousness during storage. This form was also prepared in the pure form and further characterized. Overall, this study demonstrates the potential value of nonlinear optical imaging, together with more established solid-state analysis methods, to understand complex surface crystallization behavior and its influence on drug dissolution during the development of amorphous drugs and dosage forms.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, University of Helsinki, University of Helsinki Faculty of Medicine, University of Otago

Contributors: Novakovic, D., Isomäki, A., Pleunis, B., Fraser-Miller, S. J., Peltonen, L., Laaksonen, T., Strachan, C. J.

Number of pages: 13

Pages: 5361-5373

Publication date: 5 Nov 2018

Peer-reviewed: Yes

Publication information

Journal: Molecular Pharmaceutics

Volume: 15

Issue number: 11

ISSN (Print): 1543-8384

Ratings:

Scopus rating (2018): CiteScore 4.7 SJR 1.402 SNIP 1.165

Original language: English

ASJC Scopus subject areas: Molecular Medicine, Pharmaceutical Science, Drug Discovery

Keywords: amorphous, dissolution, indomethacin, nonlinear optics, polymorphism, surface crystallization

Electronic versions:

acs.molpharmaceut.8b00840-2

DOIs:

10.1021/acs.molpharmaceut.8b00840

URLs:

<http://urn.fi/URN:NBN:fi:tty-201811222753>

Bibliographical note

EXT="Isomäki, Antti"

Source: Scopus

Source ID: 85054882971

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

Production and Synthetic Modifications of Shikimic Acid

Shikimic acid is a natural product of industrial importance utilized as a precursor of the antiviral Tamiflu. It is nowadays produced in multihundred ton amounts from the extraction of star anise (*Illicium verum*) or by fermentation processes.

Apart from the production of Tamiflu, shikimic acid has gathered particular notoriety as its useful carbon backbone and inherent chirality provide extensive use as a versatile chiral precursor in organic synthesis. This review provides an overview of the main synthetic and microbial methods for production of shikimic acid and highlights selected methods for isolation from available plant sources. Furthermore, we have attempted to demonstrate the synthetic utility of shikimic acid by covering the most important synthetic modifications and related applications, namely, synthesis of Tamiflu and derivatives, synthetic manipulations of the main functional groups, and its use as biorenewable material and in total synthesis. Given its rich chemistry and availability, shikimic acid is undoubtedly a promising platform molecule for further exploration. Therefore, in the end, we outline some challenges and promising future directions.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Research group: Chemistry & Advanced Materials, Chemistry and Bioengineering, Bulgarian Acad Sci, Bulgarian Academy of Sciences, Inst Organ Chem, Ctr Phytochem, Lab Organ Synth & Stereochem

Contributors: Candeias, N. R., Assoah, B., Simeonov, S. P.

Number of pages: 93

Pages: 10458-10550

Publication date: 24 Oct 2018

Peer-reviewed: Yes

Publication information

Journal: Chemical Reviews

Volume: 118

Issue number: 20

ISSN (Print): 0009-2665

Ratings:

Scopus rating (2018): CiteScore 54.26 SJR 22.157 SNIP 12.162

Original language: English

Keywords: OSELTAMIVIR PHOSPHATE TAMIFLU, DIELS-ALDER REACTION, ESCHERICHIA-COLI STRAIN, CHINESE STAR ANISE, HIGHLY EFFICIENT SYNTHESIS, MARINE NATURAL-PRODUCT, CARBOHYDRATE PHOSPHOTRANSFERASE SYSTEM, INFLUENZA NEURAMINIDASE INHIBITOR, INTERMEDIATES POTENTIALLY USEFUL, ABUNDANT (-)-SHILDMIC ACID

DOIs:

10.1021/acs.chemrev.8b00350

Source: WOS

Source ID: 000448754700006

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

Decane-1,2-diol derivatives as potential antitumor agents for the treatment of glioblastoma

Glioblastoma remains the most common and aggressive type of malignant brain tumor among adults thus, considerable attention has been given to discovery of novel anti-tumor drugs for its treatment. This study reports the synthesis of a series of twelve novel decane-1,2-diol derivatives and evaluation of its anti-tumor activity in mammalian glioblastoma cell lines, U87 and LN229. Starting from decane-1,2-diol, several derivatives were prepared using a diversity oriented synthesis approach through which a small library composed of esters, silyl ethers, sulfonates, sulfites, sulfates, ketals, and phosphonates was built. The decane-1,2-diol ditosylated derivative, DBT, found to have higher cytotoxicity than the standard drug cisplatin, has IC₅₀ value of 52 μM in U87 and 270 μM in LN229. Migration analysis of U87 cell line treated with the DBT indicated its ability to effectively suppress proliferation during initial hours of treatment and decrease anti-proliferative property over time. Additionally, DBT was assessed for its role in apoptosis, oxidative stress and caspase 3/7 activation in U87. Interestingly, our experiments indicated that its cytotoxicity is independent of Reactive oxygen species induced caspase 3/7 activity. The compound also exhibited caspase independent apoptosis activity in U87. DBT treatment led to G1/S cell cycle arrest and apoptosis induction of glioma cell lines. In addition, we identified 1,533 genes with significant changes at the transcriptional level, in response to DBT. A molecular docking study accounting for the interaction of DBT with NMDA receptor disclosed several hydrogen bonds and charged residue interactions with 17 amino acids, which might be the basis of the DBT cytotoxicity observed. We conclude that this molecule exerts its cytotoxicity via caspase 3/7 independent pathways in glioblastoma cells. Concisely, simple decane-1,2-diol derivatives might serve as scaffolds for the development of effective anti-glioblastoma agents.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Chemistry and Bioengineering, Research group: Computational Systems Biology, Research group: Chemistry & Advanced Materials, Research group: Predictive Society and Data Analytics (PSDA), Centre of Advanced Study in Crystallography & Biophysics, University of Madras, Chennai - 600 025.

Contributors: Viswanathan, A., Zhurina, A., Assoah, B., Paakkunainen, A., Musa, A., Kute, D., Saravanan, K. M., Yli-Harja, O., Candeias, N. R., Kandhavelu, M.

Pages: 105-116
Publication date: 15 Oct 2018
Peer-reviewed: Yes
Early online date: 1 Sep 2018

Publication information

Journal: European Journal of Pharmacology
Volume: 837
ISSN (Print): 0014-2999
Ratings:
Scopus rating (2018): CiteScore 3.24 SJR 1.001 SNIP 0.958
Original language: English
DOIs:
10.1016/j.ejphar.2018.08.041

Bibliographical note

INT=tut-bmt,"Zhurina, Anastasia"
INT=keb,"Paakkunainen, Aleks"
INT=tut-bmt,"Kute, Dinesh"
Source: PubMed
Source ID: 30179612
Research output: Contribution to journal > Article > Scientific > peer-review

Reconfigurable photoactuator through synergistic use of photochemical and photothermal effects

A reconfigurable actuator is a stimuli-responsive structure that can be programmed to adapt different shapes under identical stimulus. Reconfigurable actuators that function without control circuitry and are fueled remotely are in great demand to devise adaptive soft robotic devices. Yet, obtaining fast and reliable reconfiguration remains a grand challenge. Here we report a facile fabrication pathway towards reconfigurability, through synergistic use of photochemical and photothermal responses in light-active liquid crystal polymer networks. We utilize azobenzene photoisomerization to locally control the cis-isomer content and to program the actuator response, while subsequent photothermal stimulus actuates the structure, leading to shape morphing. We demonstrate six different shapes reconfigured from one single actuator under identical illumination conditions, and a light-fueled smart gripper that can be commanded to either grip and release or grip and hold an object after ceasing the illumination. We anticipate this work to enable all-optical control over actuator performance, paving way towards reprogrammable soft micro-robotics.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials
Contributors: Lahikainen, M., Zeng, H., Priimägi, A.
Number of pages: 9
Publication date: 8 Oct 2018
Peer-reviewed: Yes

Publication information

Journal: Nature Communications
Volume: 9
Article number: 4148
ISSN (Print): 2041-1723
Ratings:
Scopus rating (2018): CiteScore 12.19 SJR 5.992 SNIP 2.805
Original language: English
Electronic versions:
s41467-018-06647-7
DOIs:
10.1038/s41467-018-06647-7
URLs:
<http://urn.fi/URN:NBN:fi:tty-201810102393>
Research output: Contribution to journal > Article > Scientific > peer-review

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

Understanding the electrochemical properties of bio-anodes is essential to improve performance of bioelectrochemical systems. Electrochemical Impedance Spectroscopy (EIS) is often used to study these properties in detail. Analysis of the EIS response, however, is challenging due to the interfering effect of the large capacitance of typically used graphite and

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 6

Pages: 533-538

Publication date: 1 Oct 2018

Peer-reviewed: Yes

Publication information

Journal: Journal of Power Sources

Volume: 400

ISSN (Print): 0378-7753

Ratings:

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

Original language: English

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

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

Electronic versions:

1-s2.0-S0378775318308620-main

DOIs:

10.1016/j.jpowsour.2018.08.003

URLs:

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

Source: Scopus

Source ID: 85052096235

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

Removal and recovery of uranium(VI) by waste digested activated sludge in fed-batch stirred tank reactor

This study demonstrated the removal and recovery of uranium(VI) in a fed-batch stirred tank reactor (STR) using waste digested activated sludge (WDAS). The batch adsorption experiments showed that WDAS can adsorb $200 (\pm 9.0) \text{ mg}$ of uranium(VI) per g of WDAS. The maximum adsorption of uranium(VI) was achieved even at an acidic initial pH of 2.7 which increased to a pH of 4.0 in the equilibrium state. Desorption of uranium(VI) from WDAS was successfully demonstrated from the release of more than 95% of uranium(VI) using both acidic (0.5 M HCl) and alkaline (1.0 M Na_2CO_3) eluents. Due to the fast kinetics of uranium(VI) adsorption onto WDAS, the fed-batch STR was successfully operated at a mixing time of 15 min. Twelve consecutive uranium(VI) adsorption steps with an average adsorption efficiency of 91.5% required only two desorption steps to elute more than 95% of uranium(VI) from WDAS. Uranium(VI) was shown to interact predominantly with the phosphoryl and carboxyl groups of the WDAS, as revealed by in situ infrared spectroscopy and time-resolved laser-induced fluorescence spectroscopy studies. This study provides a proof-of-concept of the use of fed-batch STR process based on WDAS for the removal and recovery of uranium(VI).

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Helmholtz-Zentrum Dresden-Rossendorf, Ita-Suomen yliopisto

Contributors: Jain, R., Peräniemi, S., Jordan, N., Vogel, M., Weiss, S., Foerstendorf, H., Lakaniemi, A.

Number of pages: 9

Pages: 167-175

Publication date: 1 Oct 2018

Peer-reviewed: Yes

Publication information

Journal: Water Research

Volume: 142

ISSN (Print): 0043-1354

Ratings:

Scopus rating (2018): CiteScore 8.55 SJR 2.721 SNIP 2.426

Original language: English

ASJC Scopus subject areas: Ecological Modelling, Water Science and Technology, Waste Management and Disposal, Pollution

Keywords: Adsorption, Desorption, Infrared spectroscopy, Sludge, STR, Uranium

DOIs:

10.1016/j.watres.2018.05.042

Source: Scopus

Source ID: 85047810396

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, University of Queensland

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

Number of pages: 8

Pages: 48-55

Publication date: 12 Sep 2018

Peer-reviewed: Yes

Early online date: 2018

Publication information

Journal: Separation and Purification Technology

Volume: 203

ISSN (Print): 1383-5866

Ratings:

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

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Filtration and Separation

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

DOIs:

10.1016/j.seppur.2018.04.023

Source: Scopus

Source ID: 85045218335

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

Entangled and colloiddally stable microcrystalline cellulose matrices in controlled drug release

Drug release from a new type of matrix material consisting of partially fibrillated microcrystalline cellulose was investigated. A mechanical treatment of novel AaltoCell™ cellulose microcrystals caused partial opening of the nanofibrillary structure of the cellulose particles and entanglement of individual particles led into formation of an elastic network of microcrystalline cellulose. The rheological properties of the stable hydrogel-like materials were characterised by shear rheometry. Model compounds metronidazole and lysozyme were successfully employed in drug release experiments carried out by delignified (bleached) and lignin-containing matrices. The viscosity as well as the lignin-content played a role in the release dynamics of the drugs. Microcrystalline AaltoCell™ was proven as high-performing material for diffusion controlled release of the chosen model compounds and can be seen as a safe and economical alternative for

novel matrix materials such as nanocellulose or cellulose derivatives.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Chemistry & Advanced Materials, Chemistry and Bioengineering, Aalto University, University of Helsinki, Centre for Drug Research

Contributors: Dong, Y., Paukkonen, H., Fang, W., Kontturi, E., Laaksonen, T., Laaksonen, P.

Number of pages: 7

Pages: 113-119

Publication date: 5 Sep 2018

Peer-reviewed: Yes

Publication information

Journal: International Journal of Pharmaceutics

Volume: 548

Issue number: 1

ISSN (Print): 0378-5173

Ratings:

Scopus rating (2018): CiteScore 4.35 SJR 1.135 SNIP 1.23

Original language: English

ASJC Scopus subject areas: Pharmaceutical Science

Keywords: Cellulose hydrogel, Controlled release, Diffusion-limited release, Microcrystalline cellulose

Electronic versions:

Drug release aaltocell - revised. Embargo ended: 30/06/19

DOIs:

10.1016/j.ijpharm.2018.06.022

URLs:

<http://urn.fi/URN:NBN:fi:ty-201810262484>. Embargo ended: 30/06/19

Source: Scopus

Source ID: 85049349070

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

Post operation inactivation of acidophilic bioleaching microorganisms using natural chloride-rich mine water

The H2020 BIOMore project (www.biomore.info, Grant Agreement #642456) tests the feasibility of in situ bioleaching of copper in deep subsurface deposits in the Rudna mine, Poland. Copper is leached using biologically produced ferric iron solution, which is recycled back to the in situ reactor after re-oxidation by iron-oxidizing microorganisms. From a post operational point of view, it is important that the biological processes applied during the operation can be controlled and terminated. Our goal was to determine the possibility to use natural saline mine water for the inactivation of the introduced iron-oxidizing microorganisms remaining in the in situ reactor after completion of the leaching process of the ore block. Aerobic and anaerobic microcosms containing acid-leached (pH 2) sandstone or black shale from the Kupferschiefer in the Rudna mine were further leached with the effluent from a ferric iron generating bioreactor at 30 °C for 10 days to simulate the in situ leaching process. After the removal of the iron solution, residing iron-oxidizing microorganisms were inactivated by filling the microcosms with chloride-rich water ($65 \text{ g L}^{-1} \text{ Cl}^-$) originating from the mine. The chloride-rich water irreversibly inactivated the iron-oxidizing microorganisms and showed that the naturally occurring saline water of the mine can be used for long-term post process inactivation of bioleaching microorganisms

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, VTT Technical Research Centre of Finland

Contributors: Bomberg, M., Miettinen, H., Wahlström, M., Kaartinen, T., Ahoranta, S., Lakaniemi, A., Kinnunen, P.

Number of pages: 10

Pages: 236-245

Publication date: 1 Sep 2018

Peer-reviewed: Yes

Publication information

Journal: Hydrometallurgy

Volume: 180

ISSN (Print): 0304-386X

Ratings:

Scopus rating (2018): CiteScore 4 SJR 1.014 SNIP 1.817

Original language: English

ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Metals and Alloys, Materials Chemistry

Keywords: BIOMore, in situ bioleaching, Inactivation, Iron-oxidizing bacteria, Quantitative PCR

DOIs:

10.1016/j.hydromet.2018.06.013

Source: Scopus

Source ID: 85051388591

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

Recent progress in biohydrometallurgy and microbial characterisation

Since the discovery of microbiological metal dissolution, numerous biohydrometallurgical approaches have been developed to use microbially assisted aqueous extractive metallurgy for the recovery of metals from ores, concentrates, and recycled or residual materials. Biohydrometallurgy has helped to alleviate the challenges related to continually declining ore grades by transforming uneconomic ore resources to reserves. Engineering techniques used for biohydrometallurgy span from above ground reactor, vat, pond, heap and dump leaching to underground in situ leaching. Traditionally biohydrometallurgy has been applied to the bioleaching of base metals and uranium from sulfides and the biooxidation of sulfidic refractory gold ores and concentrates before cyanidation. More recently the interest in using bioleaching for oxide ore and waste processing, as well as extracting other commodities such as rare earth elements has been growing. Bioprospecting, adaptation, engineering and storing of microorganisms has increased the availability of suitable biocatalysts for biohydrometallurgical applications. Moreover, the advancement of microbial characterisation methods has increased the understanding of microbial communities and their capabilities in the processes. This paper reviews recent progress in biohydrometallurgy and microbial characterisation.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, CSIRO Land and Water, School of Biomedical Sciences, University of Western Australia, CSIRO Mineral Resources, Murdoch University

Contributors: Kaksonen, A. H., Boxall, N. J., Gumulya, Y., Khaleque, H. N., Morris, C., Bohu, T., Cheng, K. Y., Usher, K. M., Lakaniemi, A.

Number of pages: 19

Pages: 7-25

Publication date: 1 Sep 2018

Peer-reviewed: Yes

Publication information

Journal: Hydrometallurgy

Volume: 180

ISSN (Print): 0304-386X

Ratings:

Scopus rating (2018): CiteScore 4 SJR 1.014 SNIP 1.817

Original language: English

ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Metals and Alloys, Materials Chemistry

Keywords: Biohydrometallurgy, Bioleaching, Biooxidation, Characterisation, Microbiology

DOIs:

10.1016/j.hydromet.2018.06.018

Bibliographical note

EXT="Kaksonen, Anna H."

Source: Scopus

Source ID: 85049805480

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

Photoinduced Energy Transfer in ZnCdSeS Quantum Dot-Phthalocyanines Hybrids

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Mandal, S., Garcia Iglesias, M., Ince, M., Torres, T., Tkachenko, N. V.
Number of pages: 10
Pages: 10048-10057
Publication date: 31 Aug 2018
Peer-reviewed: Yes

Publication information

Journal: ACS Omega

Volume: 3

Issue number: 8

ISSN (Print): 2470-1343

Ratings:

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

Original language: English

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

Electronic versions:

acsomega.8b01623

DOIs:

10.1021/acsomega.8b01623

URLs:

<http://urn.fi/URN:NBN:fi:itty-201810012343>

Source: Scopus

Source ID: 85052704543

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

FLIM reveals alternative EV-mediated cellular up-take pathways of paclitaxel

In response to physiological and artificial stimuli, cells generate nano-scale extracellular vesicles (EVs) by encapsulating biomolecules in plasma membrane-derived phospholipid envelopes. These vesicles are released to bodily fluids, hence acting as powerful endogenous mediators in intercellular signaling. EVs provide a compelling alternative for biomarker discovery and targeted drug delivery, but their kinetics and dynamics while interacting with living cells are poorly understood. Here we introduce a novel method, fluorescence lifetime imaging microscopy (FLIM) to investigate these interaction attributes. By FLIM, we show distinct cellular uptake mechanisms of different EV subtypes, exosomes and microvesicles, loaded with anti-cancer agent, paclitaxel. We demonstrate differences in intracellular behavior and drug release profiles of paclitaxel-containing EVs. Exosomes seem to deliver the drug mostly by endocytosis while microvesicles enter the cells by both endocytosis and fusion with cell membrane. This research offers a new real-time method to investigate EV kinetics with living cells, and it is a potential advancement to complement the existing techniques. The findings of this study improve the current knowledge in exploiting EVs as next-generation targeted drug delivery systems.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Faculty of Pharmacy, University of Helsinki, UC Davis, Orion Corporation, Università degli Studi di Padova, Italy

Contributors: Saari, H., Lisitsyna, E., Rautaniemi, K., Rojalín, T., Niemi, L., Nivaro, O., Laaksonen, T., Yliperttula, M., Vuorimaa-Laukkanen, E.

Number of pages: 11

Pages: 133-143

Publication date: 28 Aug 2018

Peer-reviewed: Yes

Publication information

Journal: Journal of Controlled Release

Volume: 284

ISSN (Print): 0168-3659

Ratings:

Scopus rating (2018): CiteScore 7.82 SJR 2.411 SNIP 1.717

Original language: English

ASJC Scopus subject areas: Pharmaceutical Science

Keywords: Cancer, Drug delivery, Exosomes, Extracellular vesicles, Fluorescence lifetime imaging microscopy, Microvesicles, Paclitaxel, Prostate

Electronic versions:

1-s2.0-S0168365918303614-main

DOIs:

10.1016/j.jconrel.2018.06.015

URLs:

<http://urn.fi/URN:NBN:fi:tty-201807262022>

Source: Scopus

Source ID: 85048776358

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

Optimization of Fin Arrays Cooled by Forced or Natural Convection

Electronic components must be cooled to maintain their operating temperatures below the specified limits. If the maximum permissible limit of a component is exceeded, its service life decreases considerably. With increasing power densities in recent decades, the use of heat sinks to improve component cooling has become virtually mandatory in many applications. However, designing a heat sink, which optimally compromises its material weight and its heat transfer performance, is a difficult task because the result depends heavily on its geometrical structure and its operating conditions.

In this thesis, a fast way to optimize industrial heat sinks with a fixed set of heat dissipating components is presented. In a typical optimization case, several hundred temperature field evaluations are needed to find the optimal geometry. These evaluations consume a lot of CPU time if done with conventional CFD. The main objective of this thesis is, therefore, to present a new calculation model, which can handle these temperature field evaluations in a much shorter time. In the model, the speedup is obtained by replacing the slow 3D CFD -solution of air velocity and temperature distributions with 1D solutions for the mean values of these distributions, where convective heat transfer and shear stress are calculated from analytical correlations. A complete 3D numerical solution is only performed for the solid temperature field. These modifications make the new model at least a thousand times faster than CFD.

The calculation model is then tested for accuracy in many test cases, where its results are compared to those calculated with CFD and analytical solutions. These comparisons ensure that the model operates with the precision needed for optimization to predict the maximum temperature of the components. This is important because, in optimization, the maximum temperature of the components is the most crucial quantity.

After accuracy testing, the use of the model as part of an efficient multi-objective optimization algorithm is demonstrated in many distinct cases. Instead of just one optimal solution, multiobjective optimization results in a set of best compromise solutions, called the Pareto optimal set, according to the chosen criteria. Usually, the optimization criteria are the maximum temperature of the components and the weight of the material, or the external volume, of the heat sink. A wellperformed optimization can allow a significant reduction of the solid material used. In the heat sink manufacturing industry, the potential for total savings in material, energy, and CO₂ emissions is significant as the global market size of thermal management technology is vast.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Chemistry and Bioengineering

Contributors: Lampio, K.

Number of pages: 71

Publication date: 24 Aug 2018

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-4171-1

ISBN (Electronic): 978-952-15-4175-9

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Volume: 1558

ISSN (Print): 1459-2045

Electronic versions:

lampio 1558

URLs:

<http://urn.fi/URN:ISBN:978-952-15-4175-9>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Methods to design optimum heat sink geometries

This paper gives a short review of recent studies dealing with optimization of conjugated heat transfer of fin arrays. First, some results considering optimal geometries of single fins are presented to give some idea on how fin shape affects heat transfer. The main emphasis is on fin arrays, which can be solved with CFD, but it requires plenty of CPU-time and is thus

often rejected in optimization of industrial applications. If the most time consuming phase of the solution, the convective heat transfer, is handled using analytical results and only conduction is solved numerically, we have a fast performing tool for design and optimization process. With this approach, the CPU-time is many orders of magnitude smaller than in the case of pure numerical solution with CFD. The accuracy of the results is checked by comparing them to experimental, and in some simple cases, to numerically calculated results. After testing the accuracy of the model, it is applied using multi-objective optimization to fin arrays cooled by natural and forced convection. The selected optimization algorithm was a multi-objective version of particle swarm optimization (PSO) algorithm, which works well.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Mechanical Engineering and Industrial Systems, Chemistry and Bioengineering, Research group: Bio- and Circular Economy

Contributors: Karvinen, R., Lampio, K.

Number of pages: 8

Pages: 5041-5048

Publication date: 10 Aug 2018

Host publication information

Title of host publication: International Heat Transfer Conference, IHTC-16, August 10-15, 2018, Beijing, China

Article number: IHTC16-23247

DOIs:

10.1615/IHTC16.hte.023247

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

A new method to optimize natural convection heat sinks

The performance of a heat sink cooled by natural convection is strongly affected by its geometry, because buoyancy creates flow. Our model utilizes analytical results of forced flow and convection, and only conduction in a solid, i.e., the base plate and fins, is solved numerically. Sufficient accuracy for calculating maximum temperatures in practical applications is proved by comparing the results of our model with some simple analytical and computational fluid dynamics (CFD) solutions. An essential advantage of our model is that it cuts down on calculation CPU time by many orders of magnitude compared with CFD. The shorter calculation time makes our model well suited for multi-objective optimization, which is the best choice for improving heat sink geometry, because many geometrical parameters with opposite effects influence the thermal behavior. In multi-objective optimization, optimal locations of components and optimal dimensions of the fin array can be found by simultaneously minimizing the heat sink maximum temperature, size, and mass. This paper presents the principles of the particle swarm optimization (PSO) algorithm and applies it as a basis for optimizing existing heat sinks.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Mechanical Engineering and Industrial Systems

Contributors: Lampio, K., Karvinen, R.

Pages: 2571-2580

Publication date: Aug 2018

Peer-reviewed: Yes

Publication information

Journal: Heat and Mass Transfer/Waerme- und Stoffuebertragung

Volume: 54

Issue number: 8

ISSN (Print): 0947-7411

Ratings:

Scopus rating (2018): CiteScore 1.72 SJR 0.561 SNIP 0.81

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Fluid Flow and Transfer Processes

DOIs:

10.1007/s00231-017-2106-4

Source: Scopus

Source ID: 85028537040

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

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

BACKGROUND: Selenium (Se) discharged into natural waterbodies can accumulate over time and have negative impacts on the environment. Se-laden wastewater streams can be treated using biological processes. However, the presence of other electron acceptors in wastewater, such as nitrate (NO_3^-) and sulfate (SO_4^{2-}), can influence selenate (SeO_4^{2-}) reduction and impact the efficiency of biological treatment systems. **RESULTS:** SeO_4^{2-} removal by biofilms formed from an anaerobic sludge inoculum was investigated in the presence of NO_3^- and SO_4^{2-} using drip flow reactors operated continuously for 10 days at pH 7.0 and 30°C. The highest total Se (~60%) and SeO_4^{2-} (~80%) removal efficiencies were observed when the artificial wastewater contained SO_4^{2-} . A maximum amount of 68 $\mu\text{mol Se cm}^{-2}$ was recovered from the biofilm matrix in SO_4^{2-} + SeO_4^{2-} exposed biofilms and biofilm mass was 2.7-fold increased for biofilms grown in the presence of SO_4^{2-} . When SeO_4^{2-} was the only electron acceptor, biofilms were thin and compact. In the simultaneous presence of NO_3^- or SO_4^{2-} , biofilms were thicker (> 0.6mm), less compact and exhibited gas pockets. **CONCLUSION:** The presence of SO_4^{2-} had a beneficial effect on biofilm growth and the SeO_4^{2-} removal efficiency, while the presence of NO_3^- did not have a significant effect on SeO_4^{2-} removal by the biofilms.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Tan, L. C., Espinosa-Ortiz, E. J., Nancharaiyah, Y. V., van Hullebusch, E. D., Gerlach, R., Lens, P. N.

Pages: 2380-2389

Publication date: Aug 2018

Peer-reviewed: Yes

Early online date: 1 Jan 2018

Publication information

Journal: Journal of Chemical Technology and Biotechnology

Volume: 93

Issue number: 8

ISSN (Print): 0268-2575

Ratings:

Scopus rating (2018): CiteScore 2.88 SJR 0.715 SNIP 0.883

Original language: English

ASJC Scopus subject areas: Biotechnology, Chemical Engineering(all), Renewable Energy, Sustainability and the Environment, Fuel Technology, Waste Management and Disposal, Pollution, Organic Chemistry, Inorganic Chemistry

Keywords: Biofilm, Biofilm characterization, Co-electron acceptors, Nitrate, Selenate, Selenium removal, Sulfate

DOIs:

10.1002/jctb.5586

Source: Scopus

Source ID: 85043713774

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

Design aspects of all atomic layer deposited TiO₂-Fe₂O₃ scaffold-absorber photoanodes for water splitting

Iron and titanium oxides have attracted substantial attention in photoelectrochemical water splitting applications. However, both materials suffer from intrinsic limitations that constrain the final device performance. In order to overcome the limitations of the two materials alone, their combination has been proposed as a solution to the problems. Here we report on the fabrication of an atomic layer deposited (ALD) Fe₂O₃ coating on porous ALD-TiO₂. Our results show that successful implementation requires complete mixing of the TiO₂ and Fe₂O₃ layers via annealing resulting in the formation of a photoactive iron titanium oxide on the surface. Moreover, we found that incomplete mixing leads to crystallization of Fe₂O₃ to hematite that is detrimental to the photoelectrochemical performance. IPCE and transient photocurrent measurements performed using UV and visible light excitation confirmed that the iron titanium oxide extends the photocurrent generation to the visible range. These measurements were complemented by transient absorption spectroscopy (TAS), which revealed a new band absent in pristine hematite or anatase TiO₂ that we assign to charge transfer within the structure. Taken together, these results provide design guidelines to be considered when aiming to combine TiO₂ and Fe₂O₃ for photoelectrochemical applications.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Pages: 2124-2130

Publication date: 31 Jul 2018

Peer-reviewed: Yes

Publication information

Journal: Sustainable Energy & Fuels

Volume: 2

Issue number: 9

ISSN (Print): 2398-4902

Ratings:

Scopus rating (2018): CiteScore 4.94 SNIP 0.841

Original language: English

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

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

DOIs:

10.1039/C8SE00252E

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

Comparison of electron injection and recombination on TiO₂ nanoparticles and ZnO nanorods photosensitized by phthalocyanine

Titanium dioxide (TiO₂) and zinc oxide (ZnO) semiconductors have similar band gap positions but TiO₂ performs better as an anode material in dye-sensitized solar cell applications. We compared two electrodes made of TiO₂ nanoparticles and ZnO nanorods sensitized by an aggregation-protected phthalocyanine derivative using ultrafast transient absorption spectroscopy. In agreement with previous studies, the primary electron injection is two times faster on TiO₂, but contrary to the previous results the charge recombination is slower on ZnO. The latter could be due to morphology differences and the ability of the injected electrons to travel much further from the sensitizer cation in ZnO nanorods.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Publication date: 11 Jul 2018

Peer-reviewed: Yes

Publication information

Journal: Royal Society Open Science

Volume: 5

Issue number: 7

Article number: 180323

ISSN (Print): 2054-5703

Ratings:

Scopus rating (2018): CiteScore 2.71 SJR 1.131 SNIP 1.058

Original language: English

ASJC Scopus subject areas: General

Keywords: Photo-induced electron transfer, Phthalocyanine, Semiconductor-organic interface, TiO nanoparticles, ZnO nanorods

Electronic versions:

180323.full

DOIs:

10.1098/rsos.180323

URLs:

<http://urn.fi/URN:NBN:fi:tty-201808012044>

Source: Scopus

Source ID: 85050034317

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

Halogen-bond driven self-assembly of triangular macrocycles

2-Iodoethynylpyridine and 2-iodoethynyl-1-methyl-imidazole self-assemble under halogen-bonding control into discrete macrocycles, viz. supramolecular triangles.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Szell, P. M. J., Siiskonen, A., Catalano, L., Cavallo, G., Terraneo, G., Priimägi, A., Bryce, D. L., Metrangolo, P.
Number of pages: 5
Pages: 10467-10471
Publication date: 7 Jul 2018
Peer-reviewed: Yes

Publication information

Journal: New Journal of Chemistry

Volume: 42

Issue number: 13

ISSN (Print): 1144-0546

Ratings:

Scopus rating (2018): CiteScore 3.09 SJR 0.716 SNIP 0.724

Original language: English

DOIs:

10.1039/C8NJ00759D

Source: Bibtex

Source ID: urn:fbda8958063fdcff5c170b8d5cde7c

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

Metabolic pairing of aerobic and anaerobic production in a one-pot batch cultivation

Background: The versatility of microbial metabolic pathways enables their utilization in vast number of applications. However, the electron and carbon recovery rates, essentially constrained by limitations of cell energetics, are often too low in terms of process feasibility. Cocultivation of divergent microbial species in a single process broadens the metabolic landscape, and thus, the possibilities for more complete carbon and energy utilization. **Results:** In this study, we integrated the metabolisms of two bacteria, an obligate anaerobe *Clostridium butyricum* and an obligate aerobe *Acinetobacter baylyi* ADP1. In the process, a glucose-negative mutant of *A. baylyi* ADP1 first deoxidized the culture allowing *C. butyricum* to grow and produce hydrogen from glucose. In the next phase, ADP1 produced long chain alkyl esters (wax esters) utilizing the by-products of *C. butyricum*, namely acetate and butyrate. The coculture produced 24.5 ± 0.8 mmol/l hydrogen (1.7 ± 0.1 mol/mol glucose) and 28 mg/l wax esters (10.8 mg/g glucose). **Conclusions:** The cocultivation of strictly anaerobic and aerobic bacteria allowed the production of both hydrogen gas and long-chain alkyl esters in a simple one-pot batch process. The study demonstrates the potential of 'metabolic pairing' using designed microbial consortia for more optimal electron and carbon recovery.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering

Contributors: Salmela, M., Lehtinen, T., Efimova, E., Santala, S., Mangayil, R.

Publication date: 3 Jul 2018

Peer-reviewed: Yes

Publication information

Journal: Biotechnology for Biofuels

Volume: 11

Issue number: 1

Article number: 187

ISSN (Print): 1754-6834

Ratings:

Scopus rating (2018): CiteScore 5.84 SJR 1.762 SNIP 1.451

Original language: English

ASJC Scopus subject areas: Biotechnology, Applied Microbiology and Biotechnology, Renewable Energy, Sustainability and the Environment, Energy(all), Management, Monitoring, Policy and Law

Keywords: Hydrogen production, Integrated metabolism, Metabolic pairing, Synthetic microbial consortia, Wax esters

Electronic versions:

full text

DOIs:

10.1186/s13068-018-1186-9

URLs:

<http://urn.fi/URN:NBN:fi:tty-201808072056>

Source: Scopus

Source ID: 85049884043

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Publication date: 1 Jul 2018

Peer-reviewed: Yes

Publication information

Journal: Pharmaceutical Research

Volume: 35

Issue number: 7

Article number: 145

ISSN (Print): 0724-8741

Ratings:

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

Original language: English

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

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

Electronic versions:

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

DOIs:

10.1007/s11095-018-2428-z

URLs:

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

Source: Scopus

Source ID: 85047448577

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

Multielectron Dynamics Depending on Intramolecular Orientations in Pentacene Dimers: Recombination and Dissociation of Correlated Triplet Pairs

Pentacene dimers bridged by a phenylene at ortho and meta positions [denoted as o-(Pc)₂ and m-(Pc)₂] were synthesized to examine intramolecular orientation-dependent multielectron dynamics, especially focusing on singlet fission (SF) and recombination from correlated triplet pairs [(TT)]. Absorption and electrochemical measurements indicated strong intramolecular couplings of o-(Pc)₂ relative to m-(Pc)₂. Femtosecond and nanosecond TA measurements successfully demonstrated efficient SF in both dimers. In contrast, the dissociation process from the (TT) to the individual triplets [(2 × T)] was clearly observed in m-(Pc)₂, which is in sharp contrast to a major recombination process in o-(Pc)₂. Time-resolved electron spin resonance (TR-ESR) measurements demonstrated that the recombination and dissociation proceed from the quintet state of 5(TT) in m-(Pc)₂. The rate constant of the SF was 2 orders of magnitude greater in o-(Pc)₂ than that in m-(Pc)₂ and was rationalized by enhanced electronic coupling between adjacent HOMOs of the Pc units.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Sakai, H., Inaya, R., Nagashima, H., Nakamura, S., Kobori, Y., Tkachenko, N. V., Hasobe, T.
Number of pages: 7
Pages: 3354-3360
Publication date: 21 Jun 2018
Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry Letters

Volume: 9

Issue number: 12

ISSN (Print): 1948-7185

Ratings:

Scopus rating (2018): CiteScore 7.91 SJR 3.618 SNIP 1.476

Original language: English

DOIs:

10.1021/acs.jpcclett.8b01184

Source: PubMed

Source ID: 29847939

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

Light-Activated Antimicrobial Materials Based on Perylene Imides and Phthalocyanines

In the era of globalization, the spread of infectious diseases is a serious concern. The emergence of drug resistant bacteria and healthcare associated infections in particular, poses a great danger to human health. Self-disinfecting surfaces may play a significant role in controlling the spread of pathogenic diseases. Photodynamic antimicrobial chemotherapy (PACT) can be a very efficient way of inactivation of drug resistant bacteria and biofilms. However, making a self-disinfecting surface based on PACT principles requires novel photosensitizers, which can efficiently generate reactive oxygen species, and are stable and accessible. In this thesis, attempts are undertaken to synthesize novel photosensitizers based on peryleneimides and phthalocyanines. We propose a novel efficient method for the direct and regioselective amination of peryleneimides. The substitution occurs with high yields exclusively at 1,6- and 7,12-positions of the bay region of perylenediimide and perylenemonoimide diester. We also report the synthesis of novel cationic peryleneimides, which can be potentially used as photosensitizers in PACT. Phthalocyanines are known to be efficient photosensitizers. In this thesis we present the synthesis of novel pyridinyl-substituted phthalocyanine and its tetracationic derivatives. As a unique synthetic approach, pyridinyl groups are connected to α -phthalo positions of the macrocycle via direct C-C bonds. Prototype self-disinfecting materials are prepared by impregnating filter paper with the synthesized dyes. Binding of the dyes occurs via electrostatic interactions and does not require any special chemical modification. A fast and simple setup for the evaluation of antimicrobial efficacies of dyed papers is proposed. The setup employs bioluminescent bacteria and allows for a fast screening of a large number of dyes. According to the screening results, tetracationic phthalocyanines are the most efficient antimicrobial photosensitizers. The antimicrobial efficacies of phthalocyanine derivatives are evaluated quantitatively with the help of colony forming unit (CFU) counting method. The papers impregnated with as little as 80 mg/m² of cationic zinc phthalocyanine exhibit 2.7 and 3.4 log reduction in CFU against *Escherichia coli* (*E. coli*) and *Acinetobacter baylyi* (*A. baylyi*), respectively after illumination with the light intensity 18 mW/cm² in a solar simulator. Similar antimicrobial efficacies are achieved under illumination with consumer light emitting diode (LED) lights. Phthalocyanine-impregnated papers show very good stability. Incubation of the dye-impregnated papers in phosphatebuffered saline demonstrates superior binding ability of phthalocyanine, with basically no detectable leaching of the dye. Photostability of the dyed paper is also high. Continuous illumination with 42 mW/cm² LED light for 64 h decreases the absorbance of dyed papers only by 10%.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Chemistry and Bioengineering

Contributors: George, L.

Number of pages: 92

Publication date: 6 Jun 2018

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-4156-8

ISBN (Electronic): 978-952-15-4159-9

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Volume: 1554

ISSN (Print): 1459-2045

Electronic versions:

george 1554

URLs:

<http://urn.fi/URN:ISBN:978-952-15-4159-9>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Effects of wastewater constituents and operational conditions on the composition and dynamics of anodic microbial communities in bioelectrochemical systems

Over the last decade, there has been an ever-growing interest in bioelectrochemical systems (BES) as a sustainable technology enabling simultaneous wastewater treatment and biological production of, e.g. electricity, hydrogen, and further commodities. A key component of any BES degrading organic matter is the anode where electric current is biologically generated from the oxidation of organic compounds. The performance of BES depends on the interactions of the anodic microbial communities. To optimize the operational parameters and process design of BES a better comprehension of the microbial community dynamics and interactions at the anode is required. This paper reviews the abundance of different microorganisms in anodic biofilms and discusses their roles and possible side reactions with respect to their implications on the performance of BES utilizing wastewaters. The most important operational parameters affecting anodic microbial communities grown with wastewaters are highlighted and guidelines for controlling the composition of microbial communities are given.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Chemistry and Bioengineering, Laboratory for MEMS Applications, Universitat Freiburg im Breisgau, Karlsruhe Institute of Technology, Institute for Technical Physics, Germany, University of Bremen

Contributors: Kokko, M., Eppe, S., Gescher, J., Kerzenmacher, S.

Number of pages: 14

Pages: 376-389

Publication date: 1 Jun 2018

Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 258

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2018): CiteScore 7.08 SJR 2.157 SNIP 1.824

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Renewable Energy, Sustainability and the Environment, Waste Management and Disposal

Keywords: Bioelectrochemical system, Exoelectrogen, Microbial community, Wastewater

DOIs:

10.1016/j.biortech.2018.01.090

Source: Scopus

Source ID: 85043472557

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

Lewis Base Catalyzed Intramolecular Reduction of Salicylaldehydes by Pinacol-Derived Chlorohydrosilane

A newly developed stable chlorohydrosilane derived from pinacol is herein described. This was successfully used in the reduction of salicylaldehydes in reasonable to excellent yields (51–97%). The ability of the hydrosilane to react as a reducing agent is increased upon the in situ formation of a trialkoxyhydrosilane and activation with a Lewis base, as further indicated by density functional theory studies. 1,3-Dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone (DMPU) was identified to be a suitable catalyst for this metal-free reduction, promoting the regio- and chemoselective reduction of aldehydes in ortho-position to phenols, despite the presence of vicinal ketones. The performance of pinacol-derived chlorohydrosilane in the reduction of salicylaldehydes was further observed to be superior to that of well-established commercially available chlorohydrosilanes.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, CQFM, Univ Jyvaskyla, University of Jyvaskyla, Dept Chem, Nanosci Ctr

Contributors: Assoah, B., Vale, J. R., Kalenius, E., Veiros, L., Rafael Candeias, N.

Pages: 2910-2917

Publication date: 1 Jun 2018

Peer-reviewed: Yes

Publication information

Journal: European Journal of Organic Chemistry

Volume: 2018

Issue number: 23

ISSN (Print): 1434-193X

Ratings:

Scopus rating (2018): CiteScore 2.81 SJR 0.987 SNIP 0.626

Original language: English

DOIs:

10.1002/ejoc.201800544

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

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

The properties and antimicrobial efficacies of zinc complexes of tetrakis(N-methylpyridinium-4-yl) tetraiodide porphyrin and tetrakis(N-methylpyridinium-4-yl) tetraiodide phthalocyanine impregnated to paper were evaluated. Photo-inactivation of microbes using inexpensive consumer light-emitting diode lamp was assessed on surface of dyed papers. Antimicrobial experiments of phthalocyanine-dyed paper by live cell assessment through colony forming units counting demonstrated 3.72 and 4.01 log reduction against *Escherichia coli* (*E. coli*) and *Acinetobacter baylyi* (*A. baylyi*) respectively after 1 h of illumination with 35 mW/cm² light. The porphyrin-dyed paper exhibited 1.66 and 2.01 log reduction in colony forming units against *E. coli* and *A. baylyi* respectively after 1 h exposure with 4 mW/cm² light. Both dyed papers were photo-stable after 64 h of continuous exposure with 42 mW/cm² light, while phthalocyanine-dyed paper exhibited superior leaching stability in phosphate-buffered saline.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 7

Pages: 94-100

Publication date: 1 Jun 2018

Peer-reviewed: Yes

Publication information

Journal: Journal of Inorganic Biochemistry

Volume: 183

ISSN (Print): 0162-0134

Ratings:

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

Original language: English

ASJC Scopus subject areas: Biochemistry, Inorganic Chemistry

DOIs:

10.1016/j.jinorgbio.2018.03.015

Source: Scopus

Source ID: 85044575449

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

Effect of Co-Adsorbate and Hole Transporting Layer on the Photoinduced Charge Separation at the TiO₂-Phthalocyanine Interface

Understanding the primary processes of charge separation (CS) in solid-state dye-sensitized solar cells (DSSCs) and, in particular, analysis of the efficiency losses during these primary photoreactions is essential for designing new and efficient photosensitizers. Phthalocyanines (Pcs) are potentially interesting sensitizers having absorption in the red side of the optical spectrum and known to be efficient electron donors. However, the efficiencies of Pc-sensitized DSSCs are lower than that of the best DSSCs, which is commonly attributed to the aggregation tendency of Pcs. In this study, we employ ultrafast spectroscopy to discover why and how much does the aggregation affect the efficiency. The samples were prepared on a standard fluorine-doped tin oxide (FTO) substrates covered by a porous layer of TiO₂ nanoparticles, functionalized by a Pc sensitizer and filled by a hole transporting material (Spiro-MeOTAD). The study demonstrates that the aggregation can be suppressed gradually by using co-adsorbates, such as chenodeoxycholic acid (CDCA) and oleic acid, but rather high concentrations of co-adsorbate is required. Gradually, a few times improvement of quantum efficiency was observed at sensitizer/co-adsorbate ratio Pc/CDCA = 1:10 and higher. The time-resolved spectroscopy studies were

complemented by standard photocurrent measurements of the same sample structures, which also confirmed gradual increase in photon-to-current conversion efficiency on mixing Pc with CDCA.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 12

Pages: 4947-4958

Publication date: 31 May 2018

Peer-reviewed: Yes

Publication information

Journal: ACS Omega

Volume: 3

Issue number: 5

ISSN (Print): 2470-1343

Ratings:

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

Original language: English

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

DOIs:

10.1021/acsomega.8b00600

Source: Scopus

Source ID: 85046661219

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

Mesophilic and thermophilic biohydrogen and bioelectricity production from real and synthetic wastewaters

In the last century, fossil fuels have been intensively used for energy production causing a dramatic increase of CO₂ level in the atmosphere and the related environmental issues, such as global warming and ozone layer depletion. In 2015, the increased awareness about climate change led to the signature of the Paris agreement, in which 195 countries committed to cut off their greenhouse gases emission by 40% (compared to emissions in 1990) by 2030. The achievement of such an ambitious target is strictly linked to a gradual switch from fossil fuels to sustainable and renewable sources for energy production. This is driving many industries producing organic and inorganic waste towards a biorefinery concept, in which side streams, wastes and wastewaters are seen as a potential feedstocks for biofuel and/or biochemical production.

Dark fermentation and microbial fuel cells (MFCs) are two emerging technologies for biological conversion of the chemical energy of organic compounds into hydrogen (H₂) and electricity, respectively. Although these technologies can potentially replace fossil fuels for energy production, their establishment is hindered by their low energy output. Due to kinetic and thermodynamic advantages, high temperature can be the key for increasing both dark fermentative H₂ production and electricity production in MFCs. Therefore, this thesis focuses on delineating how temperature influences biological production of H₂ and electricity from organic carbon-containing wastewaters.

Start-up and selection of a suitable microbial community is a crucial phase in dark fermentation. Two heat-treated inocula (fresh and digested activated sludge) were compared, in four consecutive batch cycles, for H₂ production from xylose at 37, 55 and 70 °C. At both 37 and 55 °C, a higher H₂ yield was achieved by the fresh than the digested activated sludge, whereas a very low H₂ yield was obtained by both inocula at 70 °C. Then, four different inoculum pretreatments (acidic, alkaline, heat and freezing shocks) were evaluated, in a single-stage batch experiment, for creating an efficient mesophilic (37 °C) and thermophilic (55 °C) H₂ producing community. Acidic and alkaline shocks selected known H₂ producing microorganisms belonging to Clostridiaceae at the expenses of lactate producing bacteria, resulting in the highest H₂ yield at 37 and 55 °C, respectively. Although a heat shock resulted in a low H₂ yield in a single batch, H₂ production by the heat-treated fresh activated sludge was shown to increase in the experiment with four consecutive batch cycles. This suggests that H₂ producing microbial communities may develop in the long-term as long as culture conditions are optimized for growth of H₂ producers.

Heat-treated fresh activated sludge was selected as inoculum for continuous H₂ production from a xylose-containing synthetic wastewater in a mesophilic (37 °C) and a thermophilic (55-70 °C, increased stepwise) fluidized bed reactor (FBR). A higher H₂ yield was obtained in the thermophilic than in the mesophilic FBR. Furthermore, H₂ production at 70 °C, which failed in the earlier batch study, was successful in the FBR, with a stable yield of 1.2 mol H₂ mol⁻¹ xyloseadded, by adapting the microbial community from 55 °C to 70 °C stepwise at 5 °C intervals. Operation temperature of 70 °C was also found optimal for H₂ production from thermomechanical pulping (TMP) wastewater in a temperature gradient incubator assay, as batch cultivation at 70 °C enriched the H₂ producing *Thermoanaerobacterium* sp. and repressed homoacetogenic microorganisms.

A detailed knowledge of microbial communities, and particularly the active subpopulation, is crucial in order to adjust the conditions to favor the growth of exoelectrogenic microorganisms in MFCs. A RNA approach was used to study the structure and role of the anode-attached, membrane-attached and planktonic microbial communities in a mesophilic (37 °C) and a thermophilic (55 °C) two-chamber, xylose-fed MFC. An anodeattached community dominated by Geobacteraceae sustained electricity production at 37 °C, whereas the establishment of methanogenic and H₂ oxidizing microorganisms resulted in a low electricity production at 55 °C. However, the development of a thermophilic exoelectrogenic community can be promoted by applying a start-up strategy which includes imposing a negative potential to the anode and chemical inhibition of methanogens. At both 37 and 55 °C, aerobic membrane-attached microorganisms were likely involved in consuming the oxygen diffusing from the cathodic to the anodic chamber, thus favoring the exoelectrogenic microorganisms, which are strictly anaerobic, but competing with them for the substrate. A mesophilic exoelectrogenic community was also shown to produce electricity from TMP wastewater in an upflow MFC operated at 37 °C.

In conclusion, a higher and more stable H₂ yield can be achieved in thermophilic rather than mesophilic dark fermentation. Dark fermentation at 70 °C is particularly suitable for treatment of TMP wastewater as it is released at high temperature (50-80 °C) and could be treated on site with minimal energy requirement for heating the bioreactor. TMP wastewater can be also used as substrate for electricity production in mesophilic MFCs. Electricity production in thermophilic MFCs is feasible, but enrichment of thermophilic exoelectrogenic microorganisms may require a long start-up period with optimized conditions. The detailed RNA-level microbial community analysis performed in this study may help in selecting a start-up and operation strategy to optimize electricity production.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Chemistry and Bioengineering

Contributors: Dessi, P.

Number of pages: 89

Publication date: 23 May 2018

Publication information

Publisher: Université Paris-Est

Original language: English

Electronic versions:

Thesis Paolo. Embargo ended: 23/11/18

URLs:

<http://urn.fi/URN:NBN:fi:tty-201805141649>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Inoculum pretreatment differentially affects the active microbial community performing mesophilic and thermophilic dark fermentation of xylose

The influence of different inoculum pretreatments (pH and temperature shocks) on mesophilic (37 °C) and thermophilic (55 °C) dark fermentative H₂ production from xylose (50 mM) and, for the first time, on the composition of the active microbial community was evaluated. At 37 °C, an acidic shock (pH 3, 24 h) resulted in the highest yield of 0.8 mol H₂ mol⁻¹ xylose. The H₂ and butyrate yield correlated with the relative abundance of Clostridiaceae in the mesophilic active microbial community, whereas Lactobacillaceae were the most abundant non-hydrogenic competitors according to RNA-based analysis. At 55 °C, Clostridium and Thermoanaerobacterium were linked to H₂ production, but only an alkaline shock (pH 10, 24 h) repressed lactate production, resulting in the highest yield of 1.2 mol H₂ mol⁻¹ xylose. This study showed that pretreatments differentially affect the structure and productivity of the active mesophilic and thermophilic microbial community developed from an inoculum.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Natl. University of Ireland, Galway, ENEA/CREATE/Università Degli Studi Napoli Federico II, University of Cassino and Southern Lazio, Institute for Water Education, UNESCO-IHE

Contributors: Dessi, P., Porca, E., Frunzo, L., Lakaniemi, A., Collins, G., Esposito, G., Lens, P. N.

Pages: 9233-9245

Publication date: 10 May 2018

Peer-reviewed: Yes

Early online date: 1 Jan 2018

Publication information

Journal: International Journal of Hydrogen Energy

Volume: 43

Issue number: 19

ISSN (Print): 0360-3199

Ratings:

Scopus rating (2018): CiteScore 4.16 SJR 1.1 SNIP 1.128

Original language: English

ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Fuel Technology, Condensed Matter Physics, Energy Engineering and Power Technology

Keywords: Biohydrogen, Clostridium, Lactobacillus, MiSeq, pH shock, Temperature shock

Electronic versions:

Inoculum pretreatment differentially affects the active microbial community

DOIs:

10.1016/j.ijhydene.2018.03.117

URLs:

<http://urn.fi/URN:NBN:fi:ty-201901231146>

Source: Scopus

Source ID: 85045538153

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

Crystallization Kinetics of an Amorphous Pharmaceutical Compound Using Fluorescence-Lifetime-Imaging Microscopy

Pharmaceutical scientists are increasingly interested in amorphous drug formulations especially because of their higher dissolution rates. Consequently, the thorough characterization and analysis of these formulations are becoming more and more important for the pharmaceutical industry. Here, fluorescence-lifetime-imaging microscopy (FLIM) was used to monitor the crystallization of an amorphous pharmaceutical compound, indomethacin. Initially, we identified different solid indomethacin forms, amorphous and γ - and α -crystalline, on the basis of their time-resolved fluorescence. All of the studied indomethacin forms showed biexponential decays with characteristic fluorescence lifetimes and amplitudes. Using this information, the crystallization of amorphous indomethacin upon storage in 60 °C was monitored for 10 days with FLIM. The progress of crystallization was detected as lifetime changes both in the FLIM images and in the fluorescence-decay curves extracted from the images. The fluorescence-lifetime amplitudes were used for quantitative analysis of the crystallization process. We also demonstrated that the fluorescence-lifetime distribution of the sample changed during crystallization, and when the sample was not moved between measuring times, the lifetime distribution could also be used for the analysis of the reaction kinetics. Our results clearly show that FLIM is a sensitive and nondestructive method for monitoring solid-state transformations on the surfaces of fluorescent samples.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Rautaniemi, K., Vuorimaa-Laukkanen, E., Strachan, C. J., Laaksonen, T.

Number of pages: 8

Pages: 1964-1971

Publication date: 7 May 2018

Peer-reviewed: Yes

Publication information

Journal: Molecular Pharmaceutics

Volume: 15

Issue number: 5

ISSN (Print): 1543-8384

Ratings:

Scopus rating (2018): CiteScore 4.7 SJR 1.402 SNIP 1.165

Original language: English

ASJC Scopus subject areas: Molecular Medicine, Pharmaceutical Science, Drug Discovery

Keywords: amorphous materials, crystal growth, fluorescence, fluorescence lifetime, kinetics

Electronic versions:

[acs.molpharmaceut.8b00117](https://doi.org/10.1021/acs.molpharmaceut.8b00117)

DOIs:

10.1021/acs.molpharmaceut.8b00117

URLs:

<http://urn.fi/URN:NBN:fi:ty-201809032262>

Source: Scopus

Source ID: 85046674658

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

Investigating the kinetics and biofuel properties of *Alstonia congensis* and *Ceiba pentandra* via torrefaction

Alstonia congensis (Ahun) and *Ceiba pentandra* (Araba) were chosen as representations of tropical wood in this study. The use of untreated wood for energy recovery could lead to a high loss in efficiency. One way of circumventing this in a developing country such as Nigeria is by exposing the fuel materials to a pre-treatment, such as torrefaction, prior to deployment. Attempts were made to improve the combustion properties of these resources and also to investigate their torrefaction kinetics. Derivations of kinetic parameters using Coats-Redfern method were discontinued due to inconsistent results. A non-linear regression method was then employed and the results compared to the average value obtained by the FWO method, which was considered more viable than the Coats-Redfern method. The kinetic parameters (E_a , A and n) derived by the regression method are 134.45 kJ/mol, $1.83E+13 \text{ min}^{-1}$ and 2.15, respectively, for Araba and 143.38 kJ/mol, $1.90E+10 \text{ min}^{-1}$ and 2.28, respectively, for Ahun. The thermal behaviour of the samples showed that a lower mass yield resulted in a lower energy yield, while the heating values increased with the temperature of torrefaction. The results obtained in this study affirm the possibility of obtaining an optimum conversion of these resources for energy recovery.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, University of Borås, Laboratory of Chemistry and Bioengineering

Contributors: Oluoti, K., Doddapaneni, T. R. K., Richards, T.

Number of pages: 8

Pages: 134-141

Publication date: 1 May 2018

Peer-reviewed: Yes

Publication information

Journal: Energy

Volume: 150

ISSN (Print): 0360-5442

Ratings:

Scopus rating (2018): CiteScore 6.2 SJR 2.048 SNIP 1.822

Original language: English

ASJC Scopus subject areas: Civil and Structural Engineering, Building and Construction, Pollution, Energy(all), Mechanical Engineering, Industrial and Manufacturing Engineering, Electrical and Electronic Engineering

Keywords: *Alstonia congensis*, *Ceiba pentandra*, Energy densification, Kinetic parameters, Mini-grid, Torrefaction

DOIs:

10.1016/j.energy.2018.02.086

Source: Scopus

Source ID: 85042679330

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 6

Pages: 23-28

Publication date: May 2018

Peer-reviewed: Yes

Early online date: 7 Dec 2017

Publication information

Journal: Food Chemistry
Volume: 247
ISSN (Print): 0308-8146
Ratings:

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

Original language: English

ASJC Scopus subject areas: Analytical Chemistry, Food Science

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

Electronic versions:

Manuscript_Free amino acids and 5'-nucleotides in Finnish forest mushrooms_revised. Embargo ended: 13/12/18

DOIs:

10.1016/j.foodchem.2017.12.014

URLs:

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

Source: Scopus

Source ID: 85037999138

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

Anaerobic digestion of 30–100-year-old boreal lake sedimented fibre from the pulp industry: Extrapolating methane production potential to a practical scale

Since the 1980s, the pulp and paper industry in Finland has resulted in the accumulation of fibres in lake sediments. One such site in Lake Näsijärvi contains approximately 1.5 million m³ sedimented fibres. In this study, the methane production potential of the sedimented fibres (on average 13% total solids (TS)) was determined in batch assays. Furthermore, the methane production from solid (on average 20% TS) and liquid fractions of sedimented fibres after solid-liquid separation was studied. The sedimented fibres resulted in fast methane production and high methane yields of 250 ± 80 L CH₄/kg volatile solids (VS). The main part (ca. 90%) of the methane potential was obtained from the solid fraction of the sedimented fibres. In addition, the VS removal from the total and solid sedimented fibres was high, 61–65% and 63–78%, respectively. The liquid fraction also contained a large amount of organics (on average 8.8 g COD/L), treatment of which also has to be considered. The estimations of the methane production potentials in the case area showed potential up to 40 million m³ of methane from sedimented fibres.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering

Contributors: Kokko, M., Koskue, V., Rintala, J.

Number of pages: 9

Pages: 218-226

Publication date: 15 Apr 2018

Peer-reviewed: Yes

Publication information

Journal: Water Research

Volume: 133

ISSN (Print): 0043-1354

Ratings:

Scopus rating (2018): CiteScore 8.55 SJR 2.721 SNIP 2.426

Original language: English

ASJC Scopus subject areas: Ecological Modelling, Water Science and Technology, Waste Management and Disposal, Pollution

Keywords: Anaerobic digestion, Methane, Pulp and paper industry, Sedimented fibre

DOIs:

10.1016/j.watres.2018.01.041

Source: Scopus

Source ID: 85041395267

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

Nutrient management via struvite precipitation and recovery from various agroindustrial wastewaters: Process feasibility and struvite quality

Improving environmental protection and finding sustainable and renewable resources of nutrients are core issues in circular bioeconomy. Thus, this study evaluated the efficiency of recovering struvite, MgNH₄PO₄·6H₂O, from different agro-industrial wastewaters (four highly loaded reject waters of anaerobically co-digested agro-industrial waste and a raw swine slurry) and assessed the quality of recovered struvite crystals and their reusability as fertilizer. The efficiency of crystallization (E_c 40–80%) and amount of struvite in the precipitate (P_p 55–94%) highly varied due to the characteristics

of influent wastewaters, particularly to the content of competing elements, such as alkaline and heavy metals and total solids (TS). In particular, E_C (94, 75, 61%) and P_D (76, 66, 48%) decreased at increasing TS (0.57, 0.73, 0.99%), demonstrating the hindering effect of solid content on struvite recovery and quality. According to X-ray diffraction analysis, the structure of all isolated samples corresponded to crystalline, orthorhombic struvite, which exhibited high purity (32–48 g/kg_d N, 114–132 g/kg_d P, and 99–116 g/kg_d Mg) containing only a few foreign elements, whose amount depended on the characteristics of the influent wastewater. All struvite contained other plant macronutrients (K, Ca) and many micronutrients (Fe, Na, Cu, Mn, Co, Zn) that further enhance its agronomic value. Therefore, this study showed that struvite can be successfully recovered from a wide range of highly loaded agroindustrial wastewaters, and that the quality of the recovered struvite could be suitable for reuse in agriculture.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Materials Science, OY Scandinavian Colloids Ltd

Contributors: Taddeo, R., Honkanen, M., Kolppo, K., Lepistö, R.

Number of pages: 7

Pages: 433-439

Publication date: 15 Apr 2018

Peer-reviewed: Yes

Publication information

Journal: Journal of Environmental Management

Volume: 212

ISSN (Print): 0301-4797

Ratings:

Scopus rating (2018): CiteScore 5.32 SJR 1.206 SNIP 1.726

Original language: English

ASJC Scopus subject areas: Environmental Engineering, Waste Management and Disposal, Management, Monitoring, Policy and Law

Keywords: Crystalline purity, Heavy metals, Nutrient recycling, Solid content, Sustainable fertilizer

DOIs:

10.1016/j.jenvman.2018.02.027

Bibliographical note

EXT="Kolppo, Kari"

Source: Scopus

Source ID: 85042109316

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Pages: 11950-11960

Publication date: 11 Apr 2018
Peer-reviewed: Yes
Early online date: 15 Mar 2018

Publication information

Journal: ACS Applied Materials & Interfaces

Volume: 10

Issue number: 14

ISSN (Print): 1944-8244

Ratings:

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

Original language: English

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

DOIs:

10.1021/acsami.8b01351

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

Process Integration Approaches to Improve the Techno-Economic Feasibility of Torrefaction Process

Over the past few years, the torrefaction process has evolved into a promising pre-treatment process to improve the properties of biomass to a level at which it is competitive with coal. However, in order to make torrefied biomass pellets an economically viable alternative to coal and wood pellets, the techno-economic feasibility of the torrefaction process needs to be improved. Thus, new process configurations are required to produce torrefied biomass pellets and other high value products from the torrefaction process. This thesis presents new process configurations, which have been evaluated with laboratory experiments, process simulations and mathematical modeling.

Two different biomass samples i.e. eucalyptus clone and pinewood were used in torrefaction experiments. Initially, the effect that torrefaction pretreatment has on the kinetics, reaction mechanisms and heat flow during biomass pyrolysis was studied using TGA and DSC analysis. The results showed that the pyrolysis reaction mechanism varied significantly with torrefaction treatment. The heat flow data from DSC showed that torrefied biomass pyrolysis requires more energy than dried biomass in order to initiate the pyrolysis reactions.

In the second stage, the anaerobic digestion of torrefaction condensate for the efficient utilization of torrefaction volatiles was studied through batch anaerobic digestion assays. Torrefaction condensate produced at 225, 275 and 300 °C was used at various substrate to inoculum ratio i.e. 0.1, 0.2 and 0.5. The methane yield was in the range of 430 - 492 mL/g volatile solids (VS) and 430 - 460 mL/g VS under mesophilic and thermophilic conditions, respectively. With the higher loading, i.e. > 0.2 VS_{substrate}:VS_{inoculum}, the production of methane was inhibited because of the inhibitory compounds in the torrefaction condensate, such as furfural and guaiacol.

Large quantities of binders are required to make the pelletization process effective and to improve the quality of the pellets. An innovative process configuration is hereby proposed for detoxifying the torrefaction condensate and to reduce the binders' requirement. The removal of a major inhibitory compound, i.e. furfural, through adsorption using torrefied biomass as an adsorbent was also studied. The adsorption of furfural from the torrefaction condensate at 250 g/L dosage was around 54%. Finally, the influence of the detoxification of the torrefaction condensate on the AD process was studied through batch assays.

Finally, the experimental results were used to simulate industrial scale operations to evaluate the feasibility of integrating the torrefaction process with anaerobic digestion. In addition, different process integration approaches were studied to identify possible heat energy recovery options in the torrefaction process, on its own, and also when integrated with AD. The standalone torrefaction process was compared with three different process configurations, which varied according to the intended application for the produced biogas. The mass balance showed that biomethane can be produced at 369 m³/h, at 10 t/h of torrefied biomass pellets production capacity. A sensitivity analysis showed that the cost of the feedstock has a significant effect on the economics of the overall process. The economic analysis showed that the price of torrefied biomass pellets could be significantly reduced if the torrefaction process is integrated with AD.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Chemistry and Bioengineering

Contributors: Doddapaneni, T. R. K. C.

Number of pages: 84

Publication date: 6 Apr 2018

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-4119-3

ISBN (Electronic): 978-952-15-4125-4

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Volume: 1539

ISSN (Print): 1459-2045

Electronic versions:

doddapaneni 1539

URLs:

<http://urn.fi/URN:ISBN:978-952-15-4125-4>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Metabolic Engineering of *Acinetobacter baylyi* ADP1 for Improved Growth and Wax Ester Production Using Components of Lignocellulosic Hydrolysates as Carbon Sources

Microorganisms can be used in bioprocesses to produce various chemicals, such as fuels, cosmetics and medical products, as an environmentally friendly alternative for chemical synthesis. In these bioprocesses the raw materials (*e.g.* lignocellulose) can be converted to compounds with high complexity with a minimum energy input and waste material production. The metabolic capabilities and robustness of the bioprocess host organism limit the yield and purity of the product. Molecules that currently cannot be produced efficiently with robust microbial host organisms include wax esters, which have several industrial applications and are currently produced with the Jojoba plant.

Acinetobacter baylyi ADP1 is a non-pathogenic soil bacterium that produces wax esters that can readily incorporate foreign DNA into their genome and utilize various plant-derived molecules as a carbon source. For these reasons, *A. baylyi* ADP1 has become a model organism of bacterial genetics and metabolism, which has led to the accumulation of a vast amount of information about its biology. This Doctor of Science thesis describes experiments where the metabolism of *A. baylyi* ADP1 was engineered for improved growth and wax ester production using lignocellulose-derived molecules as raw material.

With a gene knockout (*rmlA*) and expression of a foreign gene (*pykF*), it was possible to double the growth rate of *A. baylyi* ADP1 on glucose, double the molar wax ester yield from glucose while improving product purity and collection of the cells. An additional gene knockout (*poxB*) improved growth and wax ester production in the presence of acetate, a common growth inhibitor found in lignocellulosic hydrolysates. A combination of these modifications led to a strain that produced 0.45 g/l of wax esters in a medium containing glucose, amino acids from casein hydrolysate and acetate as carbon sources. In addition, a biodegradation strain for the removal of inhibitors produced in the pretreatment of lignocellulosic biomass was produced with a single gene knockout.

While significant improvements in growth and wax ester production of *A. baylyi* ADP1 from components of lignocellulosic hydrolysates were obtained with metabolic engineering, the wax ester production needs to be further improved if this strain is going to be used in industrial applications. The strains that were produced here can be used as platform for further improvements of wax ester production by *A. baylyi* ADP1.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Chemistry and Bioengineering

Contributors: Kannisto, M.

Number of pages: 64

Publication date: 23 Mar 2018

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-4100-1

ISBN (Electronic): 978-952-15-4117-9

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Volume: 1532

ISSN (Print): 1459-2045

Electronic versions:

kannisto 1532

URLs:

<http://urn.fi/URN:ISBN:978-952-15-4117-9>

Thermal Isomerization of Hydroxyazobenzenes as a Platform for Vapor Sensing

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Aalto University

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

Number of pages: 6

Pages: 381-386

Publication date: 20 Mar 2018

Peer-reviewed: Yes

Publication information

Journal: ACS Macro Letters

Volume: 7

Issue number: 3

ISSN (Print): 2161-1653

Ratings:

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

Original language: English

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

Electronic versions:

82E3E980-7E4D-4608-8C73-F2F0ADCB6EEA

DOIs:

10.1021/acsmacrolett.8b00093

URLs:

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

Source: Scopus

Source ID: 85044222959

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

Modeling of Charge Transfer at Dye-Semiconductor Interfaces in p-Type Solar Cells

Dye-sensitized solar cells are composed of cheap and recyclable materials. These colorful and flexible cells convert sunlight into renewable energy. However, dye-sensitized solar cells are inefficient due to their low-charge current. The goal of this thesis is thus to create better understanding of the various components of these cells in order to improve their efficiencies. The main focus of dye-sensitized solar energy research lies in charge-transfer reactions between three main components: dye molecule; semiconductor surface, and electrolyte. In dye-sensitized solar cells, the charge is transferred from the excited dye molecule to the semiconductor surface. The charge is then transported to the electrode to create the electric current.

The studied components are derivatives of boron-dipyrromethene, perylene monoimide, and trisphenyl amine as dye molecules. Nickel oxide and titanium dioxide are used as semiconductor surfaces. The studied anchoring groups are carboxylate, 1,2-diol, and pyridine. These are studied in isolation, and then, their interactions in contact are investigated. In this study theoretical modeling is used, which includes the hybrid functional B3LYP and CRYSTAL09 software. The hybrid functional, B3LYP, is not widely used in studies within periodic boundary conditions such as dye-semiconductor interfaces. Thus, the mentioned systems have not been studied earlier at this level of theory.

In the first part of the study, the isolated systems, namely derivatives borondipyrromethene and titanium dioxide, are investigated. Results with BODIPY show that i) the vinylene group makes no difference for the electron transition nor orbital localization of orbitals, ii) phosphonate draws the most and carboxyl the least amount of the electron localization from the anchor, iii) methyl groups block completely the electron localization from the anchoring group, and iv) the absence of donor decreases the energy of HOMO level. BODIPY with vinylene and methyl groups were chosen for the

synthesis, because the methyl groups increase the life-time of electron-hole pair. Doping with nitrogen shows that the amount of nitrogen atoms makes difference for electronic structure, yet do not distort the lattice. The electronic structure changes due to the created empty gaps states that enhance electron conductivity.

In the second part of this study, derivatives of perylenemonoimide based dye molecules trisphenyl amine based anchoring groups on the NiO(100) surface and their interactions are investigated. The study with complete dye molecules on the nickel oxide surface is straightforward: the dyes' highest occupied molecular orbital is above nickel oxide's valence band maximum, thus, the spontaneous charge transfer is hard to obtain. Next it is shown that the anchoring group impacts the energy level alignment because of created dipole moment of the system that creates a shift within an electrostatic potential. Due to the shift, the highest occupied molecular orbitals of the dye molecule are either above (in case of carboxylate) or below (in the cases of pyridine and 1,2-diol) valence band maximum. In the case of complete molecules, which have the carboxylate as an anchoring group, HOMOs are above the VBM.

The results and analysis of the study show the importance of the size of the molecule and the anchoring group. The smaller the dye molecule, the smaller the distances are inside the interacting system, and shorter distances to transfer the charge. In the case of complete molecules, which have the carboxylate as an anchoring group, HOMOs are above the VBM. In conclusion, the largest effect is caused by the anchoring group inside the interacting system.

General information

Publication status: Published
MoE publication type: G4 Doctoral dissertation (monograph)
Organisations: Physics
Contributors: Kontkanen, O. V.
Number of pages: 117
Publication date: 2 Mar 2018

Publication information

Publisher: Tampere University of Technology
ISBN (Print): 978-952-15-4097-4
ISBN (Electronic): 978-952-15-4107-0
Original language: English

Publication series

Name: Tampere University of Technology. Publication
Volume: 1530
ISSN (Print): 1459-2045
Electronic versions:
kontkanen 1530
URLs:
<http://urn.fi/URN:ISBN:978-952-15-4107-0>
Research output: Book/Report > Doctoral thesis > Monograph

Techno-economic analysis of a power to biogas system operated based on fluctuating electricity price

This article presents a feasibility analysis of a novel operating principle based on fluctuating electricity prices for an existing biogas plant. By investing in an electrolyzer, excess electricity from renewable production can be stored as CH₄ by biological methanation of H₂ with CO₂ originating from the biogas plant. The main components of the system are an electrolyzer that is connected to an electric grid and an anaerobic digester where the methanation takes place as well as a biogas upgrading unit. First the energy flow of the system was studied, and secondly the operation costs of the system as well as the electrolyzer investment payback time were evaluated.

The study showed that up to 40% of the electricity fed into the system can be stored as biomethane, and the system energy flow is most sensitive to the electrolyzer efficiency. The economics of the studied system depend mostly on the electrolyzer investment cost and desired target price for the CH₄. The system can be run economically with current electricity prices if the electrolyzer investment costs decrease 60–72% or the price of CH₄ increases 20–76% depending on the investment interest and price fluctuation scheme.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy
Contributors: Pääkkönen, A., Tolvanen, H., Rintala, J.
Number of pages: 9
Pages: 166-174
Publication date: Mar 2018
Peer-reviewed: Yes

Early online date: 12 Oct 2017

Publication information

Journal: Renewable Energy

Volume: 117

ISSN (Print): 0960-1481

Ratings:

Scopus rating (2018): CiteScore 6.19 SJR 1.889 SNIP 2.075

Original language: English

DOIs:

10.1016/j.renene.2017.10.031

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

Critical role and modification of surface states in hematite films for enhancing oxygen evolution activity

Hematite films deposited by plasma-enhanced chemical vapor deposition of iron pentacarbonyl [Fe(CO)₅] in an oxygen plasma were modified by postdeposition (i) oxygen plasma treatment and (ii) short annealing treatments to reduce the defects and to modify the (sub)surface states and consequently the photoelectrochemical properties. The oxygen plasma treatment resulted in the increase of particle size and augmented surface roughening by densification of grains. Moreover, it induced saturated surface states with reactive oxygen species (O⁻, OH⁻), evident in the X-ray photoelectron spectroscopy (XPS). Under standard illumination (1.5 AM; 100 mW/cm²; 150 W xenon lamp), when compared to the pristine hematite coating (0.696 mA/cm²) at 1.23 V versus RHE and 0.74 V-onset) the oxygen plasma-treated films showed severe deterioration in photocurrent density of 0.035 mA/cm²) and an anodic shift in the onset potential (1.10 V-onset) due to oxygen rich surface. In a second set of experiments, the oxygen plasma-treated hematite films were briefly annealed (10 min at 750 degrees C) and the signals of Fe 2p and O 1s recovered to higher binding energies, indicating the formation of oxygen vacancies. In addition, a superior photocurrent density value of max. 1.306 mA/cm²) at 1.23 V versus RHE to that of the pristine hematite photoanode with 0.74 V-onset was obtained. Transient absorption spectroscopy further elucidated that the oxygen plasma-induced electron trap states acting as recombination centers that are unfavorable for photoelectrochemical activity. The alteration in Fe:O stoichiometry and thus photocurrent density are corroborated by determination of water oxidation rates in annealed (7.1 s⁻¹) and oxygen plasma treated (2.5 s⁻¹) samples.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Univ Cologne, University of Cologne, Inst Inorgan Chem

Contributors: Pyeon, M., Ruoko, T., Leduc, J., Goenuellue, Y., Deo, M., Tkachenko, N. V., Mathur, S.

Number of pages: 12

Pages: 455-466

Publication date: 28 Feb 2018

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Research

Volume: 33

Issue number: 4

ISSN (Print): 0884-2914

Ratings:

Scopus rating (2018): CiteScore 1.91 SJR 0.654 SNIP 0.754

Original language: English

Keywords: plasma-enhanced CVD (PECVD) (deposition), thin film, surface chemistry, RAY-ABSORPTION SPECTROSCOPY, WATER-SPLITTING PERFORMANCE, ALPHA-Fe₂O₃ PHOTOELECTRODES, SEMICONDUCTOR ELECTRODE, OXIDE PHOTOANODES, TRANSITION-METAL, XPS SPECTRA, IN-SITU, K-EDGE, OXIDATION

DOIs:

10.1557/jmr.2017.465

Source: WOS

Source ID: 000426671400007

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

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

A furan-based synthetic biopolymer composed of a bifuran monomer and ethylene glycol was synthesized through melt polycondensation, and the resulting polyester was found to have promising thermal and mechanical properties. The bifuran monomer, dimethyl 2,2'-bifuran-5,5'-dicarboxylate, was prepared using a palladium-catalyzed, phosphine ligand-free direct coupling protocol. A titanium-catalyzed polycondensation procedure was found effective at polymerizing the bifuran monomer with ethylene glycol. The prepared bifuran polyester exhibited several intriguing properties including high

tensile modulus. In addition, the bifuran monomer furnished the polyester with a relatively high glass transition temperature. Films prepared from the new polyester also had excellent oxygen and water barrier properties, which were found to be superior to those of poly(ethylene terephthalate). Moreover, the novel polyester also has good ultraviolet radiation blocking properties.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 8

Pages: 1822-1829

Publication date: 21 Feb 2018

Peer-reviewed: Yes

Early online date: 21 Feb 2018

Publication information

Journal: Macromolecules

Volume: 51

Issue number: 5

ISSN (Print): 0024-9297

Ratings:

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

Original language: English

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

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

DOIs:

10.1021/acs.macromol.7b02457

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 11

Pages: 1948-1958

Publication date: 16 Feb 2018

Peer-reviewed: Yes

Publication information

Journal: Journal of Organic Chemistry

Volume: 83

Issue number: 4

ISSN (Print): 0022-3263

Ratings:

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

Original language: English

ASJC Scopus subject areas: Organic Chemistry

Electronic versions:

acs.joc.7b02896

DOIs:

10.1021/acs.joc.7b02896

URLs:

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

Bibliographical note

INT=keb,"Vale, Joao R."

Source: Scopus

Source ID: 85042195347

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

Quantitative Real-time PCR Monitoring Dynamics Of Thermotoga Neapolitana In Synthetic Co-Culture For Biohydrogen Production

This study demonstrates the potential for biohydrogen production in a co-culture of two ecologically distant species, *Thermotoga neapolitana* and *Caldicellulosiruptor saccharolyticus*, and the development of a quantitative real-time PCR (qPCR) method for quantifying the hyperthermophilic bacterium of the genus *Thermotoga*. Substrate utilization and H₂ production performance was compared to those of their individual cultures. The highest H₂ yields obtained were 2.7 ± 0.05 , 2.5 ± 0.07 and 2.8 ± 0.09 mol H₂/mol glucose for *C. saccharolyticus*, *T. neapolitana*, and their co-culture respectively. Statistical analysis comparing the H₂ production rate of the co-culture to either *C. saccharolyticus* or *T. neapolitana* pure cultures indicated a significant difference in the H₂ production rate ($p < 0.05$: t-test), with the highest rate of H₂ production ($36.02 \text{ mL L}^{-1} \text{ h}^{-1}$) observed from the co-culture fermentations. In order to monitor the presence of *T. neapolitana* in the bioprocess, we developed a qPCR method using 16S rRNA gene and hydrogenase (*hydA*) gene targets. The qPCR data using *hydA* primers specific to *T. neapolitana* showed an increase in *hydA* gene copies from 3.32×10^7 to 4.4×10^8 *hydA* gene copies per mL confirming the influence of *T. neapolitana* in the synthetic consortium.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Okonkwo, O., Lakaniemi, A., Santala, V., Karp, M., Mangayil, R.

Number of pages: 9

Pages: 3133-3141

Publication date: 8 Feb 2018

Peer-reviewed: Yes

Publication information

Journal: International Journal of Hydrogen Energy

Volume: 43

Issue number: 6

ISSN (Print): 0360-3199

Ratings:

Scopus rating (2018): CiteScore 4.16 SJR 1.1 SNIP 1.128

Original language: English

Electronic versions:

Onyinye Okonkwo_Manuscript 1

DOIs:

[10.1016/j.ijhydene.2017.12.002](https://doi.org/10.1016/j.ijhydene.2017.12.002)

URLs:

<http://urn.fi/URN:NBN:fi:tty-201812192870>

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

Controlled Growth of Supported ZnO Inverted Nanopyramids with Downward Pointing Tips

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Supramolecular photochemistry, Chemistry and Bioengineering, Università degli Studi di Padova, Italy, Universiteit Antwerpen, VTT Technical Research Centre of Finland
Contributors: Barreca, D., Carraro, G., Maccato, C., Altantzis, T., Kaunisto, K., Gasparotto, A.
Number of pages: 9
Pages: 2579-2587
Publication date: Feb 2018
Peer-reviewed: Yes

Publication information

Journal: Crystal Growth and Design
Volume: 18
Issue number: 4
ISSN (Print): 1528-7483
Ratings:
Scopus rating (2018): CiteScore 4.01 SJR 1.046 SNIP 1.107
Original language: English
ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics
DOIs:
10.1021/acs.cgd.8b00198
Source: Scopus
Source ID: 85044992194
Research output: Contribution to journal › Article › Scientific › peer-review

Ultralong 20 Milliseconds Charge Separation Lifetime for Photoilluminated Oligophenylenevinylene–Azafullerene Systems

The synthesis and characterization of oligophenylenevinylene (OPV)–azafullerene (C59N) systems in the form of OPV–C59N donor–acceptor dyad 1 and C59N–OPV–C59N acceptor–donor–acceptor triad 2 is accomplished. Photoinduced electronic interactions between OPV and C59N within 1 and 2 are assessed by UV–vis and photoluminescence. The redox properties of 1 and 2 are investigated, revealing a set of one-electron oxidation and three one-electron reduction processes owed to OPV and C59N, respectively. The electrochemical bandgap for 1 and 2 is calculated as 1.44 and 1.53 eV, respectively, and the free energy for the formation of the charge-separated state for 1 and 2 via the singlet-excited state of OPV is found negative, proving a thermodynamically favorable the process. Photoexcitation assays are performed in toluene and o-dichlorobenzene (oDCB) and the reactions are monitored with time-resolved absorption and emission spectroscopies. Competitive photoinduced energy and electron transfer are identified to occur in both systems, with the former being dominant in 2. Markedly, the charge-separated state in oDCB exhibits a much longer lifetime compared to that in toluene, reaching 20 ms for 1, the highest ever reported value for fullerene-based materials. These unprecedented results are rationalized by considering conformational phenomena affecting the charge-separated state.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials
Contributors: Rotas, G., Stranius, K., Tkachenko, N., Tagmatarchis, N.
Publication date: Feb 2018
Peer-reviewed: Yes
Early online date: 18 Dec 2017

Publication information

Journal: Advanced Functional Materials
Volume: 28
Issue number: 7
Article number: 1702278
ISSN (Print): 1616-3028
Ratings:
Scopus rating (2018): CiteScore 14.58 SJR 5.646 SNIP 2.347
Original language: English
Keywords: azafullerenes, charge separation, oligophenylenevinylenes
DOIs:
10.1002/adfm.201702278
Source: Bibtex
Source ID: urn:2bc506961085ad4222326b1b84a9083
Research output: Contribution to journal › Article › Scientific › peer-review

Concentration-dependent photophysical switching in mixed self-assembled monolayers of pentacene and perylene-3,4,9,10-tetracarboxylic diimide on gold nanoclusters

Photophysical control and switching on organic-inorganic hybrid interfaces are of great interest in diverse fundamental and applicative research areas. 6,13-Bis(triisopropylsilylethynyl)pentacene (TP) is well-known to exhibit efficient singlet fission (SF) for generation of high-yield triplet excited states in aggregated forms, whereas perylene-3,4,9,10-tetracarboxylic diimide (PDI) ensembles show the characteristic excimer formation. Additionally, a combination of pentacene (electron donor: D) and PDI (electron acceptor: A) is expected to undergo an efficient photoinduced electron transfer (PET), and absorption of two chromophores combined covers the entire visible region. Therefore, the concentration-dependent mixed self-assembled monolayers (SAMs) composed of two chromophores enable us to control and switch the photophysical processes on a surface. In this work, a series of mixed SAMs composed of TP and PDI units on gold nanoclusters (GNCs) were newly synthesized by changing the relative molecular concentration ratios. Structural control of mixed SAMs on a gold surface based on the concentration ratios was successfully achieved. Time-resolved femtosecond and nanosecond transient absorption measurements clearly demonstrate photophysical control and switching of the above competitive reactions such as SF, electron transfer (ET) and excimer formation. The maximum quantum yields of triplet states ($\Phi_T = \sim 170\%$) and electron transfer ($\Phi_{ET} = \sim 95\%$) were quantitatively evaluated by changing the concentration ratios. The rate constants of SF and excimer processes are largely dependent on the concentration ratios, whereas the rate constants of ET processes approximately remain constant. These findings are also discussed based on the statistical framework of the assembly of chromophores on the gold surface.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Keio University, Tohoku University

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

Number of pages: 12

Pages: 8695-8706

Publication date: 1 Jan 2018

Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 20

Issue number: 13

ISSN (Print): 1463-9076

Ratings:

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

Original language: English

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

DOIs:

10.1039/c8cp00174j

Source: Scopus

Source ID: 85044838671

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 6

Pages: 9958-9963

Publication date: 1 Jan 2018

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry C

Volume: 6

Issue number: 37

ISSN (Print): 2050-7534

Ratings:

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

Original language: English

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

Electronic versions:

20180711_HBLC_REVISIED_GOA. Embargo ended: 30/08/19

DOIs:

10.1039/c8tc02611d

URLs:

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

Source: Scopus

Source ID: 85054152271

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

A Bioscreening Technique for Ultraviolet Irradiation Protective Natural Substances

Ultraviolet radiation (UV-R) causes genotoxic and aging effects on skin, and sunscreens are used to alleviate the damage. However, sunscreens contain synthetic shielding agents that can cause harmful effects in the environment. Nature-derived substances may have potential as replacement materials for the harmful sunscreen chemicals. However, screening of a broad range of samples is tedious, and often requires a separate genotoxicity assessment. We describe a simple microplate technique for the screening of UV protective substances using a recombinant *Escherichia coli* biosensor. Both absorbance-based and bioactivity-based shields can be detected with simultaneous information about the sample genotoxicity. With this technique, a controversial sunscreen compound, oxybenzone offers physical or absorbance-based shield but appears genotoxic at higher concentrations (3.3 mg/mL). We also demonstrate that pine needle extract (Pi_{Ne}) shields the biosensor from UV-R in a dose-dependent manner without showing genotoxicity. The physical shield of 5 mg/mL Pi_{Ne} was similar to that of one of the most common UV-shielding compound TiO₂ concentration 0.80 mg/mL. The bioactivity-based shield of Pi_{Ne} also reaches the extent of the physical shield with the highest concentration (3.3 mg/mL). We conclude that our technique is suitable in detecting the UV-shielding potential of natural substances, and gives simultaneous information on genotoxicity.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Pages: 1273-1280

Publication date: 2018

Peer-reviewed: Yes

Early online date: 2018

Publication information

Journal: Photochemistry and Photobiology

Volume: 94

Issue number: 6

ISSN (Print): 0031-8655

Ratings:

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

Original language: English

ASJC Scopus subject areas: Biochemistry, Physical and Theoretical Chemistry

DOIs:

10.1111/php.12954

Bibliographical note

INT=keb,"Poikulainen, Emmi"

Source: Scopus

Source ID: 85050664471

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

Adsorption of furfural from torrefaction condensate using torrefied biomass

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 11

Pages: 558-568

Publication date: 2018

Peer-reviewed: Yes

Early online date: 2017

Publication information

Journal: Chemical Engineering Journal

Volume: 334

ISSN (Print): 1385-8947

Ratings:

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

Original language: English

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

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

DOIs:

10.1016/j.cej.2017.10.053

Source: Scopus

Source ID: 85033666908

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

Archaea are prominent members of the prokaryotic communities colonizing common forest mushrooms

In this study, the abundance and composition of prokaryotic communities associated with the inner tissue of fruiting bodies of *Suillus bovinus*, *Boletus pinophilus*, *Cantharellus cibarius*, *Agaricus arvensis*, *Lycoperdon perlatum*, and *Piptoporus betulinus* were analyzed using culture-independent methods. Our findings indicate that archaea and bacteria colonize the internal tissues of all investigated specimens and that archaea are prominent members of the prokaryotic community. The ratio of archaeal 16S rRNA gene copy numbers to those of bacteria was >1 in the fruiting bodies of four out of six fungal species included in the study. The largest proportion of archaeal 16S rRNA gene sequences belonged to thaumarchaeotal classes Terrestrial group, Miscellaneous Crenarchaeotic Group (MCG), and Thermoplasmata. Bacterial communities showed characteristic compositions in each fungal species. Bacterial classes Gammaproteobacteria, Actinobacteria, Bacilli, and Clostridia were prominent among communities in fruiting body tissues. Bacterial populations in each fungal species had different characteristics. The results of this study imply that fruiting body tissues are an important habitat for abundant and diverse populations of archaea and bacteria.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Department of Microbiology, University of Helsinki, Turku University of Applied Science

Contributors: Rinta-Kanto, J. M., Pehkonen, K., Sinkko, H., Tamminen, M. V., Timonen, S.

Number of pages: 11

Pages: 716-726
Publication date: 2018
Peer-reviewed: Yes

Publication information

Journal: Canadian Journal of Microbiology

Volume: 64

Issue number: 10

ISSN (Print): 0008-4166

Ratings:

Scopus rating (2018): CiteScore 1.65 SJR 0.613 SNIP 0.649

Original language: English

ASJC Scopus subject areas: Microbiology, Immunology, Applied Microbiology and Biotechnology, Molecular Biology, Genetics

Keywords: Archaea, Bacteria, Mushroom, qPCR, Sequencing

Electronic versions:

rinta-kanto_CJM

DOIs:

10.1139/cjm-2018-0035

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201909273554>

Source: Scopus

Source ID: 85054057146

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

Bio-electrochemical conversion of industrial wastewater-COD combined with downstream methanol synthesis-an economic and life cycle assessment

Herein, a techno-economic and environmental performance evaluation (i.e. Life Cycle Assessment (LCA)) of a 45 kW Microbial Electrolysis Cell (MEC) system is presented in the context of industrial wastewater remediation. This system produces H₂ and CO₂-suitable for downstream CH₃OH synthesis-based on the bio-electrochemical conversion of chemical industry wastewater with an organic content of 3.9 g(COD) L⁻¹. A cost-benefit analysis indicates that the MEC system hardware costs, share of CO₂ captured from the MEC and MEC operating current density (i.e. 1.0 mA cm⁻²) are crucial parameters influencing the total cost and represent areas for potential cost reductions. It was established based on the present study that MEC system operation with renewable electricity leads to H₂ production costs of 4-5.7€ kg(H₂)⁻¹ (comparable to H₂O electrolysis) and CH₃OH production costs of 900€ t(CH₃OH)⁻¹. At the current CH₃OH market prices, however, the production is currently not profitable. In turn, the cost-efficient construction of the MEC system and the use of less expensive materials could lead to improved CH₃OH production economics based on this route. Our results indicate that the use of low-cost materials has greater potential with regard to cost reduction compared to reducing the internal resistance and polarization losses via the use of expensive high-performance materials in MEC construction. A complementary LCA of the proposed system, based on a "cradle-to-gate" definition, indicates that waste-based is superior to fossil-based CH₃OH production with respect to global warming potential and cumulated fossil energy demand, provided the system is operated with 100% renewable electricity and CO₂ sourced only from the MEC. However, with regard to the impact categories Metal Depletion and Freshwater Eutrophication Potential, the system was found to perform less satisfactorily (i.e. in comparison with fossil-based CH₃OH production).

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Fraunhofer Institute for Solar Energy Systems ISE, Albert-Ludwig-University of Freiburg, Karlsruhe Institute of Technology, Institute for Technical Physics, Germany, University of Freiburg, Laboratory for MEMS Applications, University of Bremen

Contributors: Streeck, J., Hank, C., Neuner, M., Gil-Carrera, L., Kokko, M., Pauliuk, S., Schadt, A., Kerzenmacher, S., White, R. J.

Number of pages: 21

Pages: 2742-2762

Publication date: 2018

Peer-reviewed: Yes

Publication information

Journal: Green Chemistry

Volume: 20

Issue number: 12

ISSN (Print): 1463-9262

Ratings:

Scopus rating (2018): CiteScore 9.43 SJR 2.517 SNIP 1.815

Original language: English
ASJC Scopus subject areas: Environmental Chemistry, Pollution
DOIs:
10.1039/c8gc00543e
Source: Scopus
Source ID: 85048986666
Research output: Contribution to journal › Article › Scientific › peer-review

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

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Natl. University of Ireland, Galway, Institute for Water Education, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education
Contributors: Dessi, P., Porca, E., Haavisto, J., Lakaniemi, A., Collins, G., Lens, P. N.
Number of pages: 12
Pages: 3069-3080
Publication date: 2018
Peer-reviewed: Yes

Publication information

Journal: RSC Advances
Volume: 8
Issue number: 6
ISSN (Print): 2046-2069
Ratings:
Scopus rating (2018): CiteScore 3.16 SJR 0.807 SNIP 0.785
Original language: English
ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all)
Electronic versions:
c7ra12316g
DOIs:
10.1039/c7ra12316g
URLs:
<http://urn.fi/URN:NBN:fi:tty-201802081202>
Source: Scopus
Source ID: 85040867034
Research output: Contribution to journal › Article › Scientific › peer-review

Conjugated Heat Transfer Simulation of a Fin-and-Tube Heat Exchanger

Heat transfer and pressure drop of a fin-and-tube heat exchanger are studied by taking into account the conjugated heat transfer between the flow and the fin. The temperature distribution of the fin is calculated in respect to the convective heat transfer of the air flowing through the tube bank channel. Contemporary enhancement methods emphasize the importance of local turbulence augmentation which effects the convective heat transfer. In this paper, the importance of conjugated heat transfer, where the temperature of the flow and fin are coupled together is emphasized and compared with a constant surface temperature boundary condition simulation and experiment, which are found in the literature.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Mechanical Engineering and Industrial Systems
Contributors: Välikangas, T., Karvinen, R.
Number of pages: 9
Pages: 1192-1200
Publication date: 2018
Peer-reviewed: Yes
Early online date: 12 Sep 2017

Publication information

Journal: Heat Transfer Engineering
Volume: 39
Issue number: 13-14
ISSN (Print): 0145-7632
Ratings:
Scopus rating (2018): CiteScore 1.83 SJR 0.818 SNIP 0.991
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanical Engineering, Fluid Flow and Transfer Processes
DOIs:
10.1080/01457632.2017.1363628
Source: Scopus
Source ID: 85029408517
Research output: Contribution to journal > Article > Scientific > peer-review

Effect of elevated nitrate and sulfate concentrations on selenate removal by mesophilic anaerobic granular sludge bed reactors

Simultaneous removal of selenate (SeO₄²⁻), nitrate (NO₃⁻) and sulfate (SO₄²⁻), typically present in Se-contaminated wastewaters, by Eerbeek anaerobic granular sludge, was investigated in batch and continuous bioreactor experiments. Batch experiments showed that SeO₄²⁻ removal was enhanced to 91% in simulated wastewater with SeO₄²⁻ + NO₃⁻ + SO₄²⁻ (1 : 40 : 100 SeO₄²⁻ : NO₃⁻ : SO₄²⁻ molar ratios) compared to simulated wastewater with SeO₄²⁻ alone (67%). SeO₄²⁻ removal was severely impacted by high concentrations of SO₄²⁻ (SeO₄²⁻ : SO₄²⁻ > 1 : 300). Removal of SeO₄²⁻, NO₃⁻ and SO₄²⁻ at a 1 : 40 : 100 ratio was studied in a 2 L lab-scale upflow anaerobic sludge blanket (UASB) reactor operated at 20 [degree]C, a 24 h hydraulic retention time and a 2 g COD L⁻¹ day⁻¹ organic loading rate using lactate as the electron donor. The removal efficiencies were stabilized at 100, 30 and 80% for NO₃⁻, SO₄²⁻ and total Se, respectively, during 92 days of UASB operation. The total Se removal efficiencies dropped to 47% or even to a negative value when, respectively, SO₄²⁻ and NO₃⁻ were sequentially excluded from the influent. Speciation of Se, particularly the microbial production of colloidal Se₀ levels, was influenced by both SO₄²⁻ and NO₃⁻. The results presented here demonstrate that UASB reactors are capable of removing SeO₄²⁻ in the presence of millimolar concentrations of NO₃⁻ and SO₄²⁻ typically found in Se-contaminated wastewaters.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, UNESCO-IHE Institute for Water Education
Contributors: Tan, L. C., Nancharaiyah, Y. V., van Hullebusch, E. D., Lens, P. N. L.
Pages: 303-314
Publication date: 2018
Peer-reviewed: Yes
Early online date: 5 Dec 2017

Publication information

Journal: Environmental Science: Water Research & Technology
Volume: 4
Issue number: 2
ISSN (Print): 2053-1400
Ratings:
Scopus rating (2018): CiteScore 4.02 SJR 1.104 SNIP 1.081
Original language: English
DOIs:
10.1039/C7EW00307B
Source: Bibtext
Source ID: urn:83b997c5e222c3328f8a2e876e3d3da8
Research output: Contribution to journal > Article > Scientific > peer-review

Effect of N/S ratio on anoxic thiosulfate oxidation in a fluidized bed reactor: Experimental and artificial neural network model analysis

Anoxic thiosulfate ($S_2O_3^{2-}$) oxidation using autotrophic denitrification by a mixed culture of nitrate reducing, sulfur oxidizing bacteria (NR-SOB) was studied in a fluidized bed reactor (FBR). The long-term performance of the FBR was evaluated for 306 days at three nitrogen-to-sulfur (N/S) molar ratios (0.5, 0.3 and 0.1) and a hydraulic retention time (HRT) of 5 h. $S_2O_3^{2-}$ removal efficiencies >99% were obtained at a N/S ratio of 0.5 and a $S_2O_3^{2-}$ and nitrate (NO_3^-) loading rate of $820 (\pm 84) \text{ mg S-S}_2\text{O}_3^{2-} \text{ L}^{-1} \text{ d}^{-1}$ and $173 (\pm 10) \text{ mg N-NO}_3^- \text{ L}^{-1} \text{ d}^{-1}$, respectively. The $S_2O_3^{2-}$ removal efficiency decreased to 76% and 26% at N/S ratios of 0.3 and 0.1, respectively, and recovered to 80% within 3 days after increasing the N/S ratio from 0.1 back to 0.5. The highest observed half-saturation (K_s) and inhibition (K_i) constants of the biofilm-grown NR-SOB obtained from batch cultivations were 172 and 800 $\text{mg S-S}_2\text{O}_3^{2-} \text{ L}^{-1}$, respectively. *Thiobacillus denitrificans* was the dominant microorganism in the FBR. Artificial neural network modeling successfully predicted $S_2O_3^{2-}$ and NO_3^- removal efficiencies and SO_4^{2-} production in the FBR. Additionally, results from the sensitivity analysis showed that the effluent pH was the most influential parameter affecting the $S_2O_3^{2-}$ removal efficiency.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education, University of Cassino and Southern Lazio, ENEA/CREATE/Università Degli Studi Napoli Federico II

Contributors: Khanongnuch, R., Di Capua, F., Lakaniemi, A., Rene, E. R., Lens, P. N.

Pages: 171-181

Publication date: 2018

Peer-reviewed: Yes

Early online date: 1 Jan 2018

Publication information

Journal: Process Biochemistry

Volume: 68

ISSN (Print): 1359-5113

Ratings:

Scopus rating (2018): SJR 0.754 SNIP 1.018

Original language: English

ASJC Scopus subject areas: Bioengineering, Biochemistry, Applied Microbiology and Biotechnology

Keywords: Anoxic thiosulfate oxidation, Artificial neural network, Kinetic constants, Nitrate reducing-sulfur oxidizing bacteria, *Thiobacillus denitrificans*

Electronic versions:

Effect of NtoS ratio on anoxic thiosulfate oxidation in a fluidized bed reactor- experimental and artificial neural network model analysis. Embargo ended: 23/02/19

DOIs:

10.1016/j.procbio.2018.02.018

URLs:

<http://urn.fi/URN:NBN:fi:tty-201811282779>. Embargo ended: 23/02/19

Source: Scopus

Source ID: 85044110451

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

Effects of Biomass Type, Carbonization Process, and Activation Method on the Properties of Bio-Based Activated Carbons

Activated carbons (AC) serve as adsorbents in various applications requiring specific functionalities. In this study, the effects of biomass type, pre-carbonization process, and activation method on the properties of ACs were investigated. Chemical (KOH and H_3PO_4) and physical (CO_2) activations were performed on slow pyrolyzed and hydrothermally carbonized (HTC) biochars produced from two feedstocks, willow and Scots pine bark (SPB). In addition, the adsorption capacities of the ACs were tested with two dyes and zinc metal. Distinct differences were found between the biochars and ACs regarding pore size distributions, surface area (238 - 3505 $\text{m}^2 \text{g}^{-1}$), and surface chemistry. KOH activation produced highly microporous ACs from all biochars, whereas with H_3PO_4 and CO_2 there was also increase in the meso- and macroporosity with the HTC biochars. Adsorption capacity for dyes was dependent on the surface area, while for zinc it depended on AC's pH. The results provide interesting insights into tailoring ACs for specific applications.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, VTT Tech Res Ctr Finland Ltd, VTT Technical Research Center Finland, Univ Oulu, University of Oulu, Res Unit Sustainable Chem, Nat Resources Inst Finland Luke, Natural Resources Institute Finland (Luke)

Contributors: Siipola, V., Tamminen, T., Kalli, A., Lahti, R., Romar, H., Rasa, K., Keskinen, R., Hyvaluoma, J., Hannula, M., Wikberg, H.
Number of pages: 27
Pages: 5976-6002
Publication date: 2018
Peer-reviewed: Yes

Publication information

Journal: BioResources
Volume: 13
Issue number: 3
ISSN (Print): 1930-2126
Ratings:

Scopus rating (2018): CiteScore 1.45 SJR 0.431 SNIP 0.728

Original language: English

Keywords: Biochar, Activated carbon, Bio-based activated carbon, Willow, Pine bark, X-ray tomography, PHOSPHORIC-ACID ACTIVATION, HYDROTHERMAL CARBONIZATION, CHEMICAL ACTIVATION, AGRICULTURAL RESIDUES, POROSITY DEVELOPMENT, H₃PO₄ ACTIVATION, POROUS CARBONS, FUEL-CELL, ADSORPTION, WASTE

URLs:

http://ojs.cnr.ncsu.edu/index.php/BioRes/article/view/BioRes_13_3_5976_Siipola_Biomass_Type_Carbonization_Process_Activation_Method/6205

Source: WOS

Source ID: 000440506300087

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering

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

Number of pages: 4

Pages: 14029-14032

Publication date: 2018

Peer-reviewed: Yes

Publication information

Journal: Chemical Communications

Volume: 54

Issue number: 99

ISSN (Print): 1359-7345

Ratings:

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

Original language: English

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

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

DOIs:

10.1039/c8cc07592a

URLs:

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

Source: Scopus

Source ID: 85058301188

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

Electronic waste as a secondary source of critical metals: Management and recovery technologies

The wealth of the society depends on several metals, including base metals, precious metals and increasingly rare earth elements (REE). They are collectively termed as technology metals. Numerous applications stimulated the use of technology metals, and their supply is at stake, owing to the high demand and uneven geographical distribution of these

metals. Their stable supply is crucial for the transition to a sustainable and circular economy. There is an increasing interest in secondary sources of these metals. This article outlines the global state of electronic waste, its management and the latest technological developments in metal recovery from various streams of electronic waste. An emphasis is given to printed circuit boards (PCB), hard disc drives (HDD) and displays regarding their critical metal content. Physical, pyrometallurgical and (bio)hydrometallurgical metal recovery technologies are overviewed. In addition, perspectives on electronic waste as a secondary source of critical metals are given.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Université Paris-Est, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education

Contributors: Işildar, A., Rene, E. R., van Hullebusch, E. D., Lens, P. N.

Pages: 296-312

Publication date: 2018

Peer-reviewed: Yes

Publication information

Journal: Resources, Conservation and Recycling

Volume: 135

ISSN (Print): 0921-3449

Ratings:

Scopus rating (2018): CiteScore 6.82 SJR 1.541 SNIP 2.258

Original language: English

ASJC Scopus subject areas: Waste Management and Disposal, Economics and Econometrics

Keywords: Critical metals, Hard disc drives (HDD), Liquid crystal displays (LCD), Printed circuit boards (PCB), Secondary source, WEEE

DOIs:

10.1016/j.resconrec.2017.07.031

Source: Scopus

Source ID: 85030839291

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

Fin-and-tube heat exchanger enhancement with a combined herringbone and vortex generator design

Vortex generators (VGs) are the most commonly investigated enhancement methods in the field of improved heat exchangers. The aim of present work is to study the effect of VGs in a fin-and-tube heat exchanger (FTHE) with herringbone fin shape. The delta winglet VG design with length (s) and height (H) is selected based on previous studies. The investigated VG design is simple and considered realistic from the manufacturing point of view. The combined enhancement with herringbone fin and the VG is evaluated by simulating the conjugate heat transfer and the air flow. The structured mesh is created for both solid and fluid domains to solve the model numerically using a coupled open source solver in OpenFOAM. The influence of flow condition on the performance enhancement is studied by changing the Reynolds number in a range $Re=1354-6157$. The study showed that VGs not only increase the heat transfer in the herringbone fin but also decrease the pressure drop. The highest and longest investigated VG design is found to perform the best because of its ability to delay the flow detachment from the tube, to feed high kinetic energy flow to the recirculation zone and to create longitudinal vortices in the downstream region from the VG. The fin with VG design $s=0.5D$ and $H=0.6F_p$ enhances the overall performance by 5.23% in comparison to the fin without VG. The results demonstrated the usefulness of VGs for the performance enhancement in connection with a herringbone fin design.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Bio- and Circular Economy, Physics, Chemistry and Bioengineering, Aalborg University

Contributors: Välikangas, T., Singh, S., Sørensen, K., Condra, T.

Number of pages: 15

Pages: 602-616

Publication date: 2018

Peer-reviewed: Yes

Early online date: 2017

Publication information

Journal: International Journal of Heat and Mass Transfer

Volume: 118

ISSN (Print): 0017-9310

Ratings:

Scopus rating (2018): CiteScore 4.73 SJR 1.624 SNIP 1.92

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Mechanical Engineering, Fluid Flow and Transfer Processes

Keywords: Conjugate heat transfer, Fin-and-tube heat exchanger, Herringbone fin, Vortex generator

DOIs:

10.1016/j.ijheatmasstransfer.2017.11.006

Source: Scopus

Source ID: 85034060389

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

Gammaproteobacterial methanotrophs dominate methanotrophy in aerobic and anaerobic layers of boreal lake waters

Small oxygen-stratified humic lakes of the boreal zone are important sources of methane to the atmosphere. Although stable isotope profiling has indicated that a substantial part of methane is already oxidized in the anaerobic water layers in these lakes, the contributions of aerobic and anaerobic methanotrophs in the process are unknown. We used next-generation sequencing of *mcrA* and 16S rRNA genes to characterize the microbial communities in the water columns of 2 boreal lakes in Finland, Lake Alinen-Mustajärvi and Lake Mekkojärvi, and complemented this with a shotgun metagenomic analysis from Alinen-Mustajärvi and an analysis of *pmoA* genes and 16S rRNA, *mcrA*, and *pmoA* transcripts from Mekkojärvi. Furthermore, we tested the effect of various electron acceptors and light on methane oxidation (¹³C-CH₄ labeling) in incubations of water samples collected from the lakes. Aerobic gamma

proteobacterial methanotrophs (order Methylococcales) exclusively dominated the methanotrophic community both above and below the oxycline in the lakes. A novel lineage within Methylococcales, *Candidatus* Methyloimidiphilus alinensis, defined here for the first time, dominated in Alinen-Mustajärvi, while methanotrophs belonging to Methylobacter were more abundant in Mekkojärvi. Light enhanced methane oxidation in the anoxic water layer, while alternative electron acceptors (SO₄²⁻, Fe³⁺, Mn⁴⁺, and anthraquinone-2,6-disulfonate), except for NO₃⁻, suppressed the process. Our results suggest that oxygenic photosynthesis potentially fuels methanotrophy below the aerobic water layers in methane-rich boreal lakes. Furthermore, incubation results, together with the detection of denitrification genes from metagenome-assembled genomes of gamma

proteobacterial methanotrophs, imply that boreal lake methanotrophs may couple methane oxidation with NO_x⁻ reduction in hypoxic conditions.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Univ Jyväskylä, University of Jyväskylä, Dept Biol & Environm Sci, Nanosci Ctr, University of Jyväskylä, University of Eastern Finland

Contributors: Rissanen, A. J., Saarenheimo, J., Tiirola, M. A., Peura, S., Aalto, S. L., Karvinen, A., Nykänen, H.

Number of pages: 20

Pages: 257-276

Publication date: 2018

Peer-reviewed: Yes

Publication information

Journal: Aquatic Microbial Ecology

Volume: 81

Issue number: 3

ISSN (Print): 0948-3055

Ratings:

Scopus rating (2018): CiteScore 2.26 SJR 0.944 SNIP 0.704

Original language: English

Electronic versions:

a081p257

DOIs:

10.3354/ame01874

URLs:

<http://urn.fi/URN:NBN:fi:tty-201806011910>

Additional files:

Supplementary material

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

High resolution E-jet printed temperature sensor on artificial skin

Skin-conformable electronics research field has grown rapidly during the recent years. Body monitoring systems are shrinking in size and integrating more seamlessly with the human skin. To make these monitoring systems feasible options, new suitable materials and manufacturing processes needs to be studied. This paper presents materials and a simple fabrication process for skin-conformable, E-jet printed silver temperature sensors. Utilizing printing processes and biodegradable substrate materials, the skin-conformable electronics may become attractive for disposable systems by decreasing the manufacturing costs and reducing the amount of waste materials. In this study, the temperature sensors

are fabricated with E-jet printed silver nanoparticle ink and the printing is done on a bacterial nanocellulose substrate. During the characterization, the silver temperature sensors were able to reach more than 0.06 % resistance change per degree Celsius sensitivity and they exhibited positive temperature dependence.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Electronics and Communications Engineering, Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Research group: Laboratory for Future Electronics

Contributors: Vuorinen, T., Laurila, M. M., Mangayil, R., Karp, M., Mäntysalo, M.

Number of pages: 4

Pages: 839-842

Publication date: 2018

Host publication information

Title of host publication: EMBEC and NBC 2017 - Joint Conference of the European Medical and Biological Engineering Conference EMBEC 2017 and the Nordic-Baltic Conference on Biomedical Engineering and Medical Physics, NBC 2017

Publisher: Springer Verlag

ISBN (Print): 9789811051210

Publication series

Name: IFMBE Proceedings

Volume: 65

ISSN (Print): 1680-0737

ASJC Scopus subject areas: Biomedical Engineering, Bioengineering

Keywords: Bacterial nanocellulose, E-jet, Printed electronics, Temperature sensor

Electronic versions:

2017-EMBEC2017

DOIs:

10.1007/978-981-10-5122-7_210

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201910113808>

Bibliographical note

jufoid=58152

Source: Scopus

Source ID: 85021718176

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

Identification of feasible pathway information for c-di-GMP binding proteins in cellulose production

In this paper, we utilize a machine learning approach to identify the significant pathways for c-di-GMP signaling proteins. The dataset involves gene counts from 12 pathways and 5 essential c-di-GMP binding domains for 1024 bacterial genomes. Two novel approaches, Least absolute shrinkage and selection operator (Lasso) and Random forests, have been applied for analyzing and modeling the dataset. Both approaches show that bacterial chemotaxis is the most essential pathway for c-di-GMP encoding domains. Though popular for feature selection, the strong regularization of Lasso method fails to associate any pathway to MshE domain. Results from the analysis may help to understand and emphasis to the supporting pathways involved in bacterial cellulose production. These findings demonstrate the need for a chassis to restrict the behavior or functionality by deactivating the selective pathways in cellulose production.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Computational Systems Biology, Chemistry and Bioengineering, BioMediTech

Contributors: Hassan, S. S., Mangayil, R., Aho, T., Yli-Harja, O., Karp, M.

Number of pages: 4

Pages: 667-670

Publication date: 2018

Host publication information

Title of host publication: EMBEC and NBC 2017 - Joint Conference of the European Medical and Biological Engineering Conference EMBEC 2017 and the Nordic-Baltic Conference on Biomedical Engineering and Medical Physics, NBC 2017

Publisher: Springer Verlag

ISBN (Print): 9789811051210

Publication series

Name: IFMBE Proceedings

Volume: 65

ISSN (Print): 1680-0737

ASJC Scopus subject areas: Biomedical Engineering, Bioengineering

Keywords: Cyclic di-guanosine monophosphate, Metabolic pathways, Random forests, Regularized logistic regression

DOIs:

10.1007/978-981-10-5122-7_167

Bibliographical note

jufoid=58152

Source: Scopus

Source ID: 85021754208

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

Light Robots: Bridging the Gap between Microrobotics and Photomechanics in Soft Materials

For decades, roboticists have focused their efforts on rigid systems that enable programmable, automated action, and sophisticated control with maximal movement precision and speed. Meanwhile, material scientists have sought compounds and fabrication strategies to devise polymeric actuators that are small, soft, adaptive, and stimuli-responsive. Merging these two fields has given birth to a new class of devices—soft microrobots that, by combining concepts from microrobotics and stimuli-responsive materials research, provide several advantages in a miniature form: external, remotely controllable power supply, adaptive motion, and human-friendly interaction, with device design and action often inspired by biological systems. Herein, recent progress in soft microrobotics is highlighted based on light-responsive liquid-crystal elastomers and polymer networks, focusing on photomobile devices such as walkers, swimmers, and mechanical oscillators, which may ultimately lead to flying microrobots. Finally, self-regulated actuation is proposed as a new pathway toward fully autonomous, intelligent light robots of the future.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, University of Warsaw, University of Florence

Contributors: Zeng, H., Wasylczyk, P., Wiersma, D. S., Priimagi, A.

Publication date: 2018

Peer-reviewed: Yes

Publication information

Journal: Advanced Materials

Volume: 30

Issue number: 24

Article number: 1703554

ISSN (Print): 0935-9648

Ratings:

Scopus rating (2018): CiteScore 23.77 SJR 10.108 SNIP 3.67

Original language: English

ASJC Scopus subject areas: Materials Science(all), Mechanics of Materials, Mechanical Engineering

Keywords: Actuators, Liquid crystals, Microrobots, Photomobile, Soft robots

Electronic versions:

20170830_Light Robots_revised_GOA. Embargo ended: 25/10/18

DOIs:

10.1002/adma.201703554

URLs:

<http://urn.fi/URN:NBN:fi:tty-201812192871>

Source: Scopus

Source ID: 85031898351

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

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

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

molecular hyperpolarizability, highlighting the unique properties of halogen bonding in supramolecular chemistry.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 8

Pages: 28810-28817

Publication date: 2018

Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 20

Issue number: 45

ISSN (Print): 1463-9076

Ratings:

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

Original language: English

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

DOIs:

10.1039/c8cp05392h

Source: Scopus

Source ID: 85056802102

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

Pathvalue: Pathways with value

This work proposes a tool called PathValue, that aims to identify commercially interesting reaction routes for bio-production. PathValue evaluates large sets of pathways using stoichiometric data, pathway properties such as compounds involved and estimates of market information. The public databases Rhea, ChEBI and IntEnz were utilized in this work for reaction, compound and enzyme data, respectively. Data were handled using Python whereas the PathValue tool was implemented as a JavaScript-based web application. The tool generates, filters and evaluates biochemical pathways. The functioning of the framework was assessed by querying pathways for ethanol and isoprene production and measuring the similarity of the generated pathways to known reference pathways. PathValue is freely available at <http://www.tut.fi/pathw/>.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

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

Contributors: Losoi, P., Aho, T.

Number of pages: 4

Pages: 583-586

Publication date: 2018

Host publication information

Title of host publication: EMBEC and NBC 2017 - Joint Conference of the European Medical and Biological Engineering Conference EMBEC 2017 and the Nordic-Baltic Conference on Biomedical Engineering and Medical Physics, NBC 2017

Publisher: Springer Verlag

ISBN (Print): 9789811051210

Publication series

Name: IFMBE Proceedings

Volume: 65

ISSN (Print): 1680-0737

ASJC Scopus subject areas: Biomedical Engineering, Bioengineering

Keywords: Commercial interest, Pathway identification, Reaction networks

DOIs:

10.1007/978-981-10-5122-7_146

Bibliographical note

jufoid=58152

INT=keb,"Losoi, Pauli"

Source: Scopus

Source ID: 85021772763

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Photoinduced Charge Separation in Semiconductor-Quantum-Dot/Organic-Molecule Hybrids

Semiconductor colloidal quantum dot/organic molecule nanohybrids are gaining momentum due to the relative ease with which an efficient photoinduced charge transfer in the desired direction can be achieved between the dot and the molecule. At the same time analysis of the experimental studies of such systems, and in particular transient absorption spectroscopy data, is a challenging task because of the statistical nature of hybrid formation and the complex kinetics of the photoreactions. This Minireview aims to find common ground for comparing the photoinduced charge-separation reactions in quantum dot/organic molecule hybrids. It also discusses a common set of parameters which would help to compare different quantum dot/molecule hybrids as well as progress in developing design principles to achieve controllable photoinduced charge separation in such hybrids.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

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

Contributors: Tkachenko, N.

Number of pages: 9

Pages: 112-120

Publication date: 2018

Peer-reviewed: Yes

Early online date: 14 Nov 2017

Publication information

Journal: ChemPhotoChem

Volume: 2

Issue number: 3

ISSN (Print): 2367-0932

Original language: English

DOIs:

10.1002/cptc.201700161

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

Programming Photoresponse in Liquid Crystal Polymer Actuators with Laser Projector

A versatile, laser-projector-based method is demonstrated for programming alignment patterns into monolithic films of liquid crystal polymer networks. Complex images can be photopatterned into the polymer films with sub-100 μm resolution, using relatively short exposure times. The method is further used to devise both photochemically and photothermally driven actuators that can undergo distinct light-induced shape changes, dictated by the programmed alignment patterns. Deformation modes such as buckling and coiling, as well as miniature robotic devices such as a gripper and a light-responsive octopod, are demonstrated. The reported technique enables easy and cost-effective programmable actuation with relatively high throughput, thus significantly facilitating the design and realization of functional soft robotic actuators.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Wani, O. M., Zeng, H., Wasylczyk, P., Priimagi, A.

Publication date: 2018

Peer-reviewed: Yes

Early online date: 2017

Publication information

Journal: Advanced Optical Materials

Volume: 6

Issue number: 1

Article number: 1700949

ISSN (Print): 2195-1071

Ratings:

Scopus rating (2018): CiteScore 7.36 SJR 2.711 SNIP 1.58

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics

Keywords: Azobenzene, Laser projectors, Liquid crystal, Patterning, Photoactuation, Photoalignment

Electronic versions:

Wani_AOM_Final_revised_GOA. Embargo ended: 4/12/18

DOIs:

10.1002/adom.201700949

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201901111061>

Source: Scopus

Source ID: 85037631675

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

Sediment diffusion method improves wastewater nitrogen removal in the receiving lake sediments

Sediment microbes have a great potential to transform reactive N to harmless N₂, thus decreasing wastewater nitrogen load into aquatic ecosystems. Here, we examined if spatial allocation of the wastewater discharge by a specially constructed sediment diffuser pipe system enhanced the microbial nitrate reduction processes. Full-scale experiments were set on two Finnish lake sites, Keuruu and Petäjavesi, and effects on the nitrate removal processes were studied using the stable isotope pairing technique. All nitrate reduction rates followed nitrate concentrations, being highest at the wastewater-influenced sampling points. Complete denitrification with N₂ as an end-product was the main nitrate reduction process, indicating that the high nitrate and organic matter concentrations of wastewater did not promote nitrous oxide (N₂O) production (truncated denitrification) or ammonification (dissimilatory nitrate reduction to ammonium; DNRA). Using 3D simulation, we demonstrated that the sediment diffusion method enhanced the contact time and amount of wastewater near the sediment surface especially in spring and in autumn, altering organic matter concentration and oxygen levels, and increasing the denitrification capacity of the sediment. We estimated that natural denitrification potentially removed 3–10% of discharged wastewater nitrate in the 33ha study area of Keuruu, and the sediment diffusion method increased this areal denitrification capacity on average 45%. Overall, our results indicate that sediment diffusion method can supplement wastewater treatment plant (WWTP) nitrate removal without enhancing alternative harmful processes.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, University of Jyväskylä, Univ Jyväskylä, University of Jyväskylä, Dept Biol & Environm Sci, Nanosci Ctr, Univ Jyväskylä, Dept Biomed & Environm Sci

Contributors: Aalto, S. L., Saarenheimo, J., Ropponen, J., Juntunen, J., Rissanen, A. J., Tirola, M.

Pages: 312-322

Publication date: 2018

Peer-reviewed: Yes

Publication information

Journal: Water Research

Volume: 138

ISSN (Print): 0043-1354

Ratings:

Scopus rating (2018): CiteScore 8.55 SJR 2.721 SNIP 2.426

Original language: English

Electronic versions:

1-s2.0-S0043135418302641-main

DOIs:

10.1016/j.watres.2018.03.068

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201804191515>

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

Simultaneous removal of tetrathionate and copper from simulated acidic mining water in bioelectrochemical and electrochemical systems

This study demonstrates (bio)electrochemical tetrathionate (S₄O₆²⁻) degradation with simultaneous elemental copper recovery from simulated acidic mining water. The effect of applied external voltage on anodic tetrathionate removal, cathodic copper removal and current density was studied using two-chamber flow-through bioelectrochemical (MEC) and abiotic electrochemical (EC) systems. At low applied cell voltages (≤ 0.5 V), the highest tetrathionate removal rate (150–170 mg L⁻¹ d⁻¹) and average current density (15–30 mA m⁻²) was obtained with MEC. At applied external voltages above 0.75 V, abiotic EC provided the highest average current density (410–3600 mA m⁻²). In bioelectrochemical systems, the current generation likely proceeds via intermediary reaction products (sulfide and/or thiosulfate), while in electrochemical system tetrathionate is oxidized directly on the electrode. The copper removal rates remained low (< 10 mg L⁻¹ d⁻¹) in all systems at applied cell voltages below 0.5 V, but increased up to a maximum of 440 mg L⁻¹ d⁻¹ in MEC and to 450 mg L⁻¹ d⁻¹ in EC at applied cell voltage of 1.5 V. After seven days of operation at applied cell voltage of 1.5 V, copper removal efficiency was 99.9% in both MEC and EC and the average tetrathionate

removal rates were $160 \text{ mg L}^{-1} \text{ d}^{-1}$ and $190 \text{ mg L}^{-1} \text{ d}^{-1}$, respectively. This study shows that by applying external voltage, tetrathionate and copper can be efficiently removed from acidic waters with bioelectrochemical and electrochemical systems.

General information

Publication status: Unpublished

MoE publication type: A1 Journal article-refereed

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

Contributors: Sulonen, M. L., Kokko, M. E., Lakaniemi, A., Puhakka, J. A.

Number of pages: 10

Pages: 129-138

Publication date: 2018

Peer-reviewed: Yes

Early online date: Feb 2018

Publication information

Journal: Hydrometallurgy

Volume: 176

ISSN (Print): 0304-386X

Ratings:

Scopus rating (2018): CiteScore 4 SJR 1.014 SNIP 1.817

Original language: English

ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Metals and Alloys, Materials Chemistry

Keywords: Bioelectrochemical system, Copper removal, Electrochemical system, Reduced inorganic sulfur compound, Tetrathionate

DOIs:

10.1016/j.hydromet.2018.01.023

Source: Scopus

Source ID: 85041488580

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

Stable blue phase polymeric Langmuir-Schaefer films based on unsymmetrical hydroxyalkadiynyl N-arylcarbamate derivatives

Unsymmetrical diynes containing N-arylcarbamate groups in the hydrophobic part and hydroxymethylene groups in the hydrophilic part of the molecules were synthesized and studied. The Langmuir monolayer formation process was followed by Brewster angle microscopy (BAM). The Langmuir-Schaefer monolayer films, transferred on solid substrates (quartz or Si), were investigated by absorption spectroscopy and atomic force microscopy (AFM). Four substances had 2 methylene groups in the hydrophilic part of the molecule (n) and 4 or 5 of these groups in the hydrophobic part (m). At the same time the aryl substituent had a hydrogen atom or a MeO group in the p-position of the benzene ring. After 20 min of UV irradiation the initially colorless monomeric films of all four compounds turned into stable blue phase polymeric films. The blue phase is unusual for alcoholic diacetylene derivatives. The BAM and AFM measurements demonstrated higher homogeneity of the films with a MeO group in the aryl substituent in comparison to the molecules with a hydrogen atom. The reasons for these different structural organizations as well as potential applications of stable blue phase polydiacetylene thin films are discussed.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, A. M. Prokhorov

General Physics Institute, Russian Academy of Sciences, Åbo Akademi University, St. Petersburg State University,

Russian Academy of Science

Contributors: Alekseev, A., Ihalainen, P., Ivanov, A., Domnin, I., Rosqvist, E., Lemmetyinen, H., Vuorimaa-Laukkanen, E., Peltonen, J., Vyaz'min, S.

Number of pages: 11

Pages: 108-118

Publication date: 2018

Peer-reviewed: Yes

Early online date: 10 Oct 2017

Publication information

Journal: Thin Solid Films

Volume: 645

ISSN (Print): 0040-6090

Ratings:

Scopus rating (2018): CiteScore 1.91 SJR 0.531 SNIP 0.815

Original language: English

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

Keywords: Absorption spectroscopy, Blue phase polydiacetylenes, Brewster angle microscopy, Langmuir-Schaefer film, Photopolymerization

DOIs:

10.1016/j.tsf.2017.10.018

Bibliographical note

EXT="Alekseev, Alexander"

Source: Scopus

Source ID: 85032302551

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

Supramolecular design principles for efficient photoresponsive polymer-azobenzene complexes

Noncovalent binding of azobenzenes to polymers allows harnessing light-induced molecular-level motions (photoisomerization) for inducing macroscopic effects, including photocontrol over molecular alignment and self-assembly of block copolymer nanostructures, and photoinduced surface patterning of polymeric thin films. In the last 10 years, a growing body of literature has proven the utility of supramolecular materials design for establishing structure-property-function guidelines for photoresponsive azobenzene-based polymeric materials. In general, the bond type and strength, engineered by the choice of the polymer and the azobenzene, influence the photophysical properties and the optical response of the material system. Herein, we review this progress, and critically assess the advantages and disadvantages of the three most commonly used supramolecular design strategies: hydrogen, halogen and ionic bonding. The ease and versatility of the design of these photoresponsive materials makes a compelling case for a paradigm shift from covalently-functionalized side-chain polymers to supramolecular polymer-azobenzene complexes.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Département de Chimie, Succ. Centre-Ville

Contributors: Vapaavuori, J., Bazuin, C. G., Priimagi, A.

Number of pages: 21

Pages: 2168-2188

Publication date: 2018

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry C

Volume: 6

Issue number: 9

ISSN (Print): 2050-7534

Ratings:

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

Original language: English

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

Electronic versions:

c7tc05005d

DOIs:

10.1039/c7tc05005d

URLs:

<http://urn.fi/URN:NBN:fi:ty-201803211417>

Source: Scopus

Source ID: 85042792061

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

Techno-economic evaluation of integrating torrefaction with anaerobic digestion

In recent days, the interest on torrefaction is increasing owing to its ability to improve biomass properties to a level of competing with coal. However, its techno-economic feasibility still need to be optimized. Integrating torrefaction with other thermochemical and biochemical processes could be a feasible option to improve the performance of the torrefaction process. In that regard, this study evaluates the techno-economic feasibility of integrating the torrefaction with anaerobic digestion (AD). In addition, new process configurations were studied to identify the possible heat energy recovery options. Technical feasibility was tested through mass and energy balance at each process unit. The economic indicators such as net present value (€), minimum selling price and internal rate on return (%) were used to evaluate the economic performance. At 10 t/h of torrefied biomass pellets production capacity, the estimated bio-methane production from AD

was 369 m³/h. The economic evaluation shows that the minimum selling price of the torrefied biomass to reach the breakeven could be reduced from 199 €/t for standalone torrefaction to 185 €/t in case of torrefaction integrated with AD. The sensitivity analysis shows that feedstock and total capital investment were the most sensitive input parameters. This study shows that integrating the torrefaction with AD has better technical and economic feasibility than standalone torrefaction.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 13

Pages: 272-284

Publication date: 2018

Peer-reviewed: Yes

Early online date: Jan 2018

Publication information

Journal: Applied Energy

Volume: 213

ISSN (Print): 0306-2619

Ratings:

Scopus rating (2018): CiteScore 9.54 SJR 3.455 SNIP 2.616

Original language: English

ASJC Scopus subject areas: Civil and Structural Engineering, Building and Construction, Energy(all), Mechanical Engineering, Management, Monitoring, Policy and Law

Keywords: Energy recovery, Minimum selling price, Process integration, Techno-economic analysis, Torrefaction – anaerobic digestion, Torrefied pellets

DOIs:

10.1016/j.apenergy.2018.01.045

Source: Scopus

Source ID: 85041461877

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

Thermophilic versus mesophilic dark fermentation in xylose-fed fluidised bed reactors: Biohydrogen production and active microbial community

Dark fermentative biohydrogen production in a thermophilic, xylose-fed (50 mM) fluidised bed reactor (FBR) was evaluated in the temperature range 55-70 °C with 5-degree increments and compared with a mesophilic FBR operated constantly at 37 °C. A significantly higher ($p = 0.05$) H₂ yield was obtained in the thermophilic FBR, which stabilised at about 1.2 mol H₂ mol⁻¹ xylose (36% of the theoretical maximum) at 55 and 70 °C, and at 0.8 mol H₂ mol⁻¹ xylose at 60 and 65 °C, compared to the mesophilic FBR (0.5 mol H₂ mol⁻¹ xylose). High-throughput sequencing of the reverse-transcribed 16S rRNA, done for the first time on biohydrogen producing reactors, indicated that *Thermoanaerobacterium* was the prevalent active microorganism in the thermophilic FBR, regardless of the operating temperature. The active microbial community in the mesophilic FBR was mainly composed of *Clostridium* and *Ruminiclostridium* at 37 °C. Thermophilic dark fermentation was shown to be suitable for treatment of high temperature, xylose-containing wastewaters, as it resulted in a higher energy output compared to the mesophilic counterpart.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Dessi, P., Porca, E., Waters, N. R., Lakaniemi, A., Collins, G., Lens, P. N.

Pages: 5473-5485

Publication date: 2018

Peer-reviewed: Yes

Early online date: 2018

Publication information

Journal: International Journal of Hydrogen Energy

Volume: 43

Issue number: 11

ISSN (Print): 0360-3199

Ratings:

Scopus rating (2018): CiteScore 4.16 SJR 1.1 SNIP 1.128

Original language: English

ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Fuel Technology, Condensed Matter Physics, Energy Engineering and Power Technology

Keywords: Active community, Biohydrogen, FBR, MiSeq, Thermoanaerobacterium, Thermophilic

Electronic versions:

Thermophilic versus mesophilic dark fermentation in xylose-fed fluidised bed reactors

DOIs:

10.1016/j.ijhydene.2018.01.158

URLs:

<http://urn.fi/URN:NBN:fi:tty-201901231143>

Source: Scopus

Source ID: 85042365131

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

Cellulose Nanofiber Alignment Using Evaporation-Induced Droplet-Casting, and Cell Alignment on Aligned Nanocellulose Surfaces

This work investigates droplet-evaporated cellulose nanofiber (CNF) alignment and cell responses on CNF surfaces. Surfaces of unmodified (u-), anionic (a-), and cationic (c-) CNFs were fabricated using an evaporation-induced droplet-casting method and characterized in terms of degree of orientation. Circular variance (CV) values obtained using Cytospectre software to analyze the degree of orientation from AFM images showed a significantly higher degree of orientation on c- and u-CNF surfaces (average CV 0.27 and 0.24, respectively) compared to a-CNF surfaces (average CV 0.76). Quantitative analysis of surface roughness plots obtained from AFM images confirmed the difference between the direction of alignment versus the direction perpendicular to alignment. AFM images as well as observations during droplet evaporation indicated c-CNF alignment parallel to a dry-boundary line during droplet evaporation. Fibroblasts were cultured on the u-, a-, and c-CNF surfaces with or without a fibronectin (FN) coating for 48 h, and the cell response was evaluated in terms of cell viability, proliferation, morphology, and degree of orientation. Cell viability and proliferation were comparable to that on a control surface on the a-CNF and c-CNF surfaces. Although an FN coating slightly enhanced cell growth on the studied surfaces, uncoated a-CNF and c-CNF surfaces were able to support cell growth as well. The results showed cell orientation on aligned c-CNF surfaces, a finding that could be further utilized when guiding the growth of cells. We also showed that the alignment direction of c-CNFs and thus the cell orientation direction can be controlled with a contact-dispensing technique.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Automation and Hydraulic Engineering, Research area: Measurement Technology and Process Control, Research group: Micro and Nanosystems Research Group, VTT Technical Research Center of Finland, Biologinkuja 7, 02150 Espoo, Finland.

Contributors: Skogberg, A., Mäki, A., Mettänen, M., Lahtinen, P., Kallio, P.

Number of pages: 18

Pages: 3936–3953

Publication date: 11 Dec 2017

Peer-reviewed: Yes

Publication information

Journal: Biomacromolecules

Volume: 18

Issue number: 12

ISSN (Print): 1525-7797

Ratings:

Scopus rating (2017): CiteScore 5.89 SJR 1.95 SNIP 1.339

Original language: English

Keywords: Journal Article

DOIs:

10.1021/acs.biomac.7b00963

Source: PubMed

Source ID: 28960956

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

Technology Development and Techno-Economic Analysis of Hydrogen Production by Thermal Decomposition of Methane

The transition to the hydrogen economy has been proposed as a sustainable solution for the simultaneous depletion of fossil fuels and the increase in global energy demand since the 1970s. However, the current fossil fuel-based hydrogen production causes significant CO₂ emissions. On the other hand, extensive hydrogen production by water electrolysis powered by renewable electricity requires a remarkable increase in the renewable electricity generation capacity.

Therefore, alternative solutions are needed in order to promote the hydrogen economy, develop hydrogen infrastructure,

and smoothen the transition to the wide-scale renewable-based hydrogen production in the future.

In this work, thermal decomposition of methane (TDM) was studied as a transition period solution towards the hydrogen economy. In TDM, methane is converted to hydrogen and solid carbon thereby avoiding the direct CO₂ emissions. A laboratory-scale test reactor was designed and constructed in this work in order to experimentally study the TDM reaction. The experimental results were combined with mathematical modeling to find a suitable TDM reaction mechanism for reactor design studies. A global reaction mechanism with reaction parameters optimized in this study was found applicable for this purpose.

The TDM product carbon utilization possibilities were evaluated by conducting a market survey. According to the experimental TDM studies in the literature, the product carbon from non-catalytic TDM at temperatures above 1450 K is carbon black. Carbon black is mainly utilized in rubber industry and its market value vary from 500 EUR per tonne to 2,000 EUR per tonne depending on the quality. As a part of the technology development, a design path was outlined to assist the selection of the reaction, reactor, and process parameters for a TDM application. The path was followed in this work when potential industrial-scale technology concepts for hydrogen production by TDM were designed. The economic feasibility of these processes was evaluated and comparison was conducted with two other hydrogen production technologies, i.e., steam methane reforming (SMR) and water electrolysis.

According to the economic analysis, a break-even value for the TDM product carbon was found as 310 EUR per tonne of carbon in the current market situation and 280 EUR per tonne of carbon in a potential market situation in 2030 above which the hydrogen production by TDM would be economically feasible in comparison with SMR. The CO₂ emissions from the hydrogen production by TDM were considerably lower than in SMR. Electrolysis could provide an economical option for the production of CO₂-free hydrogen when it is powered by inexpensive renewable electricity, but its availability is expected to remain limited in the near future. By contrast, the feedstock availability through the existing natural gas network provides a possibility for demand-driven hydrogen production by TDM. Thus, the most suitable application for TDM was identified in this work as small or medium industrial scale on-site hydrogen production, which minimizes hydrogen transportation costs. The TDM technology implementation could be further advanced by creating a sufficiently large market for the product carbon and tightening the CO₂ emission regulation.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

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

Contributors: Keipi, T.

Number of pages: 68

Publication date: 8 Dec 2017

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-4057-8

ISBN (Electronic): 978-952-15-4069-1

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Volume: 1519

ISSN (Print): 1459-2045

Electronic versions:

keipi 1519

URLs:

<http://urn.fi/URN:ISBN:978-952-15-4069-1>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Time-Resolved Fluorescence Spectroscopy Reveals Fine Structure and Dynamics of Poly(L-lysine) and Polyethylenimine Based DNA Polyplexes

Structural dynamics of the polyethylenimine-DNA and poly(L-lysine)-DNA complexes (polyplexes) was studied by steady-state and time-resolved fluorescence spectroscopy using the fluorescence resonance energy transfer (FRET) technique. During the formation of the DNA polyplexes, the negative phosphate groups (P) of DNA are bound by the positive amine groups (N) of the polymer. At N/P ratio 2, nearly all of the DNA's P groups are bound by the polymer N groups: These complexes form the core of the polyplexes. The excess polymer, added to this system to increase the N/P ratio to the values giving efficient gene delivery, forms a positively charged shell around the core polyplex. We investigated whether the exchange between the core and shell regions of PEI and PLL polyplexes takes place. Our results demonstrated a clear difference between the two studied polymers. Shell PEI can replace PEIs previously attached to DNA in the polyplex core, while PLL cannot. Such a dynamic structure of PEI polyplexes compared to a more static one found for PLL polyplexes partially explains the observed difference in the DNA transfection efficiency of these polyplexes. Moreover, the time-resolved fluorescence spectroscopy revealed additional details on the structure of PLL polyplexes: In between the

core and shell, there is an intermediate layer where both core and shell PLLs or their parts overlap.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Centre for Drug Research, University of Helsinki, Ita-Suomen yliopisto, Universita degli Studi di Padova, Italy

Contributors: Lisitsyna, E. S., Ketola, T., Morin-Picardat, E., Liang, H., Hanzlíková, M., Urtti, A., Yliperttula, M., Vuorimaa-Laukkanen, E.

Number of pages: 11

Pages: 10782-10792

Publication date: 7 Dec 2017

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry B

Volume: 121

Issue number: 48

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2017): CiteScore 3.13 SJR 1.331 SNIP 0.996

Original language: English

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

DOIs:

10.1021/acs.jpcc.7b08394

Source: Scopus

Source ID: 85037731381

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

Photodynamic self-disinfecting surface using pyridinium phthalocyanine

We have synthesized novel phthalocyanine with four pyridyl substituents connected to α -phthalocyanine positions via direct C-C bond. The Zn complex and tetracationic derivatives of phthalocyanine were also synthesized and the dyes were impregnated into filter paper to prepare photoactive antimicrobial surface. The photodynamic antimicrobial efficacy of the dyed paper samples was evaluated by a simple and fast setup using bioluminescent microbes. *Escherichia coli* and *Acinetobacter baylyi* ADP1 strains carrying bacterial luciferase genes were used in the screening experiment. The most efficient compound, tetracationic zinc derivative 8, was investigated further. The compound was highly water soluble, had high molar absorptivity and exhibited good adhesion to the filter paper without leaching into the solution. The singlet oxygen quantum yield of tetracationic zinc derivative 8 in water was found out to be $30 \pm 20\%$. According to the cell viability assay test performed on *E. coli* wild type in solution, the molecule had similar or better photo toxicity as the reference photosensitizer, tetrakis (1-methyl-pyridinium-4-yl)porphyrin (TMPyP). Antimicrobial efficacy of the dye 8 on photoactive surface was studied by live cell assessment through colony forming unit (CFU) counting. The colored surface demonstrated 3 log reduction in CFU against *E. coli* and *A. baylyi* ADP1 just after 1 h of illumination with the white light of low intensity.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Institut für Physik

Contributors: George, L., Müller, A., Röder, B., Santala, V., Efimov, A.

Number of pages: 9

Pages: 334-342

Publication date: 1 Dec 2017

Peer-reviewed: Yes

Publication information

Journal: Dyes and Pigments

Volume: 147

ISSN (Print): 0143-7208

Ratings:

Scopus rating (2017): CiteScore 3.59 SJR 0.819 SNIP 1.005

Original language: English

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

Keywords: Antimicrobial, Photodynamic antimicrobial chemotherapy, Pyridinium phthalocyanine, Self-disinfecting surface, Singlet oxygen

DOIs:

10.1016/j.dyepig.2017.08.021

Source: Scopus

Source ID: 85027896139

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

Comparison of *Scenedesmus acuminatus* and *Chlorella vulgaris* cultivation in liquid digestates from anaerobic digestion of pulp and paper industry and municipal wastewater treatment sludge

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Tao, R., Kinnunen, V., Praveenkumar, R., Lakaniemi, A., Rintala, J. A.

Number of pages: 12

Pages: 2845–2856

Publication date: Dec 2017

Peer-reviewed: Yes

Publication information

Journal: Journal of Applied Phycology

Volume: 29

Issue number: 6

ISSN (Print): 0921-8971

Ratings:

Scopus rating (2017): CiteScore 2.59 SJR 0.784 SNIP 1.022

Original language: English

ASJC Scopus subject areas: Aquatic Science, Plant Science

Keywords: Biorefinery, Chlorophyceae, Digestate, High biomass yield, Microalgae, Nutrient removal

Electronic versions:

Comparison of *Scenedesmus acuminatus* and *Chlorella vulgaris* cultivation in liquid digestates from anaerobic digestion of pulp and paper industry and municipal wastewater treatment sludge

DOIs:

10.1007/s10811-017-1175-6

URLs:

<http://urn.fi/URN:NBN:fi:ty-201812052815>

Source: Scopus

Source ID: 85020258442

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

Carbazole-based small molecule electron donors: Syntheses, characterization, and material properties

Efficient synthetic methods for carbazole-based small molecule electron donors with donor–acceptor (D–A) and A–D–A type structures were developed. In order to study the relation between chemical structures and material properties, the prepared compounds were characterized in detail using absorption spectroscopy, differential pulse voltammetry, and computational methods. In addition, symmetrical A–D–A type compounds were tested as an active layer component in bulk heterojunction based organic solar cell (OSC) devices with conventional structure. The results show that the two compound types have many similar properties. However, the extended molecular structure of A–D–A type compounds offer better film forming properties and higher molar absorption coefficients compared with the D–A type materials. Furthermore, the attachment of fluoro substituents in the A units has a positive effect on all solar cell device parameters. Moreover, the computational studies revealed that the molecular structures are twisted between the central carbazole D unit and π -bridge which may result in inefficient intramolecular charge transfer and, also, relatively limited short-circuit currents in OSC devices.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials, Research Unit of Sustainable Chemistry, IMEC PV Department

Contributors: Sippola, R. J., Hadipour, A., Kastinen, T., Vivo, P., Hukka, T. I., Aernouts, T., Heiskanen, J. P.

Number of pages: 10

Pages: 79-88

Publication date: 8 Nov 2017

Peer-reviewed: Yes

Early online date: 8 Nov 2017

Publication information

Journal: Dyes and Pigments

Volume: 150

Article number: j.dyepig.2017.11.014

ISSN (Print): 0143-7208

Ratings:

Scopus rating (2017): CiteScore 3.59 SJR 0.819 SNIP 1.005

Original language: English

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

Keywords: Absorption, DFT, Electron donor, Organic solar cell, Suzuki-Miyaura, Synthesis

DOIs:

10.1016/j.dyepig.2017.11.014

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

Multimodal Nonlinear Optical Imaging for Sensitive Detection of Multiple Pharmaceutical Solid-State Forms and Surface Transformations

Two nonlinear imaging modalities, coherent anti-Stokes Raman scattering (CARS) and sum-frequency generation (SFG), were successfully combined for sensitive multimodal imaging of multiple solid-state forms and their changes on drug tablet surfaces. Two imaging approaches were used and compared: (i) hyperspectral CARS combined with principal component analysis (PCA) and SFG imaging and (ii) simultaneous narrowband CARS and SFG imaging. Three different solid-state forms of indomethacin—the crystalline gamma and alpha forms, as well as the amorphous form—were clearly distinguished using both approaches. Simultaneous narrowband CARS and SFG imaging was faster, but hyperspectral CARS and SFG imaging has the potential to be applied to a wider variety of more complex samples. These methodologies were further used to follow crystallization of indomethacin on tablet surfaces under two storage conditions: 30 degrees C/23% RH and 30 degrees C/75% RH. Imaging with (sub)micron resolution showed that the approach allowed detection of very early stage surface crystallization. The surfaces progressively crystallized to predominantly (but not exclusively) the gamma form at lower humidity and the alpha form at higher humidity. Overall, this study suggests that multimodal nonlinear imaging is a highly sensitive, solid-state (and chemically) specific, rapid, and versatile imaging technique for understanding and hence controlling (surface) solid-state forms and their complex changes in pharmaceuticals.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Univ Helsinki, University of Helsinki, Fac Pharm, Div Pharmaceut Chem & Technol, University of Otago, University of Helsinki

Contributors: Novakovic, D., Saarinen, J., Rojalin, T., Antikainen, O., Fraser-Miller, S. J., Laaksonen, T., Peltonen, L., Isomaki, A., Strachan, C. J.

Number of pages: 8

Pages: 11460-11467

Publication date: 7 Nov 2017

Peer-reviewed: Yes

Publication information

Journal: Analytical Chemistry

Volume: 89

Issue number: 21

ISSN (Print): 0003-2700

Ratings:

Scopus rating (2017): CiteScore 6.24 SJR 2.362 SNIP 1.489

Original language: English

Keywords: RAMAN SCATTERING MICROSCOPY, CARS MICROSCOPY, AMORPHOUS INDOMETHACIN, DOSAGE FORMS, TRACE CRYSTALLINITY, T-G, CRYSTALLIZATION, DISSOLUTION, DRUG, POLYMORPHS

DOIs:

10.1021/acs.analchem.7b02639

Source: WOS

Source ID: 000414887000044

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

Azopolymer photopatterning for directional control of angiogenesis

Understanding cellular behavior in response to microenvironmental stimuli is central to tissue engineering. An increasing number of reports emphasize the high sensitivity of cells to the physical characteristics of the surrounding milieu and in particular, topographical cues. In this work, we investigated the influence of dynamic topographic signal presentation on sprout formation and the possibility to obtain a space–time control over sprouting directionality without growth factors, in order to investigate the contribution of just topography in the angiogenic process. To test our hypothesis, we employed a 3D angiogenesis assay based on the use of spheroids derived from human umbilical vein endothelial cells (HUVECs). We then modulated the in situ presentation of topographical cues during early-stage angiogenesis through real-time photopatterning of an azobenzene-containing polymer, poly (Disperse Red 1 methacrylate) (pDR1m). Pattern inscription on the polymer surface was made using the focused laser of a confocal microscope. We demonstrate that during early-stage angiogenesis, sprouts followed the pattern direction, while spheroid cores acquired a polarized shape. These findings confirmed that sprout directionality was influenced by the photo-inscribed pattern, probably through contact guidance of leader cells, thus validating the proposed platform as a valuable tool for understanding complex processes involved in cell-topography interactions in multicellular systems. **Statement of Significance** The complex relationship between endothelial cells and the surrounding environment that leads to formation of a newly formed vascular network during tissue repair is currently unknown. We have developed an innovative in vitro platform to study these mechanisms in a space and time controlled fashion simulating what happens during regeneration. In particular, we combine a “smart” surface, namely a polymer film, with a three-dimensional living cell aggregate. The polymer is activated by light through which we can design a path to guide cells toward the formation of a new vessel. Our work lies at the intersection of stimuli-responsive biointerfaces and cell biology and may be particularly inspiring for those interested in designing biomaterial surface related to angiogenesis.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Center for Advanced Biomaterials for Healthcare, Italian Institute of Technology, Dipartimento di Ingegneria Chimica dei Materiali e della Produzione Industriale, ENEA/CREATE/Università Degli Studi Napoli Federico II, Laboratory of Chemistry and Bioengineering

Contributors: Fedele, C., De Gregorio, M., Netti, P. A., Cavalli, S., Attanasio, C.

Number of pages: 9

Pages: 317-325

Publication date: 1 Nov 2017

Peer-reviewed: Yes

Publication information

Journal: Acta Biomaterialia

Volume: 63

ISSN (Print): 1742-7061

Ratings:

Scopus rating (2017): CiteScore 6.97 SJR 1.967 SNIP 1.815

Original language: English

ASJC Scopus subject areas: Biotechnology, Biomaterials, Biochemistry, Biomedical Engineering, Molecular Biology

Keywords: Angiogenesis, Azopolymers, Directional sprouting, Photopatterning, Topographical cues

DOIs:

10.1016/j.actbio.2017.09.022

Source: Scopus

Source ID: 85029628146

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

Effect of hydraulic retention time on continuous electricity production from xylose in up-flow microbial fuel cell

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Feng Chia University

Contributors: Haavisto, J. M., Kokko, M. E., Lay, C., Puhakka, J. A.

Pages: 27494-27502

Publication date: 1 Nov 2017

Peer-reviewed: Yes

Publication information

Journal: International Journal of Hydrogen Energy

Volume: 42

ISSN (Print): 0360-3199

Ratings:

Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.292

Original language: English

ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Fuel Technology, Condensed Matter

Physics, Energy Engineering and Power Technology

Keywords: Continuous operation, Hydraulic retention time, Microbial community, Microbial fuel cell, Up-flow, Xylose

Electronic versions:

Effect of hydraulic retention time on continuous electricity production from xylose in up-flow microbial fuel cell. Embargo ended: 2/11/19

DOIs:

10.1016/j.ijhydene.2017.05.068

URLs:

<http://urn.fi/URN:NBN:fi:tty-201907151963>. Embargo ended: 2/11/19

Bibliographical note

EXT="Lay, Chyi-How"

Source: Scopus

Source ID: 85019734862

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

Modelling recovery of ammonium from urine by electro-concentration in a 3-chamber cell

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Tampere University of Technology, Chemistry and Bioengineering, University of Queensland

Contributors: Thompson Brewster, E., Jermakka, J., Freguia, S., Batstone, D. J.

Number of pages: 9

Pages: 210-218

Publication date: 1 Nov 2017

Peer-reviewed: Yes

Publication information

Journal: Water Research

Volume: 124

ISSN (Print): 0043-1354

Ratings:

Scopus rating (2017): CiteScore 7.55 SJR 2.601 SNIP 2.388

Original language: English

Keywords: Ammonium bicarbonate, Electro-concentration, Electrochemical model, Nutrient recovery, Physicochemical model, Urine

DOIs:

10.1016/j.watres.2017.07.043

Source: Scopus

Source ID: 85026353513

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

Nanofibrillar cellulose hydrogels and reconstructed hydrogels as matrices for controlled drug release

Concentrated 3% and 6.5% anionic nanofibrillar cellulose (ANFC) hydrogels were introduced as matrix reservoirs for controlled delivery applications of small molecules and proteins. A further aim was to study how the freeze-drying and subsequent rehydration of ANFC hydrogel affects the rheological properties and drug release of selected model

compounds from the reconstructed hydrogels. It was demonstrated that the 3% and 6.5% ANFC hydrogels can be freeze-dried with suitable excipients into highly porous aerogel structures and redispersed back into the hydrogel form without significant change in the rheological properties. Freeze-drying did not affect the drug release properties from redispersed ANFC hydrogels, indicating that these systems could be stored in the dry form and only redispersed when needed. For large molecules, the diffusion coefficients were significantly smaller when higher ANFC fiber content was used, indicating that the amount of ANFC fibers in the hydrogel can be used to control the release rate. The release of small molecules was controlled with the ANFC fiber content only to a moderate extent. The results indicate that ANFC hydrogel can be used for controlled delivery of several types of molecules and that the hydrogel can be successfully freeze-dried and redispersed.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, University of Helsinki, Centre for Drug Research, Università degli Studi di Padova, Italy

Contributors: Paukkonen, H., Kunnari, M., Laurén, P., Hakkarainen, T., Auvinen, V., Oksanen, T., Koivuniemi, R., Yliperttula, M., Laaksonen, T.

Number of pages: 12

Pages: 269-280

Publication date: 30 Oct 2017

Peer-reviewed: Yes

Publication information

Journal: International Journal of Pharmaceutics

Volume: 532

Issue number: 1

ISSN (Print): 0378-5173

Ratings:

Scopus rating (2017): CiteScore 4.06 SJR 1.172 SNIP 1.302

Original language: English

ASJC Scopus subject areas: Pharmaceutical Science

Keywords: Aerogel, Diffusion, Drug release, Freeze-drying, Hydrogel, Nanofibrillar cellulose, Rheology

Electronic versions:

Paukkonen_IJP_2017. Embargo ended: 6/09/18

DOIs:

10.1016/j.ijpharm.2017.09.002

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201712222488>. Embargo ended: 6/09/18

Source: Scopus

Source ID: 85029371925

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

A demand-based nutrient utilization approach to urban biogas plant investment based on regional crop fertilization

This study aimed to develop a regional nutrient demand-based approach to assess the potential use of digestate nutrients from a planned biogas plant investment as a part of a regional circular economy concept. The assumed biogas plant is expected to treat urban wastes; biowastes (23,500 t/y) and sewage sludges (120,000 t/y) from the Tampere region, Finland (total population of 500,000). The calculation of the regional nutrient balance was based on the fertilizable crop areas, fertilization regimes and biomass nutrient amounts, with an assumption that livestock manures were primarily utilized in crop production. Subsequently, a Geographic Information System (GIS)-based methodology was applied to evaluate the transportation distances of nutrients from the biogas plant to the closest crop fields. As a result from the presented approach, livestock manure covered 41% and 12% of the phosphorus (P) and soluble nitrogen (N) need of the studied region. There was a residual potential for the regional utilization of biogas plant nutrients, which together with the livestock manure accounted for 50% of P and 15% of soluble-N need. Transportation of nutrients up to 40 km from the biogas plant is necessary if all nearby fields receive the waste-based nutrients, while the distance increased to 66 km if 30% of the local farmers are willing to use the nutrients. The approach presented in this study acts as a tool for planning nutrient cycles, which can be used to sustainably manage the regional nutrient flows when planning a new biogas plant investment.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Natural Resources Institute Finland (Luke)

Contributors: Tampio, E., Lehtonen, E., Kinnunen, V., Mönkäre, T., Ervasti, S., Kettunen, R., Rasi, S., Rintala, J.

Number of pages: 11

Pages: 19-29

Publication date: 15 Oct 2017

Peer-reviewed: Yes

Publication information

Journal: Journal of Cleaner Production

Volume: 164

ISSN (Print): 0959-6526

Ratings:

Scopus rating (2017): CiteScore 5.79 SJR 1.467 SNIP 2.339

Original language: English

ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Environmental Science(all), Strategy and Management, Industrial and Manufacturing Engineering

Keywords: Biogas plant, Biowaste, Digestate, Livestock manure, Nutrient recycling, Sewage sludge

DOIs:

10.1016/j.jclepro.2017.06.172

Bibliographical note

EXT="Tampio, Elina"

Source: Scopus

Source ID: 85027488845

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

Effect of natural convection and radiation inside of a hollow beam in a standard fire

In the design of steel structures, special attention must be paid on structural fire design in order to ensure a specified safe time period that the structure can withstand the fire without collapse. In the European design rules, the standard practise assumes uniform temperature for steel beam cross sections while the surrounding area is subjected to the so called standard fire. When the ambient temperature field is not uniform (e.g. at beam joint areas) neither will be the beam cross section temperature field. This paper studies the contribution of natural convection and cavity radiation to the temperature field of a hollow beam cross section in the case of non-uniform ambient temperature by using transient CFD-simulations.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Civil Engineering, Research group: Light-weight structures, Aalborg University

Contributors: Välikangas, T., Pajunen, S., Baczkiewicz, J., Singh, S., Sørensen, K.

Number of pages: 7

Pages: 121-127

Publication date: 27 Sep 2017

Host publication information

Title of host publication: Proceedings of the 58th Conference on Simulation and Modelling (SIMS 58) Reykjavik, Iceland, September 25th – 27th, 2017

Volume: 138

Place of publication: Linköping

Publisher: Linköping University Electronic Press

Editor: Jonsson, M. T.

Article number: 16

ISBN (Electronic): 978-91-7685-417-4

Publication series

Name: Linköping Electronic Conference Proceedings

Publisher: Linköping University Electronic Press

No.: 138

ISSN (Print): 1650-3686

ISSN (Electronic): 1650-3740

Electronic versions:

[ecp17138016](#)

DOIs:

[10.3384/ecp17138121](#)

URLs:

<http://urn.fi/URN:NBN:fi:ty-201712142350>

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

New Evidence for the Mechanism of Action of a Type-2 Diabetes Drug Using a Magnetic Bead-Based Automated Biosensing Platform

The mechanism of action (MOA) of the first line type-2 diabetes drug metformin remains unclear despite its widespread usage. However, recent evidence suggests that the mitochondrial copper (Cu)-binding action of metformin may contribute toward the drug's MOA. Here, we present a novel biosensing platform for investigating the MOA of metformin using a magnetic microbead-based agglutination assay which has allowed us to demonstrate for the first time the interaction between Cu and metformin at clinically relevant low micromolar concentrations of the drug, thus suggesting a potential pathway of metformin's blood-glucose lowering action. In this assay, cysteine-functionalized magnetic beads were agglutinated in the presence of Cu due to cysteine's Cu-chelation property. Addition of clinically relevant doses of metformin resulted in disaggregation of Cu-bridged bead-clusters, whereas the effect of adding a closely related but blood-glucose neutral drug propanedimidamide (PDI) showed completely different responses to the clusters. The entire assay was integrated in an automated microfluidics platform with an advanced optical imaging unit by which we investigated these aggregation-disaggregation phenomena in a reliable, automated, and user-friendly fashion with total assay time of 17 min requiring a sample (metformin/PDI) volume of 30 μL . The marked difference of Cu-binding action between the blood-glucose lowering drug metformin and its inactive analogue PDI thus suggests that metformin's distinctive Cu-binding properties may be required for its effect on glucose homeostasis. The novel automated platform demonstrating this novel investigation thus holds the potential to be utilized for investigating significant and sensitive molecular interactions via magnetic bead-based agglutination assay.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Danmarks Tekniske Universitet, DTU Informatik, University of Dundee, Academia Sinica Taiwan

Contributors: Uddin, R., Nur-E-Habiba, N., Rena, G., Hwu, E. T., Boisen, A.

Number of pages: 8

Pages: 1329-1336

Publication date: 22 Sep 2017

Peer-reviewed: Yes

Publication information

Journal: ACS Sensors

Volume: 2

Issue number: 9

ISSN (Print): 1424-8220

Ratings:

Scopus rating (2017): CiteScore 3.23 SJR 0.584 SNIP 1.567

Original language: English

ASJC Scopus subject areas: Bioengineering, Fluid Flow and Transfer Processes, Process Chemistry and Technology, Instrumentation

Keywords: agglutination assay, biosensor, magnetic beads, metformin, molecular interactions, optical imaging, type-2 diabetes

DOIs:

10.1021/acssensors.7b00384

Bibliographical note

INT=keb,"Nur-E-Habiba, N."

Source: Scopus

Source ID: 85029817525

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

Bioelectrochemical Recovery of Energy and Metals from Simulated Mining Waters

Extremely acidic water with high metal concentrations is often produced during mining and processing of sulfidic ores. Sulfur-oxidizing microorganisms contribute significantly to the acidification of the water streams and oxygen depletion by oxidizing reduced inorganic sulfur compounds (RISCs) — which are released to the mining waters during the processing of sulfide minerals — to sulfuric acid. The acidic water continues leaching metals from minerals and the metal concentrations thus further increase.

Certain metals can be recovered from acidic solutions by using them as the electron acceptor at the cathode of an electrochemical system. The metal ions accept electrons from an electrode and deposit on the surface of the electrode in pure elemental form. The electrical current required for the electrodeposition of metals is conventionally drawn from the oxidation of water. However, with the assist of electroactive microorganisms, biodegradable compounds can be used as the source of the required energy. Electroactive microorganisms oxidize a substrate and donate electrons to an anode electrode. The flow of electrons from anode to cathode creates electrical current, which can be utilized in the

electrodeposition of the metals. As mining waters do not usually contain organic compounds, RISCs are promising substrates for the recovery of metals from mining waters — they are present in the same stream and can be oxidized at lower potential than water. In addition, with the electrochemical treatment both metals and RISCs could be removed from the water streams simultaneously.

The aim of this work was to use tetrathionate (S₄O₆²⁻) as the substrate for bioelectrochemical and electrochemical current generation. The possibility to spontaneously produce electricity from tetrathionate was first studied in microbial fuel cells (Paper I). After successful electricity production was obtained, a tetrathionate-fed microbial fuel cell was monitored for over 740 days to determine the long-term stability of such systems (Paper II). The anode potential was then externally adjusted in order to determine the minimum anode potential required for bioelectrochemical and electrochemical tetrathionate degradation (Paper III). Finally, the external voltage required for the simultaneous removal of tetrathionate and copper was determined (Paper IV).

The experiments were conducted using two-chamber flow through reactors at room temperature (22±5 °C) and highly acidic conditions (pH < 2.5). The initial lag-time for electricity production from tetrathionate was relatively long in bioelectrochemical systems (approximately 100 days), but spontaneous electricity production was proven successful with ferric iron as the cathodic electron acceptor. By optimizing the external resistance, the current density was successfully improved from 80 mA m⁻² (1000 Ω) to 225 mA m⁻² (100 Ω). In the long-term experiment, biofouling or accumulating reaction products were not observed to limit the electricity production even after 740 days of operation. The minimum anode potential for tetrathionate degradation was observed to be 0.3 V vs. Ag/AgCl in the bioelectrochemical systems and 0.5 V in the abiotic electrochemical systems. Higher tetrathionate degradation rates were obtained in the bioelectrochemical systems (>110 mg L⁻¹ d⁻¹) than in the electrochemical systems (<35 mg L⁻¹ d⁻¹). The reaction products of bioelectrochemical tetrathionate degradation were sulfate and elemental sulfur, while in electrochemical systems only sulfate was detected. For the efficient removal of tetrathionate and copper, applied voltage of above 1.0 V was required. The concentrations of tetrathionate and copper were successfully decreased below the limits set for toxicity (0.5 g S₄O₆²⁻ L⁻¹) and mining effluent discharge (0.3 mg Cu²⁺ L⁻¹).

This study demonstrates for the first time that tetrathionate can be used the substrate for bioelectrochemical current generation. In bioelectrochemical systems with an efficient catholyte, tetrathionate is degraded and electricity is produced spontaneously, but abiotic electrochemical degradation requires external energy. Both bioelectrochemical and electrochemical systems provided higher current densities than a water-oxidizing control reactor when controlling the anode potential or applying external voltage. The simultaneous removal of tetrathionate and copper shows that bioelectrochemical and electrochemical systems are promising alternatives for the treatment of mining waters.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

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

Contributors: Sulonen, M.

Number of pages: 98

Publication date: 15 Sep 2017

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-3984-8

ISBN (Electronic): 978-952-15-4002-8

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Volume: 1485

ISSN (Electronic): 1459-2045

Electronic versions:

sulonen 1485

URLs:

<http://urn.fi/URN:ISBN:978-952-15-4002-8>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Hole-Transporting Materials for Printable Perovskite Solar Cells

Perovskite solar cells (PSCs) represent undoubtedly the most significant breakthrough in photovoltaic technology since the 1970s, with an increase in their power conversion efficiency from less than 5% to over 22% in just a few years. Hole-transporting materials (HTMs) are an essential building block of PSC architectures. Currently, 2,2',7,7'-tetrakis-(N,N'-di-p-methoxyphenylamine)-9,9'-spirobifluorene), better known as spiro-OMeTAD, is the most widely-used HTM to obtain high-efficiency devices. However, it is a tremendously expensive material with mediocre hole carrier mobility. To ensure wide-scale application of PSC-based technologies, alternative HTMs are being proposed. Solution-processable HTMs are crucial to develop inexpensive, high-throughput and printable large-area PSCs. In this review, we present the most recent

advances in the design and development of different types of HTMs, with a particular focus on mesoscopic PSCs. Finally, we outline possible future research directions for further optimization of the HTMs to achieve low-cost, stable and large-area PSCs.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials

Contributors: Vivo, P., Salunke, J. K., Priimagi, A.

Publication date: 15 Sep 2017

Peer-reviewed: Yes

Publication information

Journal: Materials

Volume: 10

Issue number: 9

ISSN (Print): 1996-1944

Ratings:

Scopus rating (2017): CiteScore 3.02 SJR 0.732 SNIP 1.285

Original language: English

Electronic versions:

HTM_review

DOIs:

10.3390/ma10091087

URLs:

<http://urn.fi/URN:NBN:fi:ty-201709251959>

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

Understanding selenium biogeochemistry in engineered ecosystems: Transformation and analytical methods

Selenium is used extensively in many industries, and it is necessary for human nutrition. On the other hand, it is also toxic at slightly elevated concentrations. With the advent of industrialisation, selenium concentrations in the environment due to anthropogenic activities have increased. Treatment of selenium-laden wastewaters and bioremediation are of increasing importance for counteracting contamination. Developing an effective treatment process requires the identification of all the selenium chemical species and their concentrations in engineered settings. This chapter collates the available techniques for identifying and quantifying various selenium species in gas, liquid, and solid phases, including X-ray absorption spectroscopy, electron microscopy, and liquid/gas chromatography. This chapter also throws light on isotopic fractionation and sequential extraction methods used to study the behaviour of selenium. Prior to the discussion of analytical methods, this chapter discusses selenium mineralogy and biochemistry. Finally, the chapter concludes by discussing potential future analytical techniques that will further improve our understanding of selenium biogeochemistry in engineered bioprocesses.

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Chemistry and Bioengineering, UPEM, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education, University of Applied Sciences and Arts Northwestern Switzerland (FHNW), Wageningen University and Research Centre, Laboratoire de Biochimie Théorique

Contributors: Jain, R., Van Hullebusch, E. D., Lenz, M., Farges, F.

Number of pages: 24

Pages: 33-56

Publication date: 2 Sep 2017

Host publication information

Title of host publication: Bioremediation of Selenium Contaminated Wastewater

Publisher: Springer International Publishing

ISBN (Print): 9783319578309

ISBN (Electronic): 9783319578316

ASJC Scopus subject areas: Engineering(all), Chemical Engineering(all), Environmental Science(all), Immunology and Microbiology(all), Chemistry(all)

Keywords: Bioremediation, Elemental speciation, Redox labile elements, Trace elements

DOIs:

10.1007/978-3-319-57831-6_2

Source: Scopus

Source ID: 85034980155

Research output: Chapter in Book/Report/Conference proceeding > Chapter > Scientific > peer-review

Comparison of liposomal drug formulations for transdermal iontophoretic drug delivery

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, University of Helsinki, University of Navarra, Division of Pharmaceutical Chemistry and Technology

Contributors: Malinovskaja-Gomez, K., Espuelas, S., Garrido, M. J., Hirvonen, J., Laaksonen, T.

Number of pages: 8

Pages: 294-301

Publication date: 30 Aug 2017

Peer-reviewed: Yes

Publication information

Journal: European Journal of Pharmaceutical Sciences

Volume: 106

ISSN (Print): 0928-0987

Ratings:

Scopus rating (2017): CiteScore 3.81 SJR 1.016 SNIP 1.317

Original language: English

ASJC Scopus subject areas: Pharmaceutical Science

Keywords: Diclofenac sodium, Iontophoresis, Liposome, NSAID delivery, Skin permeation, Transdermal drug delivery

Electronic versions:

Malinovskaja-Gomez_EJPS_2017. Embargo ended: 15/06/18

DOIs:

10.1016/j.ejps.2017.06.025

URLs:

<http://urn.fi/URN:NBN:fi:ty-201712222486>. Embargo ended: 15/06/18

Source: Scopus

Source ID: 85020916069

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

Locomotion of light-driven soft microrobots through a hydrogel via local melting

Soft mobile microrobots whose deformation can be directly controlled by an external field can adapt to move in different environments. This is the case for the light-driven microrobots based on liquid-crystal elastomers (LCEs). Here we show that the soft microrobots can move through an agarose hydrogel by means of light-controlled travelling-wave motions. This is achieved by exploiting the inherent rise of the LCE temperature above the melting temperature of the agarose gel, which facilitates penetration of the microrobot through the hydrogel. The locomotion performance is investigated as a function of the travelling-wave parameters, showing that effective propulsion can be obtained by adapting the generated motion to the specific environmental conditions.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Chemistry and Bioengineering, Max Planck Institute for Intelligent Systems, Max Planck ETH Center for Learning Systems, University of Florence, CNR-INO, University of Stuttgart

Contributors: Palagi, S., Mark, A. G., Melde, K., Qiu, T., Zeng, H., Parmeggiani, C., Martella, D., Wiersma, D. S., Fischer, P.

Publication date: 3 Aug 2017

Host publication information

Title of host publication: International Conference on Manipulation, Automation and Robotics at Small Scales, MARSS 2017 - Proceedings

Publisher: IEEE

ISBN (Electronic): 9781538603468

ASJC Scopus subject areas: Mechanical Engineering, Artificial Intelligence, Control and Optimization

Keywords: Hydrogels, Liquid-crystal elastomers (LCEs), Soft microrobots

DOIs:

10.1109/MARSS.2017.8001916

Source: Scopus

Source ID: 85030234395

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

Effects of different nickel species on autotrophic denitrification driven by thiosulfate in batch tests and a fluidized-bed reactor

Nickel is a common heavy metal and often occurs with nitrate (NO_3^-) in effluents from mining and metal-finishing industry. The present study investigates the effects of increasing concentrations (5–200 mg Ni/L) of NiEDTA^{2-} and NiCl_2 on autotrophic denitrification with thiosulfate ($\text{S}_2\text{O}_3^{2-}$) in batch tests and a fluidized-bed reactor (FBR). In batch bioassays, 50 and 100 mg Ni/L of NiEDTA^{2-} only increased the transient accumulation of NO_2^- , whereas 25–100 mg Ni/L of NiCl_2 inhibited denitrification by 9–19%. NO_3^- and NO_2^- were completely removed in the FBR at feed NiEDTA^{2-} and NiCl_2 concentrations as high as 100 and 200 mg Ni/L, respectively. PCR-DGGE revealed the dominance of *Thiobacillus denitrificans* and the presence of the sulfate-reducing bacterium *Desulfovibrio putealis* in the FBR microbial community at all feed nickel concentrations investigated. Nickel mass balance, thermodynamic modeling and solid phase characterization indicated that nickel sulfide, phosphate and oxide precipitated in the FBR during NiCl_2 injection.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Bio- and Circular Economy, University of Cassino and Southern Lazio, UPEM, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education

Contributors: Di Capua, F., Milone, I., Lakaniemi, A., Hullebusch, E. D., Lens, P. N., Esposito, G.

Number of pages: 8

Pages: 534–541

Publication date: 1 Aug 2017

Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 238

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2017): CiteScore 6.28 SJR 2.029 SNIP 1.823

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

Keywords: Autotrophic denitrification, EDTA, Fluidized-bed reactor, Nickel, Thiosulfate

DOIs:

10.1016/j.biortech.2017.04.082

Bibliographical note

INT=keb,"Di Capua, Fransesco"

Source: Scopus

Source ID: 85019042670

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

Nanofibrillar cellulose-alginate hydrogel coated surgical sutures as cell-carrier systems

Hydrogel nanomaterials, especially those that are of non-human and non-animal origins, have great potential in biomedical and pharmaceutical sciences due to their versatility and inherent soft-tissue like properties. With the ability to simulate native tissue function, hydrogels are potentially well suited for cellular therapy applications. In this study, we have fabricated nanofibrillar cellulose-alginate (NFCA) suture coatings as biomedical devices to help overcome some of the limitations related to cellular therapy, such as low cell survivability and distribution out of target tissue. The addition of sodium alginate 8% (w/v) increased the NFCA hydrogel viscosity, storage and loss moduli by slightly under one order of magnitude, thus contributing significantly to coating strength. Confocal microscopy showed nearly 100% cell viability throughout the 2-week incubation period within and on the surface of the coating. Additionally, typical morphologies in the

dual cell culture of spheroid forming HepG2 and monolayer type SK-HEP-1 were observed. Twelve out of 14 NFCA coated surgical sutures remained intact during the suturing operation with various mice and rat tissue; however, partial peeling off was observed in 2 of the coated sutures. We conclude that NFCA suture coatings could perform as cell-carrier systems for cellular based therapy and post-surgical treatment.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, University of Helsinki, Aalto University, Ita-Suomen yliopisto, Made Consulting, Centre for Drug Research

Contributors: Laurén, P., Somersalo, P., Pitkänen, I., Lou, Y. R., Urtti, A., Partanen, J., Seppälä, J., Madetoja, M., Laaksonen, T., Mäkitie, A., Yliperttula, M.

Publication date: 1 Aug 2017

Peer-reviewed: Yes

Publication information

Journal: PLoS ONE

Volume: 12

Issue number: 8

Article number: e0183487

ISSN (Print): 1932-6203

Ratings:

Scopus rating (2017): CiteScore 3.01 SJR 1.164 SNIP 1.144

Original language: English

ASJC Scopus subject areas: Medicine(all), Biochemistry, Genetics and Molecular Biology(all), Agricultural and Biological Sciences(all)

Electronic versions:

wjournal.pone.0183487

DOIs:

10.1371/journal.pone.0183487

URLs:

<http://urn.fi/URN:NBN:fi:ty-201709261961>

Source: Scopus

Source ID: 85028334326

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

Photoresponsive Polymer Hydrogel Coatings that Change Topography

This chapter provides a brief overview of the principles as well as the potential applications of photoresponsive hydrogel films, which change surface topography. It discusses the operating mechanisms that lead to topographical changes. Changes in topography can affect the wettability of a surface, which is an interesting characteristic for making self-cleaning coatings. The chapter also discusses polymer films that are useful for the development of self-cleaning films. It then discusses responsive materials, for cell culturing and microfluidics applications. The chapter further shows that appealing photoresponsive polymer hydrogel coatings that change topography can be fabricated, which holds great promise in a variety of fields ranging from microfluidic devices to biomedical applications. When the structures of the topography are in the micrometer size regime, they influence the wettability of the surface. Two types of wetting can be defined: Wenzel and Cassie-Baxter.

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

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

Contributors: Stumpel, J. E., ter Schiphorst, J., Schenning, A. P. H. J.

Pages: 159-173

Publication date: 21 Jul 2017

Host publication information

Title of host publication: Responsive Polymer Surfaces : Dynamics in Surface Topography

Publisher: Wiley-VCH

Editors: Liu, D., Broer, D.

ISBN (Print): 978-3-527-33869-6

ISBN (Electronic): 9783527690534

DOIs:

10.1002/9783527690534.ch7

Research output: Chapter in Book/Report/Conference proceeding > Chapter > Scientific > peer-review

Effect of alkylaminophenols on growth inhibition and apoptosis of bone cancer cells

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

General information

Publication status: Published

MoE 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: Chemistry & Advanced Materials, BioMediTech, Molecular Signaling Lab, Computational Systems Biology Research Group, BioMediTech and Faculty of Biomedical Sciences and Engineering, Tampere University of Technology, P.O.Box 553, 33101 Tampere, Finland.

Contributors: Doan, P., Nguyen, T., Yli-Harja, O., Candeias, N. R., Kandhavelu, M.

Number of pages: 9

Pages: 208–216

Publication date: 17 Jul 2017

Peer-reviewed: Yes

Publication information

Journal: European Journal of Pharmaceutical Sciences

Volume: 107

ISSN (Print): 0928-0987

Ratings:

Scopus rating (2017): CiteScore 3.81 SJR 1.016 SNIP 1.317

Original language: English

Keywords: Journal Article

DOIs:

10.1016/j.ejps.2017.07.016

Bibliographical note

INT=TUT-BMT, "Nguyen, Tien"

Source: PubMed

Source ID: 28728976

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

Long-Range Observation of Exciplex Formation and Decay Mediated by One-Dimensional Bridges

We report herein unprecedented long-range observation of both formation and decay of the exciplex state in donor (D)-bridge (B)-acceptor (A) linked systems. Zinc porphyrins (ZnP) as a donor were tethered to single-walled carbon nanotube (SWNT) as an acceptor through oligo(p-phenylene)s (ZnP-ph_n-SWNT) or oligo(p-xylene)s (ZnP-xy_{n-1}-ph₁-SWNT) with systematically varied lengths (n = 1-5) to address the issue. Exponential dependencies of rate constants for the exciplex formation (k_{FEX}) and decay (k_{DEX}) on the edge-to-edge separation distance between ZnP and SWNT through the bridges were unambiguously derived from time-resolved spectroscopies. Distance dependencies (i.e., attenuation factor, β) of k_{FEX} and k_{DEX} in ZnP-ph_n-SWNT were found to be considerably small (β = 0.10 for k_{FEX} and 0.12 Å⁻¹ for k_{DEX}) compared to those for charge separation and recombination (0.2-0.8 Å⁻¹) in D-B-A systems with the same oligo(p-phenylene) bridges. The small β values may be associated with the exciplex state with mixed characters of charge-transfer and excited states. In parallel, the substantially nonconjugated bridge of oligo(p-xylene)s exhibited larger attenuation values (β = 0.12 for k_{FEX} and 0.14 Å⁻¹ for k_{DEX}). These results provide deep insight into the unique photodynamics of electronically strongly coupled D-B-A systems involving exciplex.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Kyoto Women's University

Contributors: Baek, J., Umeyama, T., Stranius, K., Yamada, H., Tkachenko, N. V., Imahori, H.
Number of pages: 10
Pages: 13952-13961
Publication date: 29 Jun 2017
Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 121

Issue number: 25

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.135

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Surfaces, Coatings and Films, Physical and Theoretical Chemistry

DOIs:

10.1021/acs.jpcc.7b04483

Source: Scopus

Source ID: 85022231305

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

Effects of alternative electron acceptors on the activity and community structure of methane-producing and consuming microbes in the sediments of two shallow boreal lakes

The role of anaerobic CH₄ oxidation in controlling lake sediment CH₄ emissions remains unclear. Therefore, we tested how relevant EAs (SO₄²⁻, NO₃⁻, Fe³⁺, Mn⁴⁺, O₂) affect CH₄ production and oxidation in the sediments of two shallow boreal lakes. The changes induced to microbial communities by the addition of Fe³⁺ and Mn⁴⁺ were studied using next-generation sequencing targeting the 16S rRNA and methyl-coenzyme M reductase (*mcrA*) genes and *mcrA* transcripts. Putative anaerobic CH₄ oxidizing archaea (ANME-2D) and bacteria (NC 10) were scarce (up to 3.4% and 0.5% of archaeal and bacterial 16S rRNA genes, respectively), likely due to the low environmental stability associated with shallow depths. Consequently, the potential anaerobic CH₄ oxidation (0-2.1 nmol g⁻¹ dry weight (DW)d⁻¹) was not enhanced by the addition of EAs, nor important in consuming the produced CH₄ (0.6-82.5 nmol g⁻¹ DWd⁻¹). Instead, the increased EA availability suppressed CH₄ production via the outcompetition of methanogens by anaerobically respiring bacteria and via the increased protection of organic matter from microbial degradation induced by Fe³⁺ and Mn⁴⁺. Future studies could particularly assess whether anaerobic CH₄ oxidation has any ecological relevance in reducing CH₄ emissions from the numerous CH₄-emitting shallow lakes in boreal and tundra landscapes.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Rissanen, A. J., Karvinen, A., Nykänen, H., Peura, S., Tirola, M., Mäki, A., Kankaala, P.

Publication date: 15 Jun 2017

Peer-reviewed: Yes

Publication information

Journal: FEMS Microbiology Ecology

Volume: 93

Issue number: 7

ISSN (Print): 0168-6496

Ratings:

Scopus rating (2017): CiteScore 3.87 SJR 1.492 SNIP 1.086

Original language: English

Keywords: lake, sediment, methanogenesis, methane oxidation, 16S rRNA, *mcrA*

DOIs:

10.1093/femsec/fix078

Bibliographical note

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Source: PubMed

Source ID: 28637304

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

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.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Univ Seville, University of Sevilla, Chem & Environm Engn Dept, Bioenergy Grp, Escuela Super Ingenieros, Åbo Akademi University, Process Chemistry Center

Contributors: Konttinen, J., Kramb, J., DeMartini, N., Gomez-Barea, A.

Number of pages: 5

Pages: 443-447

Publication date: 13 Jun 2017

Host publication information

Title of host publication: EUBCE 2017 Online Conference Proceedings

Publisher: ETA-Florence Renewable Energies

Editors: Ek, L., Ernrooth, H., Scarlat, N., Grassi, A., Helm, P.

ISBN (Electronic): 978-88-89407-17-2

Publication series

Name: European biomass conference and exhibition proceedings

Publisher: ETA Florence renewable energies

ISSN (Electronic): 2282-5819

DOIs:

10.5071/25thEUBCE2017-2BO.6.4

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

Self-Regulating Iris Based on Light-Actuated Liquid Crystal Elastomer

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Warsaw Univ Technol, Warsaw University of Technology, Fac Phys, Opt Div, Department and Clinic of Ophthalmology, Wrocław Medical University, Wrocław, Poland

Contributors: Zeng, H., Wani, O. M., Wasylczyk, P., Kaczmarek, R., Priimägi, A.

Publication date: 7 Jun 2017

Peer-reviewed: Yes

Publication information

Journal: Advanced Materials

ISSN (Print): 0935-9648

Ratings:

Scopus rating (2017): CiteScore 21.1 SJR 10.579 SNIP 3.627

Original language: English

Electronic versions:

20170419_Iris-paper_REVISSED_GOA. Embargo ended: 7/06/18

DOIs:

10.1002/adma.201701814

URLs:

<http://urn.fi/URN:NBN:fi:tty-201901111062>

Bibliographical note

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Source: PubMed

Source ID: 28589679

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

CFD based reactivity parameter determination for biomass particles of multiple size ranges in high heating rate devolatilization

This work presents a methodology that combines experimental measurements and Computational Fluid Dynamics (CFD) modeling to determine the global reaction kinetics of high heating rate biomass devolatilization. Three particle size ranges of woody biomass are analyzed: small (SF), medium (MF) and large (LF) fractions. Devolatilization mass loss is measured for each fraction in a laminar Drop-Tube Reactor (DTR) in nitrogen atmosphere, using two nominal reactor temperatures of 873 and 1173 K. Single First Order Reaction (SFOR) kinetics are determined by coupling an optimization routine with CFD models of the DTR. The global pre-exponential factors and activation energies for the SF, MF and LF particles are 5880 1/s and 42.7 kJ/mol, 48.1 1/s and 20.2 kJ/mol, and 102 1/s and 24.8 kJ/mol, respectively. These parameters are optimized for the isothermal heat transfer model available in CFD programs, and it is recommended that the specific heat capacity that was used in the optimization (1500 J/kgK) is used together with the parameters. Using the SF kinetics for small wood particles and either of the MF or LF kinetics for large particles, it is expected that more accurate devolatilization predictions can be obtained for the whole fuel size distribution in large scale CFD simulations.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology, Valmet Technologies Oy

Contributors: Niemelä, N. P., Tolvanen, H., Saarinen, T., Leppänen, A., Joronen, T.

Number of pages: 12

Pages: 676-687

Publication date: 1 Jun 2017

Peer-reviewed: Yes

Publication information

Journal: Energy

Volume: 128

ISSN (Print): 0360-5442

Ratings:

Scopus rating (2017): CiteScore 5.6 SJR 1.99 SNIP 1.941

Original language: English

ASJC Scopus subject areas: Pollution, Energy(all)

Keywords: Biomass, Computational Fluid Dynamics (CFD), Devolatilization, High heating rate, Pyrolysis, Single First Order Reaction (SFOR)

DOIs:

10.1016/j.energy.2017.04.023

Source: Scopus

Source ID: 85018474683

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

Impact of film thickness of ultra-thin dip-coated compact TiO₂ layers on the performance of mesoscopic perovskite solar cells

Uniform and pinhole-free electron selective TiO₂ layers are of utmost importance for efficient perovskite solar cells. Here we used a scalable and low-cost dip coating method to prepare uniform and ultra-thin (5–50 nm) compact TiO₂ films on fluorine doped tin oxide (FTO) glass substrates. The thickness of the film was tuned by changing the TiCl₄ precursor concentration. The formed TiO₂ follows the texture of the underlying FTO substrates, but at higher TiCl₄ concentrations, the surface roughness is substantially decreased. This change occurs at a film thickness close to 20–30 nm. A similar TiCl₄ concentration is needed to produce crystalline TiO₂ films. Furthermore, below this film thickness, the underlying FTO might be exposed resulting in pinholes in the compact TiO₂ layer. When integrated into mesoscopic perovskite solar cells, there appears to be a similar critical compact TiO₂ layer thickness above which the devices perform more optimally. The power conversion efficiency was improved by more than 50% (from 5.5% to ~8.6%) when inserting a compact TiO₂ layer.

Devices without or with very thin compact TiO₂ layers display J-V curves with an “s-shaped” feature in the negative voltage range, which could be attributed to immobilized negative ions at the electron-extracting interface. A strong correlation between the magnitude of the s-shape feature and the exposed FTO seen in the x-ray photoelectron spectroscopy measurements indicates that the s-shape is related to pinholes in the compact TiO₂ layer when it is too thin.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Åbo Akademi, Aalto University

Contributors: Masood, M. T., Weinberger, C., Sarfraz, J., Rosqvist, E., Sandén, S., Sandberg, O., Vivo, P., Hashmi, G., Lund, P. D., Österbacka, R., Smätt, J.

Pages: 17906-17913

Publication date: 31 May 2017

Peer-reviewed: Yes

Publication information

Journal: ACS Applied Materials and Interfaces

Volume: 9

Issue number: 21

ISSN (Print): 1944-8244

Ratings:

Scopus rating (2017): CiteScore 8.15 SJR 2.784 SNIP 1.543

Original language: English

DOIs:

10.1021/acsami.7b02868

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

Charge Carrier Dynamics in Solar Water Oxidation

The search for sustainable energy sources is one of the greatest problems facing mankind in the 21st century. Most renewable sources do not have adequate potential to cover the growing need for energy in order to sustain economic and population growth. Solar power is a plausible way to fully cover mankind's continuously growing need for energy. However, sunlight is diurnal, and the amount of sunlight received at different latitudes of the Earth varies drastically. Harnessing solar energy into chemical bonds is an attractive approach to enable the storage of energy for transportation and later use. Direct photoelectrochemical water splitting produces only oxygen and hydrogen, of which hydrogen can be used to sustain a possible hydrogen based economy. The materials used in this Thesis are metal oxide semiconductors that act as photoanodes, performing the water oxidation reaction on their surface and supplying electrons for the water reduction reaction.

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

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

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

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Ruoko, T.

Number of pages: 49

Publication date: 24 May 2017

Publication information

Publisher: Tampere University of Technology
ISBN (Print): 978-952-15-3951-0
ISBN (Electronic): 978-952-15-3955-8
Original language: English

Publication series

Name: Tampere University of Technology. Publication
Volume: 1473
ISSN (Print): 1459-2045
Electronic versions:
ruoko 1473
URLs:
<http://urn.fi/URN:ISBN:978-952-15-3955-8>
Research output: Book/Report > Doctoral thesis > Collection of Articles

Biohydrogen production from xylose by fresh and digested activated sludge at 37, 55 and 70 °C

Two heat-treated inocula, fresh and digested activated sludge from the same municipal wastewater treatment plant, were compared for their H₂ production via dark fermentation at mesophilic (37 °C), thermophilic (55 °C) and hyperthermophilic (70 °C) conditions using xylose as the substrate. At both 37 and 55 °C, the fresh activated sludge yielded more H₂ than the digested sludge, whereas at 70 °C, neither of the inocula produced H₂ effectively. A maximum yield of 1.85 mol H₂ per mol of xylose consumed was obtained at 55 °C. H₂ production was linked to acetate and butyrate production, and there was a linear correlation ($R^2 = 0.96$) between the butyrate and H₂ yield for the fresh activated sludge inoculum at 55 °C. Approximately 2.4 mol H₂ per mol of butyrate produced were obtained against a theoretical maximum of 2.0, suggesting that H₂ was produced via the acetate pathway prior to switching to the butyrate pathway due to the increased H₂ partial pressure. Clostridia sp. were the prevalent species at both 37 and 55 °C, irrespectively of the inoculum type. Although the two inocula originated from the same plant, different thermophilic microorganisms were detected at 55 °C. Thermoanaerobacter sp., detected only in the fresh activated sludge cultures, may have contributed to the high H₂ yield obtained with such an inoculum.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Institute for Water Education, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education
Contributors: Dessi, P., Lakaniemi, A., Lens, P. N. L.
Number of pages: 10
Pages: 120-129
Publication date: 15 May 2017
Peer-reviewed: Yes

Publication information

Journal: Water Research
Volume: 115
ISSN (Print): 0043-1354
Ratings:
Scopus rating (2017): CiteScore 7.55 SJR 2.601 SNIP 2.388
Original language: English
ASJC Scopus subject areas: Ecological Modelling, Water Science and Technology, Waste Management and Disposal, Pollution
Keywords: Biohydrogen, Butyrate, Dark fermentation, Inocula, Temperature, Xylose
Electronic versions:
Dessi et al 2017 - Biohydrogen production from xylose. Embargo ended: 28/02/19
DOIs:
10.1016/j.watres.2017.02.063
URLs:
<http://urn.fi/URN:NBN:fi:tyy-201902051212>. Embargo ended: 28/02/19
Source: Scopus
Source ID: 85014366720
Research output: Contribution to journal > Article > Scientific > peer-review

The effects of calcium and potassium on CO₂ gasification of birch wood in a fluidized bed

Birch wood was leached of its naturally occurring ash forming elements and doped with three concentrations of calcium or potassium before being gasified in a laboratory bubbling fluidized bed reactor. The wood samples were pelletized and inserted into a fluidized bed reactor where they were first pyrolyzed with N₂ and then gasified with CO₂. In addition to

tracking the gas concentration of the exit gas, char samples were taken from the fluidized bed and analyzed to study the char properties. The presence of potassium in the biomass was found to have a significant influence on the structure of the resulting char, however potassium did not have an observable catalytic effect on the overall gasification reaction rate with CO₂ due to the formation of a unreactive coke layer on the char surface. In contrast, calcium did increase the char conversion rate and is likely the primary active catalyst in gasification of birch wood with CO₂.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Industrial Bioengineering and Applied Organic Chemistry, Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology, Universidad de Sevilla, Johan Gadolin Process Chemistry Centre, Abo Akademi University, Univ of Oulu

Contributors: Kramb, J., Gómez-Barea, A., DeMartini, N., Romar, H., Doddapaneni, T. R. K. C., Konttinen, J.

Number of pages: 10

Pages: 398-407

Publication date: 15 May 2017

Peer-reviewed: Yes

Publication information

Journal: Fuel

Volume: 196

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2017): CiteScore 5.4 SJR 1.891 SNIP 2.127

Original language: English

ASJC Scopus subject areas: Chemical Engineering(all), Fuel Technology, Energy Engineering and Power Technology, Organic Chemistry

Keywords: Biomass, Catalysts, Char, Fluidized bed, Gasification

DOIs:

10.1016/j.fuel.2017.01.101

Source: Scopus

Source ID: 85012050856

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

Photoinduced Electron Injection from Zinc Phthalocyanines into Zinc Oxide Nanorods: Aggregation Effects

Phthalocyanines (Pc) are well-known light-harvesting compounds. However, despite the tremendous efforts on phthalocyanine synthesis, the achieved energy conversion efficiencies for Pc-based dye-sensitized solar cells are moderate. To cast light on the factors reducing the conversion efficiency, we have undertaken a time-resolved spectroscopy study of the primary photoinduced reactions at a semiconductor-Pc interface. ZnO nanorods were chosen as a model semiconductor substrate with enhanced specific surface area. The use of a nanostructured oxide surface allows to extend the semiconductor-dye interface with a hole transporting layer (spiro-MeOTAD) in a controlled way, making the studied system closer to a solid-state dye-sensitized solar cell. Four zinc phthalocyanines are compared in this study. The compounds are equipped with bulky peripheral groups designed to reduce the self-aggregation of the Pcs. Almost no signs of aggregation can be observed from the absorption spectra of the Pcs assembled on a ZnO surface. Nevertheless, the time-resolved spectroscopy indicates that there are inter-Pc charge separation-recombination processes in the time frame of 1-100 ps. This may reduce the electron injection efficiency into the ZnO by more than 50%, pointing out to a remaining aggregation effect. Surprisingly, the electron injection time does not correlate with the length of the linker connecting the Pc to ZnO. A correlation between the electron injection time and the "bulkiness" of the peripheral groups was observed. This correlation is further discussed with the use of computational modeling of the Pc arrangements on the ZnO surface. (Figure Presented).

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Universidad Autónoma de Madrid, Mersin University, South-Ukrainian National Pedagogical University

Contributors: Virkki, K., Hakola, H., Urbani, M., Tejerina, L., Ince, M., Martínez-Díaz, M. V., Torres, T., Golovanova, V., Golovanov, V., Tkachenko, N. V.

Number of pages: 12

Pages: 9594-9605

Publication date: 4 May 2017

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 121

Issue number: 17

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.135

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Surfaces, Coatings and Films, Physical and Theoretical Chemistry

DOIs:

10.1021/acs.jpcc.7b01562

Source: Scopus

Source ID: 85020915273

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

Alkyl thiophene vinylene electropolymerization in C8mimPF6, potential use in solar cells

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials

Contributors: Rojas, V., Martinez, F., Bernede, J. C., Guenadez, L. C., Efimov, A., Lemmetyinen, H.

Number of pages: 13

Pages: 405-417

Publication date: May 2017

Peer-reviewed: Yes

Publication information

Journal: Materials Sciences and Applications

Volume: 8

Issue number: 5

ISSN (Print): 2153-117X

Original language: English

Electronic versions:

2017-martinez-MSA

DOIs:

10.4236/msa.2017.85013

URLs:

<http://urn.fi/URN:NBN:fi:tty-201706151598>

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

Elucidation of Compression-Induced Surface Crystallization in Amorphous Tablets Using Sum Frequency Generation (SFG) Microscopy

Purpose: To investigate the effect of compression on the crystallization behavior in amorphous tablets using sum frequency generation (SFG) microscopy imaging and more established analytical methods. Method: Tablets containing neat amorphous griseofulvin with/without excipients (silica, hydroxypropyl methylcellulose acetate succinate (HPMCAS), microcrystalline cellulose (MCC) and polyethylene glycol (PEG)) were prepared. They were analyzed upon preparation and storage using attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy, scanning electron microscopy (SEM) and SFG microscopy. Results: Compression-induced crystallization occurred predominantly on the surface of the neat amorphous griseofulvin tablets, with minimal crystallinity being detected in the core of the tablets. The presence of various types of excipients was not able to mitigate the compression-induced surface crystallization of the amorphous griseofulvin tablets. However, the excipients affected the crystallization rate of amorphous griseofulvin in the core of the tablet upon compression and storage. Conclusions: SFG microscopy can be used in combination with ATR-FTIR spectroscopy and SEM to understand the crystallization behaviour of amorphous tablets upon compression and storage. When selecting excipients for amorphous formulations, it is important to consider the effect of the excipients on

the physical stability of the amorphous formulations.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, University of Helsinki, Division of Biopharmaceutical Sciences, Biomedicum Imaging Unit, FIN-00014 University of Helsinki

Contributors: Mah, P. T., Novakovic, D., Saarinen, J., van Landeghem, S., Peltonen, L., Laaksonen, T., Isomäki, A., Strachan, C. J.

Number of pages: 14

Pages: 957-970

Publication date: May 2017

Peer-reviewed: Yes

Early online date: 13 Oct 2016

Publication information

Journal: Pharmaceutical Research

Volume: 34

Issue number: 5

ISSN (Print): 0724-8741

Ratings:

Scopus rating (2017): CiteScore 3.3 SJR 1.077 SNIP 1.054

Original language: English

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

DOIs:

10.1007/s11095-016-2046-6

Source: Scopus

Source ID: 84991051806

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

Crystallisation-enhanced bulk hole mobility in phenothiazine-based organic semiconductors

A series of three novel donor-acceptor systems based on C(3)-malononitrile-substituted phenothiazines was synthesised in good overall yields and their thermal, spectroscopic, and electrochemical properties were characterised. The compounds were prepared through a sequence of Ullmann-coupling, Vilsmeier-Haack formylation and Knoevenagel-condensation, followed by Suzuki-coupling reactions for introduction of aryl substituents at C(7) position of the phenothiazine. The introduction of a donor unit at the C(7) position exhibited a weak impact on the optical and electrochemical characteristics of the compounds and led to amorphous films with bulk hole mobilities in the typical range reported for phenothiazines, despite the higher charge delocalisation as attested by computational studies. In contrast, highly ordered films were formed when using the C(7)-unsubstituted 3-malononitrile phenothiazine, exhibiting an outstanding mobility of $1 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, the highest reported for this class of compounds. Computational conformational analysis of the new phenothiazines suggested that free rotation of the substituents at the C(7) position suppresses the ordering of the system, thereby hampering suitable packing of the new materials needed for high charge carrier mobility.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

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

Number of pages: 10

Publication date: 12 Apr 2017

Peer-reviewed: Yes

Publication information

Journal: Scientific Reports

Volume: 7

Article number: 46268

ISSN (Print): 2045-2322

Ratings:

Scopus rating (2017): CiteScore 4.36 SJR 1.533 SNIP 1.258

Original language: English

Electronic versions:

srep46268

DOIs:

10.1038/srep46268

URLs:

<http://urn.fi/URN:NBN:fi:tty-201704181303>

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Publication date: 7 Apr 2017

Peer-reviewed: Yes

Publication information

Journal: ChemPlusChem

ISSN (Print): 2192-6506

Ratings:

Scopus rating (2017): CiteScore 2.79 SJR 1.051 SNIP 0.607

Original language: English

DOIs:

10.1002/cplu.201700061

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

Halogen bonding stabilizes a cis-azobenzene derivative in the solid state: A crystallographic study

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials, Politecnico di Milano, Aalto University

Contributors: Saccone, M., Siiskonen, A., Fernandez-Palacio, F., Priimägi, A., Terraneo, G., Resnati, G., Metrangolo, P.

Number of pages: 7

Pages: 227-233

Publication date: 1 Apr 2017

Peer-reviewed: Yes

Publication information

Journal: ACTA CRYSTALLOGRAPHICA SECTION B : STRUCTURAL SCIENCE, CRYSTAL ENGINEERING AND MATERIALS

Volume: 73

Issue number: 2

ISSN (Print): 2052-5192

Ratings:

Scopus rating (2017): CiteScore 4.54

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics, Metals and Alloys, Materials Chemistry

Keywords: azobenzene, halogen bonding, isomerization

DOIs:

10.1107/S2052520617003444

Source: Scopus

Source ID: 85017113549

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

High-rate autotrophic denitrification in a fluidized-bed reactor at psychrophilic temperatures

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Di Capua, F., Milone, I., Lakaniemi, A., N.L. Lens, P., Esposito, G.

Publication date: Apr 2017

Peer-reviewed: Yes

Early online date: 25 Dec 2016

Publication information

Journal: Chemical Engineering Journal

ISSN (Print): 1385-8947

Ratings:

Scopus rating (2017): CiteScore 7.01 SJR 1.863 SNIP 1.96

Original language: English

Keywords: Autotrophic denitrification, Fluidized-bed reactor, Psychrophilic temperatures, *Thiobacillus*, Thiosulfate

DOIs:

10.1016/j.cej.2016.12.106

Source: RIS

Source ID: urn:AA12A584D952BB2C4FADD94785C8DAC9

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

Hydrophobin-nanofibrillated cellulose stabilized emulsions for encapsulation and release of BCS class II drugs

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, University of Helsinki, VTT Technical Research Centre of Finland, Università degli Studi di Padova, Italy, Division of Biopharmaceutical Sciences

Contributors: Paukkonen, H., Ukkonen, A., Szilvay, G., Yliperttula, M., Laaksonen, T.

Number of pages: 11

Pages: 238-248

Publication date: 30 Mar 2017

Peer-reviewed: Yes

Publication information

Journal: European Journal of Pharmaceutical Sciences

Volume: 100

ISSN (Print): 0928-0987

Ratings:

Scopus rating (2017): CiteScore 3.81 SJR 1.016 SNIP 1.317

Original language: English

ASJC Scopus subject areas: Pharmaceutical Science

Keywords: Drug release, Emulsions, Hydrophobin, Ibuprofen, Nanofibrillated cellulose, Naproxen

Electronic versions:

Paukkonen_EJPS_2016. Embargo ended: 24/01/18

DOIs:

10.1016/j.ejps.2017.01.029

URLs:

<http://urn.fi/URN:NBN:fi:ty-201712222487>. Embargo ended: 24/01/18

Source: Scopus

Source ID: 85011004558

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

Hexaphyrin as a Potential Theranostic Dye for Photothermal Therapy and ¹⁹F Magnetic Resonance Imaging

Two features of meso-Aryl-substituted expanded porphyrins suggest suitability as theranostic agents. They have excellent absorption in near infrared (NIR) region, and they offer the possibility of introduction of multiple fluorine atoms at structurally equivalent positions. Here, hexaphyrin (hexa) was synthesized from 2,6-bis(trifluoromethyl)-4-formyl benzoate and pyrrole and evaluated as a novel expanded porphyrin with the above features. Under NIR illumination hexa showed intense photothermal and weak photodynamic effects, which were most likely due to its low excited states, close to singlet oxygen. The sustained photothermal effect caused ablation of cancer cells more effectively than the photodynamic effect of indocyanine green (a clinical dye). In addition, hexa showed potential for use in the visualization of tumors by ¹⁹F magnetic resonance imaging (MRI), because of the multiple fluorine atoms. Our results strongly support the utility of expanded porphyrins as theranostic agents in both photothermal therapy and ¹⁹F MRI.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Kyoto Women's University, Toyama Prefectural University

Contributors: Higashino, T., Nakatsuji, H., Fukuda, R., Okamoto, H., Imai, H., Matsuda, T., Tochio, H., Shirakawa, M., Tkachenko, N. V., Hashida, M., Murakami, T., Imahori, H.

Number of pages: 9

Pages: 951-959

Publication date: 24 Mar 2017

Peer-reviewed: Yes

Publication information

Journal: ChemBioChem

Volume: 18

Issue number: 10

ISSN (Print): 1439-4227

Ratings:

Scopus rating (2017): CiteScore 2.64 SJR 1.407 SNIP 0.726

Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Medicine, Molecular Biology, Organic Chemistry

Keywords: expanded porphyrin, fluorine, MRI, NMR spectroscopy, photochemistry, theranostics

DOIs:

10.1002/cbic.201700071

Source: Scopus

Source ID: 85016610793

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

Hierarchical Self-Assembly of Halogen-Bonded Block Copolymer Complexes into Upright Cylindrical Domains

Self-assembly of block copolymers into well-defined, ordered arrangements of chemically distinct domains is a reliable strategy for preparing tailored nanostructures. Microphase separation results from the system, minimizing repulsive interactions between dissimilar blocks and maximizing attractive interactions between similar blocks. Supramolecular methods have also achieved this separation by introducing small-molecule additives binding specifically to one block by noncovalent interactions. Here, we use halogen bonding as a supramolecular tool that directs the hierarchical self-assembly of low-molecular-weight perfluorinated molecules and diblock copolymers. Microphase separation results in a lamellar-within-cylindrical arrangement and promotes upright cylindrical alignment in films upon rapid casting and without further annealing. Such cylindrical domains with internal lamellar self-assemblies can be cleaved by solvent treatment of bulk films, resulting in separated and segmented cylindrical micelles stabilized by halogen-bond-based supramolecular crosslinks. These features, alongside the reversible nature of halogen bonding, provide a robust modular approach for nanofabrication.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, VTT Technical Research Centre of Finland, Aalto University, Politecnico di Milano, Italian Institute of Technology, Università del Salento

Contributors: Milani, R., Houbenov, N., Fernandez-Palacio, F., Cavallo, G., Luzio, A., Haataja, J., Giancane, G., Saccone, M., Priimägi, A., Metrangolo, P., Ikkala, O.

Number of pages: 10

Pages: 417-426

Publication date: 9 Mar 2017

Peer-reviewed: Yes

Publication information

Journal: CheM

Volume: 2

Issue number: 3

ISSN (Print): 2451-9294

Ratings:

Scopus rating (2017): CiteScore 7.23 SJR 5.295 SNIP 2.263

Original language: English

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

Keywords: block copolymers, halogen bond, hierarchical self-assembly, nanofabrication, supramolecular complexes

Electronic versions:

Hierarchical Self-Assembly of Halogen-Bonded Block Copolymer Complexes into Upright Cylindrical Domains

DOIs:

10.1016/j.chempr.2017.02.003

URLs:

<http://urn.fi/URN:NBN:fi:tty-201703281227>

Source: Scopus

Source ID: 85014778403

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

Twin-layer biosensor for real-time monitoring of alkane metabolism

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy
Contributors: Lehtinen, T., Santala, V., Santala, S.
Publication date: 1 Mar 2017
Peer-reviewed: Yes

Publication information

Journal: FEMS Microbiology Letters
Volume: 364
Issue number: 6
Article number: fnx053
ISSN (Print): 0378-1097
Ratings:
Scopus rating (2017): CiteScore 1.8 SJR 0.79 SNIP 0.6
Original language: English
ASJC Scopus subject areas: Microbiology, Molecular Biology, Genetics
Keywords: Acinetobacter baylyi ADP1, Alkane, Biosensor, GFP, LuxAB, Real-time monitoring
Electronic versions:
Twin Sensor_R1
DOIs:
10.1093/femsle/fnx053
URLs:
<http://urn.fi/URN:NBN:fi:tuni-201910033686>
Source: Scopus
Source ID: 85019932837
Research output: Contribution to journal › Article › Scientific › peer-review

UV exposure in artificial and natural weathering: A comparative study

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

General information

Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: Materials Science, Chemistry and Bioengineering, Research area: Design, Development and LCM, Finnish Meteorological Institute, World Radiation Cent, Aalto University, Paper Converting and Packaging Technology, Independent Researcher
Contributors: Heikkilä, A., Kazadzis, S., Meinander, O., Vaskuri, A., Kärhä, P., Mylläri, V., Syrjälä, S., Koskela, T.
Publication date: 22 Feb 2017

Host publication information

Title of host publication: RADIATION PROCESSES IN THE ATMOSPHERE AND OCEAN (IRS2016): Proceedings of the International Radiation Symposium (IRC/IAMAS)
Publisher: American Institute of Physics
Article number: 110004
ISBN (Electronic): 9780735414785

Publication series

Name: AIP conference proceedings
Volume: 1810
ISSN (Print): 0094-243X
ISSN (Electronic): 1935-0465
ASJC Scopus subject areas: Physics and Astronomy(all)
DOIs:

10.1063/1.4975566

Source: Scopus

Source ID: 85015818515

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

Periodic Surface Structures Induced by a Single Laser Beam Irradiation

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Optics, Research group: Nonlinear Optics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Noga, J., Sobolewska, A., Bartkiewicz, S., Virkki, M., Priimägi, A.

Publication date: 13 Feb 2017

Peer-reviewed: Yes

Early online date: 10 Nov 2016

Publication information

Journal: Macromolecular Materials and Engineering

Volume: 302

Issue number: 2

ISSN (Print): 1439-2054

Ratings:

Scopus rating (2017): CiteScore 2.71 SJR 0.755 SNIP 0.962

Original language: English

Keywords: periodic structure, photoinduced surface patterning, supramolecular polymer-azobenzene complex, willow structure

DOIs:

10.1002/mame.201600329

Source: Bibtex

Source ID: urn:31ff2294204d45a05ab3bed0048519b5

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

Benchmarking DFT methods with small basis sets for the calculation of halogen-bond strengths

In recent years, halogen bonding has become an important design tool in crystal engineering, supramolecular chemistry and biosciences. The fundamentals of halogen bonding have been studied extensively with high-accuracy computational methods. Due to its non-covalency, the use of triple-zeta (or larger) basis sets is often recommended when studying halogen bonding. However, in the large systems often encountered in supramolecular chemistry and biosciences, large basis sets can make the calculations far too slow. Therefore, small basis sets, which would combine high computational speed and high accuracy, are in great demand. This study focuses on comparing how well density functional theory (DFT) methods employing small, double-zeta basis sets can estimate halogen-bond strengths. Several methods with triple-zeta basis sets are included for comparison. Altogether, 46 DFT methods were tested using two data sets of 18 and 33 halogen-bonded complexes for which the complexation energies have been previously calculated with the high-accuracy CCSD(T)/CBS method. The DGDZVP basis set performed far better than other double-zeta basis sets, and it even outperformed the triple-zeta basis sets. Due to its small size, it is well-suited to studying halogen bonding in large systems.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Siiskonen, A., Priimägi, A.

Publication date: 1 Feb 2017

Peer-reviewed: Yes

Publication information

Journal: Journal of Molecular Modeling

Volume: 23
Issue number: 2
Article number: 50
ISSN (Print): 1610-2940

Ratings:

Scopus rating (2017): CiteScore 1.17 SJR 0.36 SNIP 0.515

Original language: English

ASJC Scopus subject areas: Catalysis, Computer Science Applications, Physical and Theoretical Chemistry, Organic Chemistry, Computational Theory and Mathematics, Inorganic Chemistry

Keywords: Basis set, Benchmarking, Density functional theory, Halogen bonding

DOIs:

10.1007/s00894-017-3212-4

Source: Scopus

Source ID: 85011684872

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

Anaerobic batch conversion of pine wood torrefaction condensate

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology, Research group: Industrial Bioengineering and Applied Organic Chemistry

Contributors: Doddapaneni, T. R. K. C., Praveenkumar, R., Tolvanen, H., Palmroth, M. R. T., Konttinen, J., Rintala, J.

Number of pages: 9

Pages: 299-307

Publication date: Feb 2017

Peer-reviewed: Yes

Early online date: 22 Nov 2016

Publication information

Journal: Bioresource Technology

Volume: 225

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2017): CiteScore 6.28 SJR 2.029 SNIP 1.823

Original language: English

DOIs:

10.1016/j.biortech.2016.11.073

Bibliographical note

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Source: PubMed

Source ID: 27898321

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

High-rate thiosulfate-driven denitrification at pH lower than 5 in fluidized-bed reactor

Abstract This study investigated the potential of a fluidized-bed biofilm dominated by Thiobacillus denitrificans to sustain thiosulfate-driven denitrification under increasingly acidic conditions. A fluidized-bed reactor (FBR) performing denitrification via thiosulfate (S₂O₃²⁻) oxidation of a nitrate-contaminated synthetic wastewater was first operated under decreasing feed pH values from 7.00 to 5.25. Denitrification efficiency > 99% was observed even at feed and effluent pH of 5.75 and 5.30, respectively. At lower feed pH values, the denitrification efficiency decreased rapidly due to inorganic carbon deficiency. The addition of a carbonation unit continuously feeding anaerobic grade CO₂ to the FBR biofilm allowed to investigate denitrification at pH values lower than 5.0. This new configuration, i.e. FBR with a carbonation unit, was able to sustain a complete and stable denitrification even at pH as low as 4.75. Denaturing gradient gel electrophoresis (DGGE) showed the evolution of the denitrifying biofilm during the FBR operation, resulting in a robust and

high-performing mixotrophic consortium of chemolithotrophic and heterotrophic bacteria dominated by *T. denitrificans*. Batch activity tests performed at three different stages of the FBR operation (feed pH 7.0, 6.0 and 5.25) showed that low pH cultivation enhanced the denitrification activity (mg N/g VS d) of the FBR biofilm at acidic pH values.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Di Capua, F., Lakaniemi, A., Puhakka, J. A., Lens, P. N. L., Esposito, G.

Number of pages: 10

Pages: 282-291

Publication date: Feb 2017

Peer-reviewed: Yes

Early online date: 28 Oct 2016

Publication information

Journal: Chemical Engineering Journal

Volume: 310, Part 1

ISSN (Print): 1385-8947

Ratings:

Scopus rating (2017): CiteScore 7.01 SJR 1.863 SNIP 1.96

Original language: English

Keywords: Acidic wastewater treatment, Autotrophic denitrification, Chemolithotrophic denitrifiers, Fluidized-bed reactor, Mixotrophic biofilm, Thiosulfate

DOIs:

10.1016/j.cej.2016.10.117

Source: RIS

Source ID: urn:63A5AD5846B4CA4F52FF655EE34EB47C

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

The Role of Inorganics in Biomass Gasification: Catalytic Effects on Char Reactions and Toxic Emissions

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

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

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

While there are methods for modeling the effects of inorganics in catalyzing char gasification, further research into interconnected issues of surface area, pore sizes, pyrolysis conditions and inorganic concentrations is needed. Similarly, while equilibrium modeling has been shown to predict the behavior of arsenic during gasification in some cases, there are many gaps in understanding which arsenic compounds are most relevant.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

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

Contributors: Kramb, J.

Number of pages: 81

Publication date: 13 Jan 2017

Publication information

Publisher: Tampere University of Technology
ISBN (Print): 978-952-15-3883-4
ISBN (Electronic): 978-952-15-3897-1
Original language: English

Publication series

Name: Tampere University of Technology. Publication
Volume: 1450
ISSN (Print): 1459-2045
Electronic versions:
kramb 1450
URLs:
<http://urn.fi/URN:ISBN:978-952-15-3897-1>
Research output: Book/Report > Doctoral thesis > Collection of Articles

Enhancing the activity of iron-oxidising bacteria: A case study with process liquors from heap bioleaching of a complex sulphide ore

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry
Contributors: Ahoranta, S. H., Peltola, M. K., Lakaniemi, A., Puhakka, J. A.
Pages: 163-172
Publication date: Jan 2017
Peer-reviewed: Yes
Early online date: 30 Nov 2016

Publication information

Journal: Hydrometallurgy
Volume: 167
ISSN (Print): 0304-386X
Ratings:
Scopus rating (2017): CiteScore 3.43 SJR 1.208 SNIP 1.962
Original language: English
Keywords: Iron-oxidising bacteria, Heap bioleaching, Bacterial community composition, Inhibition, Nutrient limitation, Aluminium toxicity
DOIs:
[10.1016/j.hydromet.2016.11.010](https://doi.org/10.1016/j.hydromet.2016.11.010)

Bibliographical note

INT=keb,"Peltola, Minna K."
Source: RIS
Source ID: urn:01F974DF5D153BB114C1E139A4861A1B
Research output: Contribution to journal > Article > Scientific > peer-review

The Orange Side of Disperse Red 1: Humidity-Driven Color Switching in Supramolecular Azo-Polymer Materials Based on Reversible Dye Aggregation

Humidity detection, and the quest for low-cost facile humidity-sensitive indicator materials is of great interest for many fields, including semi-conductor processing, food transport and storage, and pharmaceuticals. Ideal humidity-detection materials for these applications might be based on simple clear optical readout with no power supply, i.e.: a clear color change observed by the naked eye of any untrained observer, since it doesn't require any extra instrumentation or

interpretation. Here, the introduction of a synthesis-free one-step procedure, based on physical mixing of easily available commercial materials, for producing a humidity memory material which can be easily painted onto a wide variety of surfaces and undergoes a remarkable color change (approximately 100 nm blue-shift of λ_{MAX}) upon exposure to various thresholds of levels of ambient humidity is reported. This strong color change, easily visible to as a red-to-orange color switch, is locked in until inspection, but can then be restored reversibly if desired, after moderate heating. By taking advantage of spontaneously-forming reversible 'soft' supramolecular bonds between a red-colored azo dye and a host polymer matrix, a reversible dye 'migration' aggregation appearing orange, and dis-aggregation back to red can be achieved, to function as the sensor.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, McGill University

Contributors: Schoelch, S., Vapaavuori, J., Rollet, F., Barrett, C. J.

Publication date: Jan 2017

Peer-reviewed: Yes

Early online date: 23 Nov 2016

Publication information

Journal: Macromolecular Rapid Communications

Volume: 38

Issue number: 1

ISSN (Print): 1022-1336

Ratings:

Scopus rating (2017): CiteScore 4.08 SJR 1.452 SNIP 0.959

Original language: English

DOIs:

10.1002/marc.201600582

Bibliographical note

© 2016 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

Source: PubMed

Source ID: 27879028

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

A comparison of fate and toxicity of selenite, biogenically and chemically synthesized selenium nanoparticles to zebrafish (*Danio rerio*) embryogenesis

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Mal, J., Veneman, W. J., Nancharaiah, Y. V., van Hullebusch, E. D., Peijnenburg, W. J. G. M., Vijver, M. G., Lens, P. N. L.

Number of pages: 34

Pages: 1-34

Publication date: 2017

Peer-reviewed: Yes

Early online date: 23 Dec 2016

Publication information

Journal: Nanotoxicology

Volume: 11

Issue number: 1

ISSN (Print): 1743-5390

Ratings:

Scopus rating (2017): CiteScore 5.99 SJR 1.63 SNIP 1.204

Original language: English

DOIs:

10.1080/17435390.2016.1275866

Source: PubMed

Source ID: 28008795

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

A light-driven artificial flytrap

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Wani, O. M., Zeng, H., Priimägi, A.

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Nature Communications

Volume: 8

Article number: 15546

ISSN (Print): 2041-1723

Ratings:

Scopus rating (2017): CiteScore 12.41 SJR 6.582 SNIP 2.934

Original language: English

Keywords: Journal Article

Electronic versions:

A light-driven artificial flytrap

DOIs:

10.1038/ncomms15546

URLs:

<http://urn.fi/URN:NBN:fi:ty-201705311568>

Source: PubMed

Source ID: 28534872

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

Base catalysed N-functionalisation of boroxazolidones

A method for the condensation of boroxazolidones derived from L-valine with aromatic aldehydes, catalysed by 1,5,7-triazabicyclo[4.4.0]dec-5-ene was developed. The preparation and isolation of a series of highly functionalised stable ketimines derived from the reaction of 2,2-diaryl-1,3,2-oxazaborolidin-5-ones with aryl aldehydes is herein described. Several unreported boroxazolidones were prepared by condensation of triethylammonium tetra-arylborates with L-valine in up to 98% yield. The newly synthesised compounds were determined to be moderately cytotoxic against colorectal adenocarcinoma cells, with the best compound in this series having an IC₅₀ of 76 µM. A brief inspection of the effect of the same compound against human brain astrocytoma cells showed an IC₅₀ of 268 µM.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Faculty of Biomedical Sciences and Engineering, Research group: Molecular Signaling Lab, BioMediTech, Department of Chemistry and Bioengineering

Contributors: J., R., Mannoja, J., Nguyen, T., N., A., N. M., K., Franzén, R. G., Kandhavelu, M., Candeias, N. R.

Number of pages: 8

Pages: 20620-20627

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: RSC Advances

Volume: 7

Issue number: 33

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2017): CiteScore 3.01 SJR 0.863 SNIP 0.736

Original language: English

Electronic versions:

Base catalysed N-functionalisation of boroxazolidones

DOIs:

10.1039/c7ra03266h

URLs:

<http://urn.fi/URN:NBN:fi:tty-201704181305>

Bibliographical note

INT=keb,"Raunio, J."

INT=tut-bmt,"Nguyen, T."

INT=tut-bmt,"Ahmad, N."

INT=keb,"Kempainen, N. M."

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

Bioelectrochemical Systems for Heavy Metal Removal and Recovery

Although metal bearing wastes are toxic, they possess economic value and hence need attention towards remediation/recovery. Various physical and chemical methods are being practiced for treating metal laden wastewaters, but are limited owing to the problems associated with maintenance and operational costs. Biological methods that use microbes as catalyst are cost effective and easy to operate, but only a little progress has been made in terms of recovery than the treatment. Recently, there is a shift in focus from bioremediation of metal wastes towards the recovery of valuable metals which are scanty. In this context, bioelectrochemical systems (BES) have emerged as a potential technological platform for recovery of metal ions from metallurgical waste (end-of-life products), process streams and wastewaters. In bioelectrochemical systems, microbial oxidation of organic substrate at the anode is coupled to abiotic or biotic reduction of metal ions at the cathode. With this perspective, this chapter gives an insight on the redox mechanisms of bacteria towards metal recovery along with the influence of in situ and ex situ potentials in bioelectrochemical systems. The exo-electron transport mechanism in bacteria for metal reduction and speciation is also discussed. Besides, the chapter also provides an overview on the metal speciation in bioelectrochemical systems along with electrochemical, physical and chemical methods for metal removal and recovery from wastewaters. Emerging metal recovery concepts based on bioelectrochemical systems are also presented in detail.

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Chemistry and Bioengineering

Contributors: Modestra, J. A., Velvizhi, G., Krishna, K. V., Arunasri, K., Lens, P. N. L., Nancharaiyah, Y., Venkata Mohan, S.

Number of pages: 34

Pages: 165-198

Publication date: 2017

Host publication information

Title of host publication: Sustainable Heavy Metal Remediation : Volume 1: Principles and Processes

Place of publication: Cham

Publisher: Springer International Publishing

Editors: Rene, E. R., Sahinkaya, E., Lewis, A., Lens, P. N.

ISBN (Print): 978-3-319-58622-9

Publication series

Name: Environmental Chemistry for a Sustainable World

ISSN (Print): 2213-7114

DOIs:

10.1007/978-3-319-58622-9_6

Source: Bibtex

Source ID: urn:876e5b6ca410fd8901e3ed4c94c08ff5

Research output: Chapter in Book/Report/Conference proceeding > Chapter > Scientific > peer-review

Biological removal of selenate and ammonium by activated sludge in a sequencing batch reactor

Wastewaters contaminated by both selenium and ammonium need to be treated prior to discharge into natural water bodies, but there are no studies on the simultaneous removal of selenium and ammonium. A sequencing batch reactor (SBR) was inoculated with activated sludge and operated for 90 days. The highest ammonium removal efficiency achieved was 98%, while the total nitrogen removal was 75%. Nearly a complete chemical oxygen demand removal efficiency was attained after 16 days of operation, whereas complete selenate removal was achieved only after 66 days. The highest total Se removal efficiency was 97%. Batch experiments showed that the total Se in the aqueous phase decreased by 21% with increasing initial ammonium concentration from 50 to 100 mg L⁻¹. This study showed that SBR can remove both selenate and ammonium via, respectively, bioreduction and partial nitrification-denitrification and thus offer possibilities for treating selenium and ammonium contaminated effluents.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, UPEM, Homi Bhabha National Institute, Mumbai, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education

Contributors: Mal, J., Nancharaiah, Y. V., van Hullebusch, E. D., Lens, P. N.

Number of pages: 9

Pages: 11-19

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 229

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2017): CiteScore 6.28 SJR 2.029 SNIP 1.823

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

Keywords: Activated sludge, Elemental selenium, Selenate bioreduction, Sequencing batch reactor, Simultaneous nitrification and denitrification

DOIs:

10.1016/j.biortech.2016.12.112

Source: Scopus

Source ID: 85009200824

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

Biological Sulphate Reduction

During construction, renovation and/or demolition activities, large amounts of construction and demolition debris are created. This debris contains high sulphate concentrations and toxic metals, which can create a lot of environmental problems, especially at landfill sites. The disposal of the debris can cause odour problems and possible health impacts to landfill staff and surrounding inhabitants due to hydrogen sulphide gas generation. In order to reuse this debris, sulphate and heavy metal have to be removed. This chapter reviews the technologies used for sulphate and heavy metal removal from the debris both by chemical and biological processes. Moreover, possible ways for sulphur recovery has been reviewed. A sulphate removal efficiency up to 99% can be achieved from the chemical sulphate removal process. However, for this high performance, toxic chemicals such as barium and lead compounds have to be used. The biological sulphate reduction process is an alternative method for sulphate removal and recovery of sulphur and heavy metals from debris. Sulphide which is the product of this bio-process can be easily precipitated together with dissolved metal as metallic sulphides. Moreover, sulphide produced in this process can also be recovered as elemental sulphur or sulphuric acid.

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Chemistry and Bioengineering
Contributors: Kijjanapanich, P., Lens, P. N. L.
Number of pages: 18
Pages: 115-132
Publication date: 2017

Host publication information

Title of host publication: Sustainable Heavy Metal Remediation: Volume 2: Case studies
Place of publication: Cham
Publisher: Springer International Publishing
Editors: Rene, E. R., Sahinkaya, E., Lewis, A., Lens, P. N.
ISBN (Print): 978-3-319-61146-4
ISBN (Electronic): 978-3-319-61146-4

Publication series

Name: Environmental Chemistry for a Sustainable World
ISSN (Print): 2213-7114
DOIs:

10.1007/978-3-319-61146-4_4

Source: Bibtex

Source ID: urn:0fb003eb03e7d35d9d8d037bbf1dd2ab

Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific › peer-review

Biorecovery of Metals from Electronic Waste

Electronic waste, termed interchangeably as e-waste and/or waste electrical and electronic equipment (WEEE), is the fastest-growing segment of solid waste. The global electronic waste generation has reached 42 million tons in 2014, and is expected to reach 50 million tons in 2020. In addition to being a hazardous waste type, WEEE also includes relatively high concentrations of metals. Modern devices contain up to 60 different elements at various concentrations, encompassing base metals, critical metals, and platinum group metals mixed in a complex matrix of metallic and non-metallic materials. The emergence of numerous new electronic products and occurrence of complex metal mixtures make this waste stream an important secondary source of metals. Improper and informal end-of-life (EoL) processing of electronic waste has detrimental consequences on the environment and public health. Microbial processing of metals from their primary ores is an established technology with many full-scale applications. Bioprocessing of waste materials for metal recovery, on the other hand, is an emerging and promising technology with low environmental impact and high cost-effectiveness. This chapter overviews bioprocessing of electronic waste as a secondary source of metals to recover metals. Additionally, biologically-driven metal extraction technologies, (e.g. bioleaching) and metal recovery techniques (e.g. biomineralisation) are reviewed.

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Chemistry and Bioengineering

Contributors: Iildar, A., van de Vossenbergh, J., Rene, E. R., van Hullebusch, E. D., Lens, P. N. L.

Number of pages: 38

Pages: 241-278

Publication date: 2017

Host publication information

Title of host publication: Sustainable Heavy Metal Remediation : Volume 2: Case studies
Place of publication: Cham
Publisher: Springer International Publishing
Editors: Rene, E. R., Sahinkaya, E., Lewis, A., Lens, P. N.
ISBN (Print): 978-3-319-61146-4

Publication series

Name: Environmental Chemistry for a Sustainable World
ISSN (Print): 2213-7114
DOIs:

10.1007/978-3-319-61146-4_8

Source: Bibtex

Source ID: urn:c24f3ec79128445d46ff52e4787ae612

Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific › peer-review

Biosynthesis of CdSe nanoparticles by anaerobic granular sludge

This study investigated the feasibility of combining bioremediation of selenium (Se) containing wastewater and biorecovery of Se as cadmium selenide nanoparticles (CdSe NPs). A microbial community of anaerobic granular sludge was enriched for 300 days in the presence of Cd(ii) and selenite (Se(iv)). Complete Se(iv) (79 mg L⁻¹) reduction in the presence of Cd (30 mg L⁻¹) was observed after the 16th transfer (8 months) with the formation of both elemental selenium (Se(0)) and dissolved selenide (Se(-ii)). Cd either was associated with Se(0) or remained in the aqueous phase as free Cd(ii) ions and/or CdSe. The absorption and the fluorescence spectra of the aqueous phase showed formation of CdSe NPs. UV-vis and X-ray photoelectron spectroscopy (XPS) confirmed that the CdSe NPs were capped by extracellular polymeric substances (EPS) originating from the anaerobic granular sludge. Raman spectroscopy and XPS analysis further confirmed the presence of CdSe NPs in the aqueous phase, while Cd present in the Se(0) pellet after centrifugation was mainly precipitated as a Se(0)-Cd complex. A CdSe/CdS core/shell structure was found in the sludge, suggesting that Cd(ii) ions on the surface of the CdSe core interact with the sulfhydryl (-SH) groups present in the EPS of the UASB granules.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, UPEM, Homi Bhabha National Institute, Mumbai, Universite de Technologie de Compiègne, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education

Contributors: Mal, J., Nancharaiyah, Y. V., Bera, S., Maheshwari, N., Van Hullebusch, E. D., Lens, P. N.

Number of pages: 10

Pages: 824-833

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Environmental Science: Nano

Volume: 4

Issue number: 4

ISSN (Print): 2051-8153

Ratings:

Scopus rating (2017): CiteScore 6.52 SJR 1.676 SNIP 1.393

Original language: English

ASJC Scopus subject areas: Materials Science (miscellaneous), Environmental Science(all)

DOIs:

10.1039/c6en00623j

Source: Scopus

Source ID: 85017546806

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

Controlling azobenzene photoswitching through combined ortho-fluorination and -amination

We present a series of visible-light-absorbing azobenzene photoswitches with cis-lifetimes ranging from one second to three days. We combine ortho-fluorination to control the cis-lifetimes, and ortho-amination to boost the visible-light absorption. The synthesis is accomplished by selectively replacing one or more ortho-fluorines with amines in the ortho-fluoroazobenzene precursors.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group:

Chemistry & Advanced Materials, Research area: Optics

Contributors: Ahmed, Z., Siiskonen, A., Virkki, M., Priimägi, A.

Number of pages: 4

Pages: 12520-12523

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Chemical Communications

Volume: 53

Issue number: 93

ISSN (Print): 1359-7345

Ratings:

Scopus rating (2017): CiteScore 6.03 SJR 2.555 SNIP 1.127

Original language: English

Electronic versions:

c7cc07308a

DOIs:

10.1039/C7CC07308A

URLs:

<http://urn.fi/URN:NBN:fi:tty-201712042303>

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

Cultivation of *Scenedesmus acuminatus* in different liquid digestates from anaerobic digestion of pulp and paper industry biosludge

Different undiluted liquid digestates from mesophilic and thermophilic anaerobic digesters of pulp and paper industry biosludge with and without thermal pretreatment were characterized and utilized for cultivating *Scenedesmus acuminatus*. Higher *S. acuminatus* biomass yields were obtained in thermophilic digestates (without and with pretreatment prior to anaerobic digestion (AD): 10.2 ± 2.2 and $10.8 \pm 1.2 \text{ g L}^{-1}$, respectively) than in pretreated mesophilic digestates ($7.8 \pm 0.3 \text{ g L}^{-1}$), likely due to differences in concentration of sulfate, iron, and/or other minor nutrients. *S. acuminatus* removed over 97.4% of ammonium and 99.9% of phosphate and sulfate from the digestates. Color (74–80%) and soluble COD (29–39%) of the digestates were partially removed. Different AD processes resulted in different methane yields (18–126 L $\text{CH}_4 \text{ kg}^{-1} \text{ VS}$), digestate compositions, and microalgal yields. These findings emphasize the importance of optimizing each processing step in wood-based biorefineries and provide information for pulp and paper industry development for enhancing value generation.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Tao, R., Lakaniemi, A., Rintala, J. A.

Number of pages: 8

Pages: 706–713

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 245

Issue number: A

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2017): CiteScore 6.28 SJR 2.029 SNIP 1.823

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Renewable Energy, Sustainability and the Environment, Waste Management and Disposal

Keywords: Digestate characteristics, Microalgal growth, Nutrient recovery, Pulp and paper industry, Wastewater treatment

Electronic versions:

Cultivation of *Scenedesmus acuminatus* in different liquid digestates from anaerobic digestion of pulp and paper industry biosludge

Cultivation of *Scenedesmus acuminatus* in different liquid digestates from anaerobic digestion of pulp and paper industry biosludge. Embargo ended: 14/09/19

DOIs:

10.1016/j.biortech.2017.08.218

URLs:

<http://urn.fi/URN:NBN:fi:tty-201812052814>

Source: Scopus

Source ID: 85029373417

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

Difference in the core-shell dynamics of polyethyleneimine and poly(L-lysine) DNA polyplexes

Electrostatic polymer-DNA complexes (polyplexes) have been widely investigated for DNA delivery, and remarkable differences in transfection efficacy have been seen among the materials. For example, polyethyleneimine (PEI) mediates DNA transfection more effectively than poly(L-lysine) (PLL). Biophysical properties of the polyplexes may explain their different properties in gene delivery. We investigated the structural dynamics in DNA polyplexes, especially the material exchange between the core and shell regions of the PEI and PLL polyplexes. Steady-state fluorescence spectroscopy and double labeling based fluorescence resonance energy transfer (FRET) techniques were used to study the DNA

polyplexes. According to our results there is a clear difference between these two polymers: core exchange takes place in PEI but not in PLL polyplexes. Such differences in structural dynamics of polyplexes explain, at least partly, the differences in DNA release and transfection efficacy at cellular level.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, University of Helsinki, Ita-Suomen yliopisto, Universita degli Studi di Padova, Italy

Contributors: Vuorimaa-Laukkanen, E., Lisitsyna, E. S., Ketola, T., Morin-Pickardat, E., Liang, H., Hanzlíková, M., Yliperttula, M.

Pages: 122-127

Publication date: 2017

Peer-reviewed: Yes

Early online date: 2017

Publication information

Journal: European Journal of Pharmaceutical Sciences

Volume: 103

ISSN (Print): 0928-0987

Ratings:

Scopus rating (2017): CiteScore 3.81 SJR 1.016 SNIP 1.317

Original language: English

ASJC Scopus subject areas: Pharmaceutical Science

Keywords: DNA complexation, Fluorescence spectroscopy, Non-viral gene delivery, Poly-l-lysine, Polyethylene imine, Polyplex

DOIs:

10.1016/j.ejps.2017.03.025

Source: Scopus

Source ID: 85017349792

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

Effects of orientation at the phthalocyanine-CdSe interface on the electron transfer characteristics

A phthalocyanine molecule adsorbed on the (1010) surface of wurtzite CdSe is theoretically modeled by the DFT method. We have found that a linker does not affect substantially the redox properties of phthalocyanine, while saturation of the macrocycle with peripheral substituent groups causes a downward shift in the energy position of its frontier orbitals that can hinder electron injection to the CdSe surface. Tilting of the phthalocyanine molecule relative to the surface also leads to the lowering of its molecular electronic levels relative to the bands of CdSe. At a tilting angle of 30°, the LUMO level of the dye appears to be lower than the conduction band minimum of cadmium selenide, which makes the electron transfer to its hybridized surface unfavorable. By contrast, the HOMO level of the phenylbutyric acid linker provides a suitable intermediate channel for the hole transfer from the valence band of CdSe to the phthalocyanine that points to the possible acceptor behavior of the phthalocyanine molecule in its hybrids with CdSe nanostructures.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Research group: Electronic Structure Theory, Research area: Computational Physics, Center of Innovation Technologies

Contributors: Golovanov, V. V., Nazarchuk, B. V., Golovanova, V. V., Tkachenko, N. V., Rantala, T. T.

Number of pages: 7

Pages: 10511-10517

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 19

Issue number: 16

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.075

Original language: English

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

DOIs:

10.1039/c7cp00833c

Source: Scopus

Source ID: 85019969347

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

Evaluation of long-term post process inactivation of bioleaching microorganisms

The H2020 BioMORe project (www.biomore.info, Grant Agreement #642456) tests the feasibility of in-situ bioleaching of copper in deep subsurface deposits in the Rudna Mine, Poland. Copper is leached using biologically produced ferric iron solution, which is recycled back to the in-situ reactor after re-oxidation by iron-oxidizing bacteria (IOB). From a post operational point of view, it is important that the biological processes applied during the operation can be controlled and terminated. Our goal was to determine the possibility to use natural saline mine water for the inactivation of introduced IOB remaining in the in-situ reactor after completion of the leaching process of the Kupferschiefer ore. Aerobic and anaerobic microcosms containing acid-leached (pH 2) sandstone or black shale from the Kupferschiefer in the Rudna mine were further leached with the effluent from an iron-oxidizing bioreactor, at a temperature of 30°C, for 10 days, to simulate in-situ leaching. After the removal of the iron solution, residing IOB were inactivated by filling the microcosms with saline water (65 g L⁻¹ Cl⁻) originating from the mine. The saline water completely inactivated the IOB and the naturally occurring saline water of the mine can be used for long-term post process inactivation of bioleaching microorganisms.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, VTT Technical Research Centre of Finland

Contributors: Bomberg, M., Miettinen, H., Wahlström, M., Kaartinen, T., Ahoranta, S., Lakaniemi, A., Kinnunen, P.

Number of pages: 4

Pages: 57-60

Publication date: 2017

Host publication information

Title of host publication: 22nd International Biohydrometallurgy Symposium

Publisher: Trans Tech Publications Ltd

ISBN (Print): 9783035711806

Publication series

Name: Solid State Phenomena

Volume: 262 SSP

ISSN (Electronic): 1662-9779

ASJC Scopus subject areas: Atomic and Molecular Physics, and Optics, Materials Science(all), Condensed Matter Physics

Keywords: In situ bioleaching, Inactivation, Iron-oxidizing bacteria

DOIs:

10.4028/www.scientific.net/SSP.262.57

Bibliographical note

EXT="Kinnunen, Päivi"

Source: Scopus

Source ID: 85028980141

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Fate of metallic engineered nanomaterials in constructed wetlands: prospection and future research perspectives

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Laboratory of Industrial Water and Ecotechnology, Universiteit Gent, Laboratory of Analytical Chemistry and Applied Ecochemistry, Laboratory of Chemistry and Bioengineering, Royal Military College of Canada

Contributors: Auvinen, H., Gagnon, V., Rousseau, D. P. L., du Laing, G.

Number of pages: 16

Pages: 207–222

Publication date: 2017

Peer-reviewed: Yes

Early online date: 5 Apr 2017

Publication information

Journal: Reviews in Environmental Science and Bio-Technology

Volume: 16

Issue number: 2

ISSN (Print): 1569-1705

Ratings:

Scopus rating (2017): CiteScore 6.27 SJR 1.615 SNIP 2.347

Original language: English

ASJC Scopus subject areas: Environmental Engineering, Applied Microbiology and Biotechnology, Waste Management and Disposal, Pollution

Keywords: Discharge, Effluent, Nanoparticle, Transformation, TSS, Wastewater

DOIs:

10.1007/s11157-017-9427-0

Source: Scopus

Source ID: 85021244022

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

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

General information

Publication status: Published

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials, Univ Helsinki, University of Helsinki, Ctr Drug Res, Div Pharmaceut Biosci, Univ Eastern Finland, University of Eastern Finland, Sch Pharm, Univ Helsinki, University of Helsinki, Fac Pharm, Ctr Drug Res, Div Biopharmaceut Sci, Division of Biopharmaceutical Sciences, Faculty of Pharmacy, Helsinki University

Contributors: Vuorimaa-Laukkanen, E., Lisitsyna, E. S., Ketola, T., Morin-Pickardat, E., Liang, H., Hanzlikova, M., Urtti, A., Yliperttula, M. L., Lisitsyna, E., Laaksonen, T.

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: Other conference contribution › Paper, poster or abstract › Scientific

Influence of TiO₂ compact layer precursor on the performance of perovskite solar cells

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Åbo Akademi, Aalto University, VTT

Contributors: Vivo, P., Ojanperä, A., Smått, J., Sänden, S., Hashmi, S. G., Kaunisto, K., Ihalainen, P., Masood, M. T., Österbacka, R., Lund, P. D., Lemmetyinen, H.

Pages: 287-293

Publication date: 2017

Peer-reviewed: Yes

Early online date: 17 Nov 2016

Publication information

Journal: Organic Electronics

Volume: 41

ISSN (Print): 1566-1199

Ratings:

Scopus rating (2017): CiteScore 3.44 SJR 1.085 SNIP 0.884

Original language: English

DOIs:

10.1016/j.orgel.2016.11.017

Bibliographical note

EXT="Kaunisto, Kimmo"

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

Leaching and Recovery of Metals

Sludges, dusts, residues and other wastes originating from ferrous and non-ferrous metallic industries pose a serious environmental threat, if not disposed properly. Disposal of these wastes is expensive and remediation is a necessary step to be implemented to control the adverse environmental effects if disposal is done improperly. Since the past couple of decades, the world's high-grade metal reserves have been depleted considerably, but the demand for metals in day-to-day life in this electronic era is growing rapidly. The depletion of high-grade ores urges the mineral industry to look for alternative resources for metal extraction. Sludges, dusts, and other wastes generated by the metallurgical industries are interesting options as they still contain significant amounts of valuable base and heavy metals, sometimes even precious metals like gold and silver and also rare earth elements, depending on the nature of the mining site and composition of the primary ores used. This chapter overviews various hydrometallurgical and bio-hydrometallurgical leaching processes for the extraction of metals from these wastes. Different strategies of metal recovery such as solvent-extraction, electrowinning, bio/chemical sorption and bio/chemical precipitation from the wastes generated by various ferrous and non-ferrous metallic industries are overviewed.

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Chemistry and Bioengineering

Contributors: Sethurajan, M., Lens, P. N. L., Horn, H. A., Figueiredo, L. H. A., van Hullebusch, E. D.

Number of pages: 46

Pages: 161-206

Publication date: 2017

Host publication information

Title of host publication: Sustainable Heavy Metal Remediation : Volume 2: Case studies

Place of publication: Cham

Publisher: Springer International Publishing

Editors: Rene, E. R., Sahinkaya, E., Lewis, A., Lens, P. N.

ISBN (Print): 978-3-319-61146-4

Publication series

Name: Environmental Chemistry for a Sustainable World

ISSN (Print): 2213-7114

DOIs:

10.1007/978-3-319-61146-4_6

Source: Bibtex

Source ID: urn:3f4f7edc2f43f3e98e85ddb80c33ea09

Research output: Chapter in Book/Report/Conference proceeding > Chapter > Scientific > peer-review

Leaching and Recovery of Molybdenum from Spent Catalysts

Spent catalysts are generated in large quantities as solid waste on a yearly basis. Owing to their hazardous nature, environmental regulations for discarded spent catalysts are very strict. Consequently, from the ecological and economical viewpoint, metal recovery from spent catalysts is very important. Molybdenum (Mo) is one of the elements present in spent catalysts at high concentrations. The rapidly growing demands for Mo and its products create a need to develop novel recovery processes from secondary resources, i.e. spent catalysts, as there is a projected shortage of the primary resources for this element. This chapter overviews: (i) the general characteristics of Mo along with the research conducted in recent years concerning Mo chemical leaching, i.e. with strong inorganic acids, sodium hydroxide, hydrogen peroxide and acid mixtures, (ii) Mo bioleaching, i.e. with bacteria *Acidithiobacillus ferrooxidans*, *Acidithiobacillus thiooxidans* and *Acidianus brierleyi* or fungi *Penicillium simplicissimum* and *Aspergillus niger* and (iii) Mo recovery, i.e. precipitation, adsorption, ion exchange and solvent extraction, from spent catalysts. Chemical leaching offers Mo leaching yields exceeding 90%. Sulphuric acid seems to be the best leachant owing to its high oxidising power. Bioleaching offers more

cost-efficient, simpler and more environmentally friendly processes. However, bioleaching has relatively long leaching cycles (usually around 20 days) and extraction efficiencies of Mo are below 70%. Among the recovery techniques, solvent extraction is well-established in hydrometallurgy for commercial production of high purity Mo.

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Chemistry and Bioengineering

Contributors: Vemic, M., Bordas, F., Guibaud, G., Lens, P. N. L., van Hullebusch, E. D.

Number of pages: 33

Pages: 207-239

Publication date: 2017

Host publication information

Title of host publication: Sustainable Heavy Metal Remediation : Volume 2: Case studies

Place of publication: Cham

Publisher: Springer International Publishing

Editors: Rene, E. R., Sahinkaya, E., Lewis, A., Lens, P. N.

ISBN (Print): 978-3-319-61146-4

Publication series

Name: Environmental Chemistry for a Sustainable World

ISSN (Print): 2213-7114

DOIs:

10.1007/978-3-319-61146-4_7

Source: Bibtex

Source ID: urn:149b1a76ad0b466b4222266cd292817e

Research output: Chapter in Book/Report/Conference proceeding > Chapter > Scientific > peer-review

Light-Driven, Caterpillar-Inspired Miniature Inching Robot

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Research group: Supramolecular photochemistry, Univ Warsaw, University of Warsaw, Fac Phys, Inst Expt Phys

Contributors: Zeng, H., Wani, O. M., Wasylczyk, P., Priimägi, A.

Pages: 1700224

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Macromolecular Rapid Communications

Volume: 39

Issue number: 1

ISSN (Print): 1022-1336

Ratings:

Scopus rating (2017): CiteScore 4.08 SJR 1.452 SNIP 0.959

Original language: English

Keywords: Journal Article

Electronic versions:

20170427_MRC_Inching-walker-revised_GOA. Embargo ended: 31/05/18

DOIs:

10.1002/marc.201700224

URLs:

<http://urn.fi/URN:NBN:fi:tty-201901111064>

Bibliographical note

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Source: PubMed

Source ID: 28561989

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

Metal Recovery from Industrial and Mining Wastewaters

Biological sulphate-reduction is a microbial-mediated process where sulphate is reduced to sulphide, which can be used to recover metals as sulphidic precipitates. To date, this technology has been assessed at full scale to recover valuable metals such as Cu, Ni and Zn. Despite this, research gaps are still encountered in this technology for improving and expanding its scope. Accordingly, the present review discusses: (1) the state of the art of the sulphate-reduction process, (2) the substrate options available that can meet the needs of the process, (3) the bioreactor configurations and their suitability for metal recovery, (4) the principles and factors affecting metal sulphide-precipitation and (5) the basis and advances on modelling and control of the process. The high diversity and versatility of sulphate-reducing bacteria allows exploring the use of substrates and operational conditions that facilitate the recovery of metals in bioreactors. Due to the lack of organics on industrial and mining waste streams that can sustain sulphate-reducing bacteria, the selection of a degradable, cost-effective, available, and non-pollutant substrate becomes crucial for the process. Different bioreactor configurations have been tested for the removal of metals from waste streams upon variations of the several operational conditions, concentration and type of metals tested, but metal recovery is hardly reported. Sulphate-reduction modelling has been developed to predict sulphide-inhibition/toxicity, microbial competition, kinetic parameters, biofilm and granulation development, sulphide-equilibrium and for scale-up design. Physicochemical reactions such as sorption/desorption and precipitation/solubilisation are not included in sulphate-reduction models despite that they are highly important for metal recovery in these systems. Sulphide and pH control in sulphate-reducing bioreactors is inherently essential to achieve metal recovery and to avoid unnecessary electron donor addition and over production of sulphide.

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Chemistry and Bioengineering

Contributors: Gómez, D. K. V., Lens, P. N. L.

Number of pages: 34

Pages: 81-114

Publication date: 2017

Host publication information

Title of host publication: Sustainable Heavy Metal Remediation : Volume 2: Case studies

Place of publication: Cham

Publisher: Springer International Publishing

Editors: Rene, E. R., Sahinkaya, E., Lewis, A., Lens, P. N.

ISBN (Print): 978-3-319-61146-4

ISBN (Electronic): 978-3-319-61146-4

Publication series

Name: Environmental Chemistry for a Sustainable World

ISSN (Print): 2213-7114

DOIs:

10.1007/978-3-319-61146-4_3

Source: Bibtex

Source ID: urn:76f93689415b9fff46ad3436e7c07ca1

Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific › peer-review

Microbial community response on wastewater discharge in boreal lake sediments

Despite high performance, municipal wastewater treatment plants (WWTPs) still discharge significant amounts of organic material and nitrogen and even microbes into the receiving water bodies, altering physico-chemical conditions and microbial functions. In this study, we examined how nitrified wastewater affects the microbiology of boreal lake sediments. Microbial community compositions were assessed with next generation sequencing of the 16S rRNA gene, and a more detailed view on nitrogen transformation processes was gained with qPCR targeting on functional genes (*nirS*, *nirK*, *nosZI*, *nosZII*, *amoA*Archaea, and *amoA*Bacteria). In both of the two studied lake sites, the microbial community composition differed significantly between control point and wastewater discharge point, and a gradual shift toward natural community composition was seen downstream following the wastewater gradient. SourceTracker analysis predicted that ~2% of sediment microbes were of WWTP-origin on the study site where wastewater was freely mixed with the lake water, while when wastewater was specially discharged to the sediment surface, ~6% of microbes originated from WWTP, but the wastewater-influenced area was more limited. In nitrogen transformation processes, the ratio between nitrifying archaea (AOA) and bacteria (AOB) was affected by wastewater effluent, as the AOA abundance decreased from the control point

(AOA:AOB 28:1 in Keuruu, 11:1 in Petäjavesi) to the wastewater-influenced sampling points, where AOB dominated (AOA:AOB 1:2–1:15 in Keuruu, 1:3–1:19 in Petäjavesi). The study showed that wastewater can affect sediment microbial community through importing nutrients and organic material and altering habitat characteristics, but also through bringing wastewater-originated microbes to the sediment, and may thus have significant impact on the freshwater biogeochemistry, especially in the nutrient-poor boreal ecosystems.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, University of Jyväskylä, Univ Jyväskylä, University of Jyväskylä, Dept Biol & Environm Sci, Nanosci Ctr, Univ Jyväskylä, Dept Biomed & Environm Sci

Contributors: Saarenheimo, J., Aalto, S. L., Rissanen, A. J., Tirola, M.

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: *Frontiers in Microbiology*

Volume: 8

Article number: 750

ISSN (Print): 1664-302X

Ratings:

Scopus rating (2017): CiteScore 4.19 SJR 1.699 SNIP 1.201

Original language: English

Electronic versions:

fmicb-08-00750

DOIs:

10.3389/fmicb.2017.00750

URLs:

<http://urn.fi/URN:NBN:fi:tty-201705121381>

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

Molding Optical Waveguides with Nematicons

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Research area: Optics, Research group: Nonlinear Optics, Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Research group: Supramolecular photochemistry, Physics, Univ Southampton, University of Southampton, Sch Phys & Astron, University of Southampton, United Kingdom

Contributors: Karimi, N., Virkki, M., Alberucci, A., Buchnev, O., Kauranen, M., Priimägi, A., Assanto, G.

Number of pages: 5

Publication date: 2017

Peer-reviewed: Yes

Early online date: 29 May 2017

Publication information

Journal: *Advanced Optical Materials*

Volume: 5

Issue number: 14

Article number: 1700199

ISSN (Print): 2195-1071

Ratings:

Scopus rating (2017): CiteScore 6.99 SJR 3.121 SNIP 1.699

Original language: English

DOIs:

10.1002/adom.201700199

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

Occurrence of photoinduced charge separation by the modulation of the electronic coupling between pyrene dimers and chemically converted graphenes

The photoexcitation of the pyrene dimer on graphene resulted in the final formation of a charge-separated state following an exciplex formation, while that of the pyrene monomer on graphene generated the corresponding exciplex solely due to the difference in the electronic coupling between the pyrene and the graphene.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials

Contributors: Umeyama, T., Baek, J., Mihara, J., Tkachenko, N. V., Imahori, H.

Pages: 1025-1028

Publication date: 2017

Peer-reviewed: Yes

Early online date: 8 Dec 2016

Publication information

Journal: Chemical Communications

Volume: 53

ISSN (Print): 1359-7345

Ratings:

Scopus rating (2017): CiteScore 6.03 SJR 2.555 SNIP 1.127

Original language: English

DOIs:

10.1039/c6cc07985g

Source: PubMed

Source ID: 27929165

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

Optimization of convectively cooled heat sinks

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Mechanical Engineering and Industrial Systems

Contributors: Lampio, K., Karvinen, R.

Pages: 473-479

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Microelectronics Reliability

Volume: 79

ISSN (Print): 0026-2714

Ratings:

Scopus rating (2017): CiteScore 1.52 SJR 0.388 SNIP 0.907

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Safety, Risk, Reliability and Quality, Surfaces, Coatings and Films, Electrical and Electronic Engineering

Keywords: Fin array, Forced convection, Heat sink, Multi-objective optimization, Natural convection, Pin fins
DOIs:

10.1016/j.microrel.2017.06.011

Source: Scopus

Source ID: 85020690970

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

Optimizing ammonium adsorption on natural zeolite for wastewaters with high loads of ammonium and solids

Ion exchange (IE) has been so far limited to treating waters and wastewaters low in solids (TS) and ammonium (NH_4^+). This study provides a new insight into the application of IE for NH_4^+ removal from wastewaters with high NH_4^+ and TS, using natural zeolite as adsorbent medium. Assays were carried out in continuously stirred batch reactors to study the effect of initial NH_4^+ , pH, TS, contact time, and zeolite pore size (0.2–0.5 and 0.6–2.0 mm). Results confirmed the suitability of this zeolite to remove NH_4^+ from wastewater with high amounts of solids (up to 2%TS) and NH_4^+ (up to 2500 mg NH_4^+ -N/L). Ammonium adsorption capacity (q_t) was faster with 0.2–0.5 mm size because of the greater specific surface area and shorter diffusion path than 0.6–2.0 mm zeolite. Both zeolites showed increasing q_t with increasing initial NH_4^+ due to the higher driving force produced by higher concentrations. The process followed a pseudo-second order kinetic and was best described by the Freundlich isotherm. Varying the pH (6–8.5) of the wastewater had no effect on NH_4^+ removal capacity. In conclusion, this natural zeolite showed high affinity for NH_4^+ in wastewater with high loads of NH_4^+ and solids, returning a viable treatment method when other techniques are not applicable.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering

Contributors: Taddeo, R., Prajapati, S., Lepistö, R.

Number of pages: 10

Pages: 1545–1554

Publication date: 2017

Peer-reviewed: Yes

Early online date: 3 Mar 2017

Publication information

Journal: Journal of Porous Materials

Volume: 24

Issue number: 6

ISSN (Print): 1380-2224

Ratings:

Scopus rating (2017): CiteScore 1.84 SJR 0.5 SNIP 0.697

Original language: English

ASJC Scopus subject areas: Materials Science(all), Mechanics of Materials, Mechanical Engineering

Keywords: Ammonium, Ion exchange, Kinetics, Solids, Zeolite

DOIs:

10.1007/s10934-017-0394-1

Bibliographical note

INT=keb,"Prajapati, Sumitra"

Source: Scopus

Source ID: 85014222281

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

Orientational optical nonlinearities in polymer-stabilized dye-doped liquid crystals

Dye-doped liquid crystals have drawn much attention for their potential in nonlinear optical applications. To invoke nonlinear optical effects, high light intensities are typically required. This review briefly introduces our group's efforts on developing highly nonlinear, dye-doped LC systems. By (i) using an effective oligothiophene dye, (ii) introducing polymer stabilization of the LC host and (iii) using hybrid molecular alignment, we have achieved self-focusing, a common third-order nonlinear process, even using a low-power, handheld laser-pointer.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Tokyo Inst Technol, Tokyo Institute of Technology, Chem Resources Lab, Midori Ku, JST, Japan Science & Technology Agency (JST), PRESTO, Tokyo Institute of Technology

Contributors: Wang, J., Aihara, Y., Kinoshita, M., Mamiya, J., Priimägi, A., Shishido, A.

Number of pages: 11

Pages: 57-67

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: The Japanese Liquid Crystal Society journal EKISHO

Volume: 21

Issue number: 1

ISSN (Print): 2189-2512

Original language: English

URLs:

https://bunken.org/jlcs/paper/Paper/detail?pdf=21-1_57.pdf&&year=2017&month=1

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

Origin and fate of methane in the Eastern Tropical North Pacific oxygen minimum zone

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Department of Environmental Sciences, University of Helsinki, Faculty of Life Sciences, University of Manchester, School of Biological and Chemical Sciences, Queen Mary University of London

Contributors: Chronopoulou, P., Shelley, F., Pritchard, W. J., Maanoja, S. T., Trimmer, M.

Number of pages: 14

Pages: 1386–1399

Publication date: 2017

Peer-reviewed: Yes

Early online date: 28 Feb 2017

Publication information

Journal: ISME Journal

Volume: 11

ISSN (Print): 1751-7362

Ratings:

Scopus rating (2017): CiteScore 9.5 SJR 4.813 SNIP 2.33

Original language: English

Electronic versions:

ismej20176a

DOIs:

10.1038/ismej.2017.6

URLs:

<http://urn.fi/URN:NBN:fi:tty-201703241222>

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

Photoinduced Electron Transfer in 9-Substituted 10-Methylacridinium Ions

A series of 9-substituted 10-methylacridinium ions (Acr⁺-R) in which an electron-donor moiety (R) is directly linked with an electron-acceptor moiety (Acr⁺) at the 9-position was synthesized, and the photodynamics was fully investigated to

determine the rate constants of photoinduced electron transfer (ET) and back electron transfer. The driving forces of photoinduced electron transfer and back electron transfer were determined by means of electrochemical and photophysical measurements. The dependence of the ET rate constants on driving force was well analyzed in the light of the Marcus theory of ET. The quantum yields of formation of the triplet ET states vary significantly, depending on the interaction between the donor (R) and acceptor (Acr⁺) moieties. Among the Acr⁺-R examined, the 9-mesityl-10-methylacridinium ion (Acr⁺-Mes) exhibits the best performance in terms of the lifetime of the triplet ET state and the quantum yield. Photoexcitation of Acr⁺-Mes results in formation of the triplet ET state [3(Acr⁺-Mes.⁺)], which has a long lifetime, a high energy (2.37 eV), and a high quantum yield (>75%) in acetonitrile. The triplet ET state exhibits both the oxidizing and reducing activity of the Mes.⁺ and Acr. moieties, respectively.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials

Contributors: Tsudaka, T., Kotani, H., Ohkubo, K., Nakagawa, T., Tkachenko, N. V., Lemmetyinen, H., Fukuzumi, S.

Pages: 1306-1317

Publication date: 2017

Peer-reviewed: Yes

Early online date: 14 Dec 2016

Publication information

Journal: Chemistry: A European Journal

Volume: 23

Issue number: 6

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2017): CiteScore 4.97 SJR 2.265 SNIP 1.033

Original language: English

DOIs:

10.1002/chem.201604527

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

Photophysical properties of porphyrin dimer-single-walled carbon nanotube linked systems

Porphyrin dimers were covalently grafted onto electron-accepting single-walled carbon nanotube (SWNT) sidewalls by direct aryl radical addition reaction with an m- or p-phenylene linker with the help of p-p interaction between the porphyrins. A splitting of the porphyrin Soret band and DFT calculations supported the selective formation of the porphyrin dimers on the sidewall of SWNTs. Photoexcitation of the porphyrin dimers on the SWNT resulted in the formation of the exciplex state, which directly decayed to the ground state without yielding the complete charge-separated state. Lifetimes of the porphyrin dimer-SWNT exciplex were longer than that of a porphyrin monomer-SWNT exciplex due to the stabilization by p-electron interaction over two porphyrin rings. In addition, the weaker electronic coupling through the meta-linkage than the para-one may be responsible for the exciplex lifetime of the porphyrin dimer-SWNT with the m-phenylene linker (49 ps) longer than that with the p-phenylene one (24 ps). The results obtained here provide the basic information on the effect of the donor dimerization on the photodynamic behavior of the exciplex state in donor-acceptor linked systems. [Figure presented]

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Kyoto Women's University

Contributors: Baek, J., Umeyama, T., Mizuno, S., Tkachenko, N. V., Imahori, H.

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 121

Issue number: 39

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.135

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Physical and Theoretical Chemistry, Surfaces, Coatings and Films

DOIs:

10.1021/acs.jpcc.7b08594

Source: Scopus

Source ID: 85032629899

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

Photoresponsive ionic liquid crystals assembled: Via halogen bond: En route towards light-controllable ion transporters

We demonstrate that halogen bonding (XB) can offer a novel approach for the construction of photoresponsive ionic liquid crystals. In particular, we assembled two new supramolecular complexes based on 1-ethyl-3-methylimidazolium iodides and azobenzene derivatives containing an iodotetrafluoro-benzene ring as XB donor, where the iodide anion acted as an XB acceptor. DSC and X-ray diffraction analyses revealed that the preferred stoichiometry between the XB donors and acceptors is 2:1, and that the iodide anions act as bidentate XB-acceptors, binding two azobenzene derivatives. Due to the high directionality of the XB, calamitic superanions are obtained, while the segregation occurring between the charged and uncharged parts of the molecules gives rise to a layered structure in the crystal lattice. Despite the fact that the starting materials are non-mesomorphic, the halogen-bonded supramolecular complexes exhibited monotropic lamellar liquid-crystalline phases over broad temperature ranges, as confirmed with polarized optical microscopy. Due to the presence of the azobenzene moieties, the LCs were photoresponsive, and a LC-to-isotropic phase transition could be obtained by irradiation with UV light. We envisage that the light-induced phase transition, in combination with the ionic nature of the LC, provides a route towards light-induced control over ion transport and conductance in these supramolecular complexes.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Politecnico di Milano, Aalto University

Contributors: Saccone, M., Palacio, F. F., Cavallo, G., Dichiarante, V., Virkki, M., Terraneo, G., Priimagi, A., Metrangolo, P.

Number of pages: 16

Pages: 407-422

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Faraday Discussions

Volume: 203

ISSN (Print): 1359-6640

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1039/c7fd00120g

Source: Scopus

Source ID: 85031726639

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

Release of Potassium during Devolatilization of Spruce Bark

The spruce bark with different particle sizes were devolatilized under various final temperatures and heating rates. The char yield and potassium release from the spruce bark at studied conditions were quantified. Lower char yields realized from the smaller fuel particles at high temperature and heating rate. It is mainly attributed to shorter residence time of volatiles in the fuel/char particles and less intensive secondary reaction of volatiles consequently. The devolatilization temperature has the most significant effects on alkali release from the studied spruce bark. At 600°C, less than 5% of alkali released from the both small and large particles regardless of heating rate. However, at 850°C, release of potassium from the small spruce bark particles sharply increased from 2.63% and 4.71% to 12.87% and 17.89%, as they were heated under heating rate of 50 K/min and 500 K/min, respectively. Large fraction of alkali released from studied fuel particles as they were devolatilized under a high heating rate. Additionally, more potassium release from small particles (125 <d<180 μm) than the larger ones (500 <d<600 μm) and this tendency increased with devolatilization temperature. In brief, intensive devolatilization conditions may limit secondary reactions of potassium containing compounds in the volatiles and thereby formation of more stable phases. The results obtained in the present work are of importance for understanding of potassium release during thermal conversion of spruce bark and proposing measures for mitigating potassium related operational problems.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, SINTEF Energy Research, Andritz AG
Contributors: Wang, L., Moilanen, A., Lehtinen, J., Konttinen, J., Matas, B. G.
Number of pages: 7
Pages: 1295-1301
Publication date: 2017
Peer-reviewed: Yes

Publication information

Journal: Energy Procedia
Volume: 105
ISSN (Print): 1876-6102
Ratings:

Scopus rating (2017): CiteScore 1.44 SJR 0.495 SNIP 0.811

Original language: English

ASJC Scopus subject areas: Energy(all)

Keywords: char, devolatilization, ICP-OES, potassium, SEM-EDX, Spruce bark

Electronic versions:

Release of Potassium During Devolatilization of Spruce Bark

DOIs:

10.1016/j.egypro.2017.03.463

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201708011639>

Source: Scopus

Source ID: 85020700355

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

Shape change of biogenic elemental selenium nanomaterials from nanospheres to nanorods decreases their colloidal stability

Microbial reduction of selenium oxyanions under mesophilic (30 °C) and thermophilic (55 °C) conditions produces biogenic elemental selenium nanospheres (BioSe-Nanospheres) and nanorods (BioSe-Nanorods), respectively. While the properties of BioSe-Nanospheres are well studied, the colloidal properties of BioSe-Nanorods have not yet been investigated. Therefore, this study characterized the surface properties of BioSe-Nanorods, compared their colloidal properties with BioSe-Nanospheres and elucidated the formation of BioSe-Nanorods in the presence of a capping agent. This study demonstrated that BioSe-Nanorods, like BioSe-Nanospheres, are capped by extracellular polymeric substances (EPS) as evidenced by infrared spectroscopy. The EPS capped BioSe-Nanorods were less colloidally stable than EPS capped BioSe-Nanospheres as demonstrated by the former's less negative zeta potential values when exposed to 10 mM NaCl. In fresh lake water, BioSe-Nanospheres showed a 91.6 (±0.5)% settling efficiency, while BioSe-Nanorods displayed a settling efficiency of 97.1 (±0.5)%. The lower colloidal stability and higher settling efficiency was due to a 7 times less negative surface charge of BioSe-Nanorods compared to BioSe-Nanospheres at pH 7.2. Further, this study observed that the formation of BioSe-Nanorods might proceed via BioSe-Nanospheres through orientation attachment followed by anisotropic growth as well as a solid-solution-solid mechanism. This study demonstrates the importance of the shape of nanoparticles in determining their bioremediation effectiveness and fate in the environment.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Helmholtz-Zentrum Dresden-Rossendorf, Institute for Water Education

Contributors: Jain, R., Jordan, N., Tsushima, S., Hübner, R., Weiss, S., Lens, P. N.

Number of pages: 10

Pages: 1054-1063

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Environmental Science: Nano

Volume: 4

Issue number: 5

ISSN (Print): 2051-8153

Ratings:

Scopus rating (2017): CiteScore 6.52 SJR 1.676 SNIP 1.393

Original language: English

ASJC Scopus subject areas: Materials Science (miscellaneous), Environmental Science(all)

DOIs:

10.1039/c7en00145b

Source: Scopus

Source ID: 85022015980

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

Structural and Photophysical Properties of Pentacene Alkanethiolate Monolayer-Protected Gold Nanoclusters and Nanorods: Supramolecular Intercalation and Photoinduced Electron Transfer with C60

6,13-Bis(triisopropylsilylethynyl)-pentacene (TIPS-pentacene: TP) alkanethiolate monolayer-protected gold nanoclusters (TP-Cn-X-MPCs: X stands for small (S) and large (L) nanocluster sizes) and nanorods (TP-Cn-MPRs) with different alkyl chain lengths ($n = 7, 11$) were synthesized to examine the structural and photophysical properties as well as intercalation trends with C60. The syntheses of TP-Cn-X-MPCs and TP-Cn-MPRs were successfully performed using two different precursors: TP disulfides and TP alkanethiols. The detailed structural properties were confirmed by ^1H NMR, elemental analyses, and transmission electron micrograph (TEM). In the spectroscopic absorption and fluorescence excitation measurements, spectral shapes of TP units on the gold surface were clearly observed, whereas fluorescence intensities of TP units were strongly quenched as compared to the corresponding reference monomer (TP-Ref). Then, fluorescence quenching titration experiments to determine the association constants (K_{app}) between C60 and TP assemblies (TP-Cn-X-MPCs and TP-Cn-MPRs) were performed by adding C60 in toluene. The K_{app} values were largely dependent on the sizes of nanoclusters and alkyl chain lengths in TP-Cn-X-MPC. For example, the K_{app} value of TP-C7-S-MPC ($73\,800\text{ M}^{-1}$) was much larger than those of TP-C11-S-MPC ($37\,800\text{ M}^{-1}$) and TP-C7-L-MPC (5350 M^{-1}). This trend is in sharp contrast with the similar K_{app} values ($\sim 66\,000\text{ M}^{-1}$) in TP-Cn-MPR ($n = 7, 11$). These results suggest that the intercalation behaviors are dependent on the surface structures (nanocluster vs nanorod). Such fluorescence quenching processes by photoinduced electron transfer (PET) in the complex between TP-C7-S-MPC and C60 were directly observed by femtosecond transient absorption measurements, monitoring the TP radical cation and C60 radical anion.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials

Contributors: Kato, D., Sakai, H., Saegusa, T., Tkachenko, N. V., Hasobe, T.

Number of pages: 10

Pages: 9043-9052

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 121

Issue number: 16

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.135

Original language: English

DOIs:

10.1021/acs.jpcc.7b01164

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

Structural characterization, spectroscopic, thermal, AC conductivity and dielectric properties and antimicrobial studies of $(\text{C}_8\text{H}_{12}\text{N})_2[\text{SnCl}_6]$

A new inorganic-organic hybrid material produced from 2,6-dimethylanilinium cations and tin halide $(\text{SnCl}_6)^{2-}$ has been synthesized and structurally determined by X-ray diffraction method. The title compound crystallizes in the monoclinic system, space group C2/m with $a = 19.8772(4)$, $b = 6.9879(1)$, $c = 8.3001(2)$ Å, $\beta = 98.487(2)^\circ$ and $V = 1140.26(4)$ Å³. The crystal structure is built up of sheets of $(\text{SnCl}_6)^{2-}$ octahedral anions and 2,6-xylidinium cations. The optical band gap was calculated and found to be 4.11 eV. At high temperature this compound exhibits a structural phase transition at 338 K. This has been characterized by differential scanning calorimetric and dielectric studies. Measurements of AC conductivity as a function of frequency at different temperatures indicated the hopping conduction mechanism. The bioassay results showed that the structure exhibits significant antibacterial activity.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Carthage University

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

Number of pages: 16

Pages: 399-414
Publication date: 2017
Peer-reviewed: Yes
Early online date: 1 Jul 2016

Publication information

Journal: PHASE TRANSITIONS

Volume: 90

Issue number: 4

ISSN (Print): 0141-1594

Ratings:

Scopus rating (2017): CiteScore 0.8 SJR 0.233 SNIP 0.61

Original language: English

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

Keywords: antibacterial activity, Crystal structure, fluorescent properties, phase transition, spectroscopies

DOIs:

10.1080/01411594.2016.1212194

Source: Scopus

Source ID: 84979648011

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

Supramolecular control of liquid crystals by doping with halogen-bonding dyes

Introducing photochromic or polymeric dopants into nematic liquid crystals is a well-established method to create stimuli-responsive photonic materials with the ability to "control light with light". Herein, we demonstrate a new material design concept by showing that specific supramolecular interactions between the host liquid crystal and the guest dopants enhance the optical performance of the doped liquid crystals. By varying the type and strength of the dopant-host interaction, the phase-transition temperature, the order parameter of the guest molecules, and the diffraction signal in response to interference irradiation, can be accurately engineered. Our concept points out the potential of supramolecular interactions in liquid-crystal photonics, being valuable for optimizing the design of dye-doped functional liquid-crystalline systems.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials, Département de Chimie, Succ. Centre-Ville, Politecnico di Milano, Università degli Studi di Milano, Tokyo Institute of Technology, VTT Technical Research Centre of Finland

Contributors: Vapaavuori, J., Siiskonen, A., Dichiarante, V., Forni, A., Saccone, M., Pilati, T., Pellerin, C., Shishido, A., Metrangolo, P., Priimagi, A.

Number of pages: 6

Pages: 40237-40242

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: RSC Advances

Volume: 7

Issue number: 64

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2017): CiteScore 3.01 SJR 0.863 SNIP 0.736

Original language: English

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

Electronic versions:

c7ra06397k

DOIs:

10.1039/c7ra06397k

URLs:

<http://urn.fi/URN:NBN:fi:ty-201712122322>

Source: Scopus

Source ID: 85028088976

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

Surface-Relief Gratings in Halogen-Bonded Polymer–Azobenzene Complexes: A Concentration-Dependence Study

In recent years, supramolecular complexes comprising a poly(4-vinylpyridine) backbone and azobenzene-based halogen bond donors have emerged as a promising class of materials for the inscription of light-induced surface-relief gratings (SRGs). The studies up to date have focused on building supramolecular hierarchies, i.e., optimizing the polymer–azobenzene noncovalent interaction for efficient surface patterning. They have been conducted using systems with relatively low azobenzene content, and little is known about the concentration dependence of SRG formation in halogen-bonded polymer–azobenzene complexes. Herein, we bridge this gap, and study the concentration dependence of SRG formation using two halogen-bond-donating azobenzene derivatives, one functionalized with a tetrafluoriodophenyl and the other with an iodoethynylphenyl group. Both have been previously identified as efficient molecules in driving the SRG formation. We cover a broad concentration range, starting from 10 mol % azobenzene content and going all the way up to equimolar degree of complexation. The complexes are studied as spin-coated thin films, and analyzed by optical microscopy, atomic force microscopy, and optical diffraction arising during the SRG formation. We obtained diffraction efficiencies as high as 35%, and modulation depths close to 400 nm, which are significantly higher than the values previously reported for halogen-bonded polymer–azobenzene complexes.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Research group: Supramolecular photochemistry, Politecn Milan, Polytechnic University of Milan, NFMLab, DCMIC Giulio Natta, Politecnico di Milano, VTT Technical Research Centre of Finland, Polimi Ist Italiano TecnoI, Istituto Italiano di Tecnologia - IIT, Ctr Nano Sci & Technol, VTT Tech Res Ctr Finland, VTT Technical Research Center Finland

Contributors: Stumpel, J. E., Saccone, M., Dichiarante, V., Lehtonen, O., Virkki, M., Metrangolo, P., Priimagi, A.

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Molecules

Volume: 22

Issue number: 11

ISSN (Print): 1420-3049

Ratings:

Scopus rating (2017): CiteScore 3.29 SJR 0.855 SNIP 1.184

Original language: English

Electronic versions:

molecules-22-01844

DOIs:

[10.3390/molecules22111844](https://doi.org/10.3390/molecules22111844)

URLs:

<http://urn.fi/URN:NBN:fi:tty-201710302091>

<http://www.mdpi.com/1420-3049/22/11/1844>

URLs:

<http://www.mdpi.com/1420-3049/22/11/1844>

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

Sustainable Heavy Metal Remediation: Volume 2: Case studies

General information

Publication status: Published

MoE publication type: C2 Edited books

Organisations: Chemistry and Bioengineering, Wageningen University and the UNESCO-IHE Institute for Water Education, Delft, The Netherlands, 18.10.2013, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education

Contributors: Rene, E. R. (ed.), Sahinkaya, E. (ed.), Lewis, A. (ed.), Lens, P. N. L. (ed.)

Number of pages: 278

Publication date: 2017

Publication information

Publisher: Springer International Publishing

Volume: 2

ISBN (Print): 978-3-319-61145-7

ISBN (Electronic): 978-3-319-61146-4

Original language: English

Publication series

Name: Environmental Chemistry for a Sustainable World
ISSN (Print): 2213-7114
DOIs:
10.1007/978-3-319-61146-4

Bibliographical note

EXT="Sahinkaya, Erkan"

Research output: Book/Report > Anthology > Scientific > peer-review

Synthesis of new acylsilanes

General information

Publication status: Published

Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Chemistry & Advanced Materials

Contributors: Rafael Candeias, N., Campos Do Vale, J.

Publication date: 2017

Peer-reviewed: Unknown

Event: Paper presented at XXV Portuguese Chemical Society Meeting , Lisbon, Portugal.

Research output: Other conference contribution > Paper, poster or abstract > Scientific

Synthesis of phenol-derivatives and biological screening for anticancer activity

Phenolic compounds are known for their cytotoxic properties against cancer cells despite their still unclear general mechanism of action. Herein is reported the evaluation of the cytotoxic effects of on human osteosarcoma cells of nine phenol derivatives against osteosarcoma cells, and some insights on their mechanism. The cytotoxicity was characterized by cell viability, scratch assay, cellular DNA content measurement, Annexin V apoptosis, mitochondrial calcium and caspase 3/7 assays. The study shows that out of the nine compounds used in this study, a tetrahydroquinoline derivative, 2-((1,2,3,4-tetrahydroquinolin-1-yl)(4-methoxyphenyl)methyl)phenol, was found to exhibit strong inhibitory response with IC₅₀ of 50.5 ± 3.8 μM, and therefore can be a potential chemotherapeutic agent. Further experiments revealed that this compound induces cell death by apoptosis and also act as a migration inhibitor. Analysis of the mitochondrial calcium following treatment with the compound on U2OS cells showed a significant reduction in the level of mitochondrial calcium concentration suggesting a mitochondrial calcium-independent mechanism in triggering apoptosis. Treatment of HEK293 cells with the compound confirmed the cytotoxic effects of the compound, however, an increase in the level of mitochondrial calcium was observed. Moreover, the caspase 3/7 mediated cell death was also observed in both cell types. Overall, the study suggests that the derivatives of this compound can be used for development of new therapeutics for osteosarcoma and other cancers.

General information

Publication status: Published

MoE 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

Contributors: Karjalainen, A., Doan, P., Sandberg, O., Chandraseelan, J. G., Yli-Harja, O., R. Candeias, N., Kandhavelu, M.

Pages: 1710-1720

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Anti-Cancer Agents in Medicinal Chemistry

Volume: 17

Issue number: 12

ISSN (Print): 1871-5206

Ratings:

Scopus rating (2017): CiteScore 2.16 SJR 0.674 SNIP 0.687

Original language: English

DOIs:

10.2174/1871520617666170327142027

Bibliographical note

INT=tut-bmt,"Karjalainen, Anzhelika"

INT=tut-bmt,"Sandberg, Ossi"

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

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

A new organic–inorganic hybrid material of formula $(C_{10}H_{15}N_2)_7 Sb_2Cl_{10} Sb_2Cl_9 (SbCl_5)_2 SbCl_4 \cdot 2Cl \cdot 7H_2O$ was synthesized and characterized by an X-ray diffraction analysis. It crystallizes in the triclinic system with the P (Formula presented.) space group and the following unit cell parameters $a = 11.8127(3) \text{ \AA}$, $b = 15.7557(4) \text{ \AA}$, $c = 35.4511(8) \text{ \AA}$, $\alpha = 89.409(1)^\circ$, $\beta = 84.04(1)^\circ$, $\gamma = 71.116(1)^\circ$, $Z = 2$ and $V = 6207.3(3) \text{ \AA}^3$. The examination of the structure shows that the two dimensional frameworks are produced by O–H...Cl, N–H...Cl and N–H...O hydrogen bonding. In addition, the most important features of crystal packing and intermolecular interactions in the title complex were quantified via Hirshfeld surface analysis. Differential scanning calorimetry has revealed a dehydration phenomenon at around 348 K. The investigation of the antioxidant activity of the title compound was carried out using the 2,2-diphenyl-1-picrylhydrazyl and ferrous iron chelating methods.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Carthage University

Contributors: Lahbib, I., Valkonen, A., Rzaigui, M., Smirani, W.

Number of pages: 14

Pages: 2239–2252

Publication date: 2017

Peer-reviewed: Yes

Early online date: 29 Apr 2017

Publication information

Journal: Journal of Cluster Science

Volume: 28

Issue number: 4

ISSN (Print): 1040-7278

Ratings:

Scopus rating (2017): CiteScore 1.4 SJR 0.332 SNIP 0.455

Original language: English

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

Keywords: Antimonates, Antioxidant activity, Crystal structure, Hirshfeld surface, Photoluminescence

DOIs:

10.1007/s10876-017-1217-x

Source: Scopus

Source ID: 85018336645

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

The impact of long-term water level draw-down on microbial biomass: A comparative study from two peatland sites with different nutrient status

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, University of Jyväskylä, University of Eastern Finland

Contributors: Mpamah, P. A., Taipale, S., Rissanen, A. J., Biasi, C., Nykänen, H. K.

Number of pages: 10

Pages: 59-68
Publication date: 2017
Peer-reviewed: Yes

Publication information

Journal: EUROPEAN JOURNAL OF SOIL BIOLOGY

Volume: 80

ISSN (Print): 1164-5563

Ratings:

Scopus rating (2017): CiteScore 2.68 SJR 0.886 SNIP 1.132

Original language: English

Electronic versions:

the_impact_of_long_term_water_2017. Embargo ended: 2/05/19

DOIs:

10.1016/j.ejsobi.2017.04.005

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201910234039>

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

Vapor Phase Fabrication of Nanoheterostructures Based on ZnO for Photoelectrochemical Water Splitting

Nanoheterostructures based on metal oxide semiconductors have emerged as promising materials for the conversion of sunlight into chemical energy. In the present study, ZnO-based nanocomposites have been developed by a hybrid vapor phase route, consisting in the chemical vapor deposition of ZnO systems on fluorine-doped tin oxide substrates, followed by the functionalization with Fe₂O₃ or WO₃ via radio frequency-sputtering. The target systems are subjected to thermal treatment in air both prior and after sputtering, and their properties, including structure, chemical composition, morphology, and optical absorption, are investigated by a variety of characterization methods. The obtained results evidence the formation of highly porous ZnO nanocrystal arrays, conformally covered by an ultrathin Fe₂O₃ or WO₃ overlayer. Photocurrent density measurements for solar-triggered water splitting reveal in both cases a performance improvement with respect to bare zinc oxide, that is mainly traced back to an enhanced separation of photogenerated charge carriers thanks to the intimate contact between the two oxides. This achievement can be regarded as a valuable result in view of future optimization of similar nanoheterostructured photoanodes.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Universita degli Studi di Padova, Italy, Universiteit Antwerpen

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

Publication date: 2017

Peer-reviewed: Yes

Publication information

Journal: Advanced Materials Interfaces

Volume: 4

Issue number: 18

Article number: 1700161

ISSN (Print): 2196-7350

Ratings:

Scopus rating (2017): CiteScore 4.13 SJR 1.796 SNIP 0.839

Original language: English

ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering

Keywords: FeO, Nanoheterostructures, Water splitting, WO, ZnO

DOIs:

10.1002/admi.201700161

Source: Scopus

Source ID: 85019578018

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

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

Abstract Block copolymers microphase separate into a variety of bulk morphologies that serve as scaffolds, templates, masks and source for polymeric nano-particles. While supramolecular additives are common to complex within diblock copolymers to modify the morphology, the subtle effects of complexation on ABC triblock terpolymer morphologies are less explored. Here, we describe the manipulation of polystyrene-block-poly(4-vinylpyridine)-block-poly(tert-butyl methacrylate) (PS-b-P4VP-b-PT or S4VT) triblock terpolymer bulk morphologies through supramolecular complexation

with rod-like 4-(4-pentylphenylazo)phenol (5PAP). The 5PAP molecule hydrogen bonds by phenolic groups to the 4VP repeating units and with increasing molar fraction of 5PAP, initially observed P4VP cylinders flatten into elliptic cylinders until a morphological transition occurs into a third (P4VP/5PAP) lamella. At sufficient 5PAP loadings, the cylinders can even merge into a perforated P4VP lamella located at the PS/PT interface. Quaternization of the P4VP phase and re-dispersion in organic solvent allows liberating S4VT Janus nanostructures from the bulk, including Janus cylinders, nanoporous Janus membranes and Janus sheets. The manipulation of "sandwiched" microphases through supramolecular binding motifs could allow the preparation of previously inaccessible terpolymer bulk morphologies and, in case of cross-linkable phases, lead to a larger library of Janus nano-objects.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Hiekkataipale, P., Löbbling, T. I., Poutanen, M., Primägi, A., Abetz, V., Ikkala, O., Gröschel, A. H.

Pages: 456-465

Publication date: 19 Dec 2016

Peer-reviewed: Yes

Publication information

Journal: Polymer

Volume: 107

ISSN (Print): 0032-3861

Ratings:

Scopus rating (2016): CiteScore 3.77 SJR 1.207 SNIP 1.253

Original language: English

Keywords: Triblock terpolymers, Self-assembly, Bulk morphologies, Janus nanostructures, Perforated lamellae, Supramolecular chemistry

DOIs:

10.1016/j.polymer.2016.05.076

Source: RIS

Source ID: urn:3E8044B61832565B2BF0DA97188BBC1C

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

Influence of torrefaction pretreatment on the pyrolysis of Eucalyptus clone: A study on kinetics, reaction mechanism and heat flow

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Jyväskylän yliopisto

Contributors: Doddapaneni, T. R. K. C., Konttinen, J., Hukka, T. I., Moilanen, A.

Number of pages: 11

Pages: 244-254

Publication date: 15 Dec 2016

Peer-reviewed: Yes

Publication information

Journal: Industrial Crops and Products

Volume: 92

ISSN (Print): 0926-6690

Ratings:

Scopus rating (2016): CiteScore 3.78 SJR 1.06 SNIP 1.709

Original language: English

ASJC Scopus subject areas: Agronomy and Crop Science

Keywords: Eucalyptus clone torrefaction, Non-isothermal kinetics, Pyrolysis, Reaction mechanism, Torrefied biomass, Torrefied biomass pyrolysis

DOIs:

10.1016/j.indcrop.2016.08.013

Source: Scopus

Source ID: 84981318598

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

Remarkable Dependence of Exciplex Decay Rate on Through-Space Separation Distance Between Porphyrin and Chemically Converted Graphene

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Umeyama, T., Hanaoka, T., Baek, J., Higashino, T., Abou-Chahine, F., Tkachenko, N., Imahori, H.

Pages: 28337-28344

Publication date: 7 Dec 2016

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 120

Issue number: 49

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.189

Original language: English

DOIs:

10.1021/acs.jpcc.6b10325

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

The effect of low-temperature pretreatment on the solubilization and biomethane potential of microalgae biomass grown in synthetic and wastewater media

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Kinnunen, V., Rintala, J.

Number of pages: 7
Pages: 78-84
Publication date: 1 Dec 2016
Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 221

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2016): CiteScore 5.94 SJR 2.215 SNIP 1.932

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

Keywords: Anaerobic digestion, Digestate, Microalgae, Pulp and paper industry, Wastewater

DOIs:

10.1016/j.biortech.2016.09.017

Source: Scopus

Source ID: 84988027316

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

Anaerobic digestion of microalgae and pulp and paper biosludge

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

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

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

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

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

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Department of Chemistry and Bioengineering

Contributors: Kinnunen, V.

Number of pages: 67

Publication date: 25 Nov 2016

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-3853-7

ISBN (Electronic): 978-952-15-3876-6
Original language: English

Publication series

Name: Tampere University of Technology. Publication

Volume: 1434

ISSN (Print): 1459-2045

Electronic versions:

kinnunen 1434

URLs:

<http://urn.fi/URN:ISBN:978-952-15-3876-6>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Efficient Light-Induced Phase Transitions in Halogen-Bonded Liquid Crystals

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Fernandez-Palacio, F., Poutanen, M., Saccone, M., Siiskonen, A., Terraneo, G., Resnati, G., Ikkala, O., Metrangolo, P., Priimägi, A.

Number of pages: 8

Pages: 8314-8321

Publication date: 22 Nov 2016

Peer-reviewed: Yes

Publication information

Journal: Chemistry of Materials

Volume: 28

Issue number: 22

ISSN (Print): 0897-4756

Ratings:

Scopus rating (2016): CiteScore 8.89 SJR 4.136 SNIP 1.883

Original language: English

Electronic versions:

8BC5E230-7E65-4338-974C-D04123C8FABB

DOIs:

[10.1021/acs.chemmater.6b03460](http://dx.doi.org/10.1021/acs.chemmater.6b03460)

URLs:

<http://urn.fi/URN:NBN:fi:tty-201901111079>

Source: PubMed

Source ID: 27917024

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

Magnesium aminoclay enhances lipid production of mixotrophic *Chlorella* sp. KR-1 while reducing bacterial populations

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

(to ~410 mg FAME/L/d) compared with the untreated control.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Chungnam National University, Korea Institute of Energy Research, Gachon University

Contributors: Kim, B., Praveenkumar, R., Lee, J., Nam, B., Kim, D. M., Lee, K., Lee, Y. C., Oh, Y. K.

Number of pages: 6

Pages: 608-613

Publication date: 1 Nov 2016

Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 219

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2016): CiteScore 5.94 SJR 2.215 SNIP 1.932

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

Keywords: Aminoclay, Bacteria, Chlorella, Lipid, Mixotrophic culture

DOIs:

10.1016/j.biortech.2016.08.034

Source: Scopus

Source ID: 84982219447

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

Mild pressure induces rapid accumulation of neutral lipid (triacylglycerol) in *Chlorella* spp.

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Chungnam National University, Korea Institute of Energy Research

Contributors: Ramasamy, P., Kim, B., Lee, J., Vijayan, D., Lee, K., Nam, B., Jeon, S. G., Kim, D. M., Oh, Y. K.

Number of pages: 5

Pages: 661-665

Publication date: 1 Nov 2016

Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 220

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2016): CiteScore 5.94 SJR 2.215 SNIP 1.932

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

Keywords: Induction, Microalgae, Neutral lipid, Pressure stress, Triacylglycerol

DOIs:

10.1016/j.biortech.2016.09.025

Source: Scopus

Source ID: 84989931657

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

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 lixivants.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, UNESCO-IHE Institute for Water Education, Université Paris-Est

Contributors: Işildar, A., van de Vossen, J., Rene, E. R., van Hullebusch, E. D., Lens, P. N. L.

Pages: 149–157

Publication date: Nov 2016

Peer-reviewed: Yes

Publication information

Journal: Waste Management

Volume: 57

ISSN (Print): 0956-053X

Ratings:

Scopus rating (2016): CiteScore 4 SJR 1.407 SNIP 2.177

Original language: English

ASJC Scopus subject areas: Waste Management and Disposal

Keywords: Bioleaching, Copper, Gold, PCB, Secondary resource, Two-step, WEEE

DOIs:

10.1016/j.wasman.2015.11.033

Source: Scopus

Source ID: 84950236733

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

Recombinant antibodies for specific detection of clostridial [Fe-Fe] hydrogenases

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Univ Turku, University of Turku, Dept Biotechnol

Contributors: Mangayil, R., Karp, M., Lamminmäki, U., Santala, V.

Number of pages: 9

Publication date: 27 Oct 2016

Peer-reviewed: Yes

Publication information

Journal: Scientific Reports

Volume: 6

Article number: 36034

ISSN (Print): 2045-2322

Ratings:

Scopus rating (2016): CiteScore 4.63 SJR 1.692 SNIP 1.364

Original language: English

DOIs:

10.1038/srep36034

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

Elimination of arsenic-containing emissions from gasification of chromated copper arsenate wood

The behavior of arsenic in chromated copper arsenate containing wood during gasification was modeled using thermodynamic equilibrium calculations. The results of the model were validated using bench-scale gasification tests. It is shown that over 99.6% of arsenic can be removed from the product gas by a hot filter when the gas is cooled below the predicted condensation temperature.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Energy Technology and Thermal Process Chemistry, Gasification Technologies Inc., Gas Technology Institute

Contributors: Kramb, J., Konttinen, J., Backman, R., Salo, K., Roberts, M.

Number of pages: 6

Pages: 319-324

Publication date: 1 Oct 2016

Peer-reviewed: Yes

Publication information

Journal: Fuel

Volume: 181

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2016): CiteScore 4.9 SJR 1.736 SNIP 2.185

Original language: English

ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

Keywords: Arsenic, CCA wood, Equilibrium modeling, Gasification

DOIs:

10.1016/j.fuel.2016.04.109

Source: Scopus

Source ID: 84965081806

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

Impacts of sulfur source and temperature on sulfur-driven denitrification by pure and mixed cultures of Thiobacillus

This study investigated the impacts of thiosulfate (S₂O₃²⁻) as well as chemically synthesized and biogenic elemental sulfur (S₀) on the rates of sulfur-based denitrification in batch bioassays. The use of S₂O₃²⁻ resulted in the highest denitrification rate (52.5 mg N-NO₃⁻/L d), whereas up to 10 times slower nitrate (NO₃⁻) removal was observed with S₀. Biogenic S₀ was tested for the first time as electron donor for chemolithotrophic denitrification, resulting in 1.7-fold faster NO₃⁻ removal than that achieved with chemically synthesized S₀. The effects of increasing concentrations of S₂O₃²⁻ and chemically synthesized S₀ on denitrification were evaluated testing three different sulfur-to-nitrogen (S/N) molar ratios (1.8, 3.5 and 5.1) on a pure culture of Thiobacillus denitrificans and a mixotrophic enrichment dominated by Thiobacillus thioautotrophicus. S₂O₃²⁻ concentrations exceeding 2.2 g/L inhibited the activity of T. denitrificans, whereas a stimulatory effect was observed on mixotrophic denitrification. The increase in S₀ concentration slightly enhanced denitrification by both microbial cultures due to the low solubility of chemically synthesized S₀. The temperature dependence of the thiosulfate-driven denitrification by T. denitrificans was investigated to further optimize the process and modeled by the Arrhenius equation with an apparent activation energy E_a of 76.6 kJ/mol and a temperature coefficient Q₁₀ of 3.0.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, University of Cassino and Southern Lazio, Department of Civil and Mechanical Engineering

Contributors: Di Capua, F., Ahoranta, S. H., Papirio, S., Lens, P. N., Esposito, G.
Pages: 1576-1584
Publication date: 1 Oct 2016
Peer-reviewed: Yes

Publication information

Journal: Process Biochemistry
Volume: 51
Issue number: 10
ISSN (Print): 1359-5113
Ratings:
Scopus rating (2016): CiteScore 2.87 SJR 0.825 SNIP 1.087
Original language: English
DOIs:
10.1016/j.procbio.2016.06.010

Bibliographical note

EXT="Papirio, Stefano"
Research output: Contribution to journal > Article > Scientific > peer-review

Fossil Feedstock-free Preparation of Hydroquinone

General information

Publication status: Published
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry
Contributors: Rafael Candeias, N., Assoah, B.
Publication date: 23 Sep 2016
Peer-reviewed: Unknown
Event: Paper presented at 3rd Ibero-American Symposium of Organic Chemistry, Porto, Portugal.
Research output: Other conference contribution > Paper, poster or abstract > Scientific

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

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

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

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

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

General information

Publication status: Published
MoE publication type: G5 Doctoral dissertation (article)
Organisations: Department of Chemistry and Bioengineering
Contributors: Tampio, E.
Number of pages: 75
Publication date: 10 Sep 2016

Publication information

Publisher: Tampere University of Technology
ISBN (Print): 978-952-15-3792-9
ISBN (Electronic): 978-952-15-3798-1
Original language: English

Publication series

Name: Tampere University of Technology. Publication
Volume: 1405
ISSN (Print): 1459-2045
Electronic versions:
Tampio 1405
URLs:
<http://urn.fi/URN:ISBN:978-952-15-3798-1>
Research output: Book/Report > Doctoral thesis > Collection of Articles

Photoinduced hole transfer in QD–phthalocyanine hybrids

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

General information

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

Publication information

Journal: Physical Chemistry Chemical Physics
Volume: 18
Issue number: 39
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.117
Original language: English
Electronic versions:
Arvani et al. - Photoinduced hole transfer in QD–phthalocyanine hybrids . Embargo ended: 5/09/17
DOIs:
10.1039/c6cp04374g
URLs:
<http://urn.fi/URN:NBN:fi:tyy-201610044583> . Embargo ended: 5/09/17

Additional files:

Supporting Information (SI)

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

Long-term stability of bioelectricity generation coupled with tetrathionate disproportionation

To prevent uncontrolled acidification of the environment, reduced inorganic sulfur compounds (RISCs) can be bioelectrochemically removed from water streams. The long-term stability of bioelectricity production from tetrathionate ($S_4O_6^{2-}$) was studied in highly acidic conditions (pH <2.5) in two-chamber fed-batch microbial fuel cells (MFCs). The maximum current density was improved from previously reported 80 mA m^{-2} to 225 mA m^{-2} by optimizing the external resistance. The observed reaction products of tetrathionate disproportionation were sulfate and elemental sulfur. In long-term run, stable electricity production was obtained for over 700 days with the average current density of 150 mA m^{-2} . The internal resistance of the MFC decreased over time and no biofouling was observed. This study shows that tetrathionate is an efficient substrate also for long-term bioelectricity production.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Sulonen, M. L. K., Lakaniemi, A. M., Kokko, M. E., Puhakka, J. A.

Number of pages: 7

Pages: 876-882

Publication date: 1 Sep 2016

Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 216

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2016): CiteScore 5.94 SJR 2.215 SNIP 1.932

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

Keywords: Acidophile, Disproportionation, Long-term stability, Microbial fuel cell, Tetrathionate

DOIs:

10.1016/j.biortech.2016.06.024

Source: Scopus

Source ID: 8497477755

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

Selenium: environmental significance, pollution, and biological treatment technologies

Selenium is an essential trace element needed for all living organisms. Despite its essentiality, selenium is a potential toxic element to natural ecosystems due to its bioaccumulation potential. Though selenium is found naturally in the earth's crust, especially in carbonate rocks and volcanic and sedimentary soils, about 40% of the selenium emissions to atmospheric and aquatic environments are caused by various industrial activities such as mining-related operations. In recent years, advances in water quality and pollution monitoring have shown that selenium is a contaminant of potential environmental concern. This has practical implications on industry to achieve the stringent selenium regulatory discharge limit of $5 \mu\text{g Se L}^{-1}$ for selenium containing wastewaters set by the United States Environmental Protection Agency. Over the last few decades, various technologies have been developed for the treatment of selenium-containing wastewaters. Biological selenium reduction has emerged as the leading technology for removing selenium from wastewaters since it offers a cheaper alternative compared to physico-chemical treatments and is suitable for treating dilute and variable selenium-laden wastewaters. Moreover, biological treatment has the advantage of forming elemental selenium nanospheres which exhibit unique optical and spectral properties for various industrial applications, i.e. medical, electrical, and manufacturing processes. However, despite the advances in biotechnology employing selenium reduction, there are still several challenges, particularly in achieving stringent discharge limits, the long-term stability of biogenic selenium and predicting the fate of bio-reduced selenium in the environment. This review highlights the significance of selenium in the environment, health, and industry and biotechnological advances made in the treatment of selenium contaminated wastewaters. The challenges and future perspectives are overviewed considering recent biotechnological advances in the management of these selenium-laden wastewaters.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Department of Chemistry and Bioengineering, UNESCO-IHE Institute for Water Education, Bhabha Atomic Research Centre, UPEM

Contributors: Tan, L. C., Nancharaiah, Y. V., van Hullebusch, E. D., Lens, P. N. L.
Number of pages: 22
Pages: 886-907
Publication date: 1 Sep 2016
Peer-reviewed: Yes

Publication information

Journal: Biotechnology Advances
Volume: 34
Issue number: 5
ISSN (Print): 0734-9750
Ratings:

Scopus rating (2016): CiteScore 11.05 SJR 2.747 SNIP 3.195

Original language: English

ASJC Scopus subject areas: Biotechnology

Keywords: Bioreactors, Bioremediation, Selenium bioreduction, Selenium environmental impact, Selenium nanoparticles, Selenium pollution, Selenium recovery, Selenium wastewaters

DOIs:

10.1016/j.biotechadv.2016.05.005

Source: Scopus

Source ID: 84992046700

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

Vesi-insinöörit arvojen välittäjinä: Infrastruktuurien hallinta muodostaa kivijalan kestäväälle tulevaisuudelle

General information

Publication status: Published
MoE publication type: D1 Article in a trade journal
Organisations: Department of Chemistry and Bioengineering
Contributors: Heino, O.
Number of pages: 2
Pages: 14-15
Publication date: 1 Sep 2016
Peer-reviewed: Unknown

Publication information

Journal: Kuntatekniikka
Volume: 75
Issue number: 5
ISSN (Print): 1238-125X
Original language: Finnish
Research output: Contribution to journal › Article › Professional

Higher Cd adsorption on biogenic elemental selenium nanoparticles

Cadmium (Cd) is a carcinogenic metal contaminating the environment and ending up in wastewaters. There is therefore a need for improved methods to remove Cd by adsorption. Biogenic elemental selenium nanoparticles have been shown to adsorb Zn, Cu and Hg, but these nanoparticles have not been tested for Cd removal. Here we studied the time-dependency and adsorption isotherm of Cd onto biogenic elemental selenium nanoparticles using batch adsorption experiments. We measured ζ -potential values to assess the stability of nanoparticles loaded with Cd. Results show that the maximum Cd adsorption capacity amounts to 176.8 mg of Cd adsorbed per g of biogenic elemental selenium nanoparticles. The ζ -potential of Cd-loaded nanoparticles became less negative from -32.7 to -11.7 mV when exposing nanoparticles to an initial Cd concentration of 92.7 mg L^{-1} . This is the first study that demonstrates the high Cd uptake capacity of biogenic elemental selenium nanoparticles, of 176.8 mg g^{-1} , when compared to that of traditional adsorbents such as carboxyl-functionalized activated carbon, of 13.5 mg g^{-1} . An additional benefit is the easy solid-liquid separation by gravity settling due to coagulation of Cd-loaded biogenic elemental selenium nanoparticles.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Institute for Water Education, UNESCO-IHE Institute for Water Education, Helmholtz-Zentrum Dresden-Rossendorf, Laboratoire Géomatériaux et Environnement (EA 4508)
Contributors: Jain, R., Dominic, D., Jordan, N., Rene, E. R., Weiss, S., van Hullebusch, E. D., Hübner, R., Lens, P. N. L.
Number of pages: 6

Pages: 381–386
Publication date: Sep 2016
Peer-reviewed: Yes

Publication information

Journal: ENVIRONMENTAL CHEMISTRY LETTERS

Volume: 14

Issue number: 3

ISSN (Print): 1610-3653

Ratings:

Scopus rating (2016): CiteScore 3.7 SJR 1.05 SNIP 1.604

Original language: English

ASJC Scopus subject areas: Environmental Chemistry

Keywords: Adsorption isotherm, Cd, Intraparticle diffusion, Pseudo-second order, Selenium nanoparticles, ζ -Potential

DOIs:

10.1007/s10311-016-0560-8

Source: Scopus

Source ID: 84966447038

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

Multicomponent Petasis-borono Mannich Preparation of Alkylaminophenols and Antimicrobial Activity Studies

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Neto, Í., Andrade, J., Pinto Reis, C., Salunke, J. K., Priimagi, A., R. Candeias, N., Rijo, P.

Pages: 2015-2023

Publication date: Sep 2016

Peer-reviewed: Yes

Early online date: 2016

Publication information

Journal: CHEMMEDCHEM

Volume: 11

Issue number: 18

ISSN (Print): 1860-7179

Ratings:

Scopus rating (2016): CiteScore 3.11 SJR 1.156 SNIP 0.925

Original language: English

Electronic versions:

chemmedchem. Embargo ended: 26/07/17

DOIs:

10.1002/cmdc.201600244

URLs:

<http://urn.fi/URN:NBN:fi:tty-201707281635>. Embargo ended: 26/07/17

Bibliographical note

Kysytty pre-printtiä (voi laittaa Restricted) HO/12.8.2016

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

Methodological approaches for fractionation and speciation to estimate trace element bioavailability in engineered anaerobic digestion ecosystems: An overview

Optimal supply of trace elements (TE) is a prerequisite for microbial growth and activity in anaerobic digestion (AD) bioprocesses. However, the required concentrations and ratios of essential TE for AD biotechnologies strongly depend on prevailing operating conditions as well as feedstock composition. Furthermore, TE in AD bioreactors undergo complex

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Université Paris-Est, Groupement de Recherche Eau Sol Environnement, Wageningen University and Research Centre, Linköping University, Campus Universidad Pablo de Olavide, Federal Institute of Hydrology, University of Birmingham, Université Reims Champagne Ardenne, Swedish University of Agricultural Sciences, Univ Porto, Universidade do Porto, Fac Med, Dept Med Imaging, Centro Ricerche Produzioni Animali (CRPA), ENEA/CREATE/Università Degli Studi Napoli Federico II, University of Cassino and Southern Lazio, BIOENERGY 2020 GmbH, Natl. University of Ireland, Galway

Contributors: van Hullebusch, E. D., Guibaud, G., Simon, S., Lenz, M., Yekta, S. S., Feroso, F. G., Jain, R., Duester, L., Roussel, J., Guillon, E., Skyllberg, U., Almeida, C. M. R., Pechaud, Y., Garuti, M., Frunzo, L., Esposito, G., Carliell-Marquet, C., Ortner, M., Collins, G.

Number of pages: 43

Pages: 1324-1366

Publication date: 17 Aug 2016

Peer-reviewed: Yes

Publication information

Journal: Critical Reviews in Environmental Science and Technology

Volume: 46

Issue number: 16

ISSN (Print): 1064-3389

Ratings:

Scopus rating (2016): CiteScore 5.58 SJR 1.75 SNIP 2.168

Original language: English

ASJC Scopus subject areas: Environmental Engineering, Water Science and Technology, Waste Management and Disposal, Pollution

Keywords: Anaerobic digestion, analytical methods, bioavailability, fractionation, speciation, trace elements

DOIs:

10.1080/10643389.2016.1235943

Source: Scopus

Source ID: 84991813353

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

Structural photoactivation of a full-length bacterial phytochrome

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, University of Jyväskylä

Contributors: Björling, A., Berntsson, O., Lehtivuori, H., Takala, H., Hughes, A. J., Panman, M., Hoernke, M., Niebling, S., Henry, L., Henning, R., Kosheleva, I., Chukharev, V., Tkachenko, N. V., Menzel, A., Newby, G., Khakhulin, D., Wulff, M., A. Ihalainen, J., Westenhoff, S.

Number of pages: 9

Publication date: 12 Aug 2016

Peer-reviewed: Yes

Publication information

Journal: Science Advances

Volume: 2

Issue number: 8

Article number: e1600920

ISSN (Print): 2375-2548

Ratings:

Scopus rating (2016): SJR 4.8 SNIP 2.93

Original language: English

Electronic versions:

e1600920.full

DOIs:

10.1126/sciadv.1600920

URLs:

<http://urn.fi/URN:NBN:fi:tty-201609274552>

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

The red, purple and blue modifications of polymeric unsymmetrical hydroxyalkadiynyl-N-arylcarbamate derivatives in Langmuir-Schaefer films

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, A. M.

Prokhorov General Physics Institute, Russian Academy of Sciences, Åbo Akademi University, St. Petersburg State

University, NRC Kurchatov Institute, Russian Acad Sci, Russian Academy of Sciences, Kotelnikov Inst Radio Engrn & Elect

Contributors: Alekseev, A., Ihalainen, P., Ivanov, A., Domnin, I., Klechkovskaya, V., Orekhov, A., Lemmetyinen, H.,

Vuorimaa-Laukkanen, E., Peltonen, J., Vyaz'min, S.

Number of pages: 9

Pages: 463-471

Publication date: 1 Aug 2016

Peer-reviewed: Yes

Publication information

Journal: Thin Solid Films

Volume: 612

ISSN (Print): 0040-6090

Ratings:

Scopus rating (2016): CiteScore 1.83 SJR 0.639 SNIP 0.866

Original language: English

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

Keywords: Langmuir monolayer, Langmuir-Schaefer film, Polydiacetylenes with urethane group, Solid topochemical photopolymerization

DOIs:

Bibliographical note

EXT="Alekseev, Alexander"

Source: Scopus

Source ID: 84976884439

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

Characterization and Potential Use of Source-Separated Urine

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

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

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

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

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

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

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

Contributors: Jaatinen, S.

Number of pages: 95

Publication date: 1 Jul 2016

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-3765-3

ISBN (Electronic): 978-952-15-3781-3

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Volume: 1391

ISSN (Print): 1459-2045

Electronic versions:

Jaatinen 1391

URLs:

<http://urn.fi/URN:ISBN:978-952-15-3781-3>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Liquid fertilizer products from anaerobic digestion of food waste: Mass, nutrient and energy balance of four digestate liquid treatment systems

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Natural Resources Institute Finland (Luke)

Contributors: Tampio, E., Marttinen, S., Rintala, J.

Number of pages: 11

Pages: 22–32

Publication date: Jul 2016

Peer-reviewed: Yes

Publication information

Journal: Journal of Cleaner Production

Volume: 125

ISSN (Print): 0959-6526

Ratings:

Scopus rating (2016): CiteScore 5.83 SJR 1.659 SNIP 2.53

Original language: English

ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Renewable Energy, Sustainability and the Environment, Environmental Science(all), Strategy and Management

Keywords: Anaerobic digestion, Digestate liquid treatment, Evaporation, Food waste, Reverse osmosis, Stripping
DOIs:

10.1016/j.jclepro.2016.03.127

Source: Scopus

Source ID: 84963538041

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

Structurally Controlled Dynamics in Azobenzene-Based Supramolecular Self-Assemblies in Solid State

Light-responsive supramolecular self-assemblies exhibit interplay between order and dynamics of the self-assembling motifs, through which the thermal isomerization rate of azobenzene chromophores can be tuned by orders of magnitude. By using supramolecular complexes of 4-(4-alkylphenylazo)phenols hydrogen-bonded to poly(4-vinylpyridine) as model systems, we demonstrate that the thermal isomerization rate of the hydroxyazobenzene derivatives increases 5700-fold when the material undergoes a transformation from a disordered, low-azobenzene-concentration state to a high-concentration state exhibiting lamellar, smectic-like self-assembly. Drastically smaller thermal isomerization rates are observed in disordered structures. This allows us to attribute the change to a combination of increased number density of the hydroxyazobenzenes inducing plasticization, and cooperativity created by the chromophore-chromophore interactions through self-assembled molecular order and alignment. Our results pinpoint the importance of molecular self-assembly and intermolecular interactions in modifying the dynamics in supramolecular complexes in a controlled manner. We

foresee this to be important in light-controlled dynamic materials.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Aalto University

Contributors: Poutanen, M., Ikkala, O., Priimägi, A.

Number of pages: 7

Pages: 4095-4101

Publication date: 14 Jun 2016

Peer-reviewed: Yes

Publication information

Journal: Macromolecules

Volume: 49

Issue number: 11

ISSN (Print): 0024-9297

Ratings:

Scopus rating (2016): CiteScore 5.76 SJR 2.564 SNIP 1.483

Original language: English

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

DOIs:

10.1021/acs.macromol.6b00562

Source: Scopus

Source ID: 84975044511

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

Indocyanine Green-Loaded Liposomes for Light-Triggered Drug Release

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Department of Chemistry and Bioengineering

Contributors: Lajunen, T., Kontturi, L., Viitala, L., Manna, M., Cramariuc, O., Róg, T., Bunker, A., Laaksonen, T., Viitala, T., Murtomäki, L., Urtti, A.

Number of pages: 13

Pages: 2095-2107

Publication date: 6 Jun 2016

Peer-reviewed: Yes

Publication information

Journal: Molecular Pharmaceutics

Volume: 13

Issue number: 6

ISSN (Print): 1543-8384

Ratings:

Scopus rating (2016): CiteScore 4.84 SJR 1.538 SNIP 1.216

Original language: English

ASJC Scopus subject areas: Pharmaceutical Science, Molecular Medicine, Drug Discovery

Keywords: indocyanine green, light activation, liposome, macromolecules, molecular dynamics, triggered release

DOIs:

10.1021/acs.molpharmaceut.6b00207

Source: Scopus

Source ID: 84973635764

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

Photoactive ZnO-Organic Nanostructures: Development and Characterization

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

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Hakola, H.

Number of pages: 60

Publication date: 27 May 2016

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-3748-6

ISBN (Electronic): 978-952-15-3759-2

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Volume: 1385

ISSN (Print): 1459-2045

Keywords: Digital hydraulics, Power management, Energy efficiency

Electronic versions:

hakola 1385

URLs:

<http://urn.fi/URN:ISBN:978-952-15-3759-2>

Research output: Book/Report > Doctoral thesis > Collection of Articles

Electronic structure of p-type perylene monoimide-based donor-acceptor dyes on the nickel oxide (100) surface: a DFT approach

A p-type dye-sensitized solar cell, where the dye injects a hole to the semiconductor, could be combined with typical Grätzel cell to create an efficient tandem device. However, the current p-type devices suffer from low efficiency. Here, geometries and electronic structures of four perylenemonoimide-based dyes (1–4) both as free and adsorbed on the NiO (100) semiconductor surface have been investigated to gain better understanding of the p-type devices. In particular, the electronic transitions relevant to charge transfer between the dye and the surface have been identified. Excitations have been evaluated by using the time dependent DFT calculations and the roles of frontier orbitals and band edges in transitions have been assessed. The adsorbed dyes can take either upright or slightly tilted geometries depending on the

structure of the anchoring group and the binding mode of the dye. The adsorption slightly lowers the NiO band gap, from 4.06 eV to 3.90–3.96 eV depending on the surface–adsorbate system, and the band gaps of the dye molecules by 0.1–0.2 eV. Additionally, the adsorption mode of dye 1 moves the LUMO+1 level down by 0.5 eV. The effective mass of the charge carrier holes is significantly smaller at the NiO surface than in the bulk indicating the importance of the surface conductivity. We also found that the potential drop, i.e. the driving force for charge transfer from NiO to dye molecule depends on the adsorption mode of 1.

General information

Publication status: Published

MoE 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.

Contributors: Kontkanen, O., Niskanen, M., Hukka, T., Rantala, T.

Pages: 14382-14389

Publication date: May 2016

Peer-reviewed: Yes

Early online date: 12 May 2016

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 18

Issue number: 21

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.117

Original language: English

DOIs:

10.1039/C6CP02510B

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

Photoexcitation and electron transfer at inorganic–organic interface — a DFT approach

General information

Publication status: Published

Organisations: Department of Physics, Research group: Electronic Structure Theory, Research area: Computational Physics, Department of Chemistry and Bioengineering

Contributors: Niskanen, M. O., Kontkanen, O. V., Hukka, T. I., Rantala, T. T.

Number of pages: 1

Publication date: May 2016

Peer-reviewed: Unknown

Event: Paper presented at Optics and Photonics days, Tampere, Finland.

Research output: [Other conference contribution](#) > [Paper, poster or abstract](#) > [Scientific](#)

Synthesis and biological screening for cytotoxic activity of N-substituted indolines and morpholines

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Signal Processing, Research group: Laboratory of Biosystem Dynamics-LBD, Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Molecular Signaling Lab, Tampere Univ Technol, Tampere University of Technology, Dept Chem & Bioengn

Contributors: Doan, P., Karjalainen, A., Chandraseelan, J. G., Sandberg, O., Yli-Harja, O., Rosholm, T., Franzén, R., R. Candeias, N., Kandhavelu, M.

Pages: 296-303
Publication date: May 2016
Peer-reviewed: Yes

Publication information

Journal: European Journal of Medicinal Chemistry
Volume: 120
ISSN (Print): 0223-5234
Ratings:
Scopus rating (2016): CiteScore 4.35 SJR 1.289 SNIP 1.521
Original language: English
DOIs:
10.1016/j.ejmech.2016.05.024

Bibliographical note

INT=sgn,"Doan, Phuong"
INT=sgn,"Karjalainen, Anzhelika"
INT=sgn,"Sandberg, Ossi"
INT=keb,"Rosholm, Tomi"
Research output: Contribution to journal > Article > Scientific > peer-review

Effect of Hole Transporting Material on Charge Transfer Processes in Zinc Phthalocyanine Sensitized ZnO Nanorods

The photoinduced electron transfer processes were studied for hybrid systems consisting of self-assembled monolayer of zinc phthalocyanine (ZnPc) assembled on ZnO nanorods and a film of organic hole transporting material (HTM) atop. Polythiophene (P3HT) or Spiro-OMeTAD were used as HTM. The study was carried out by ultrafast transient absorption spectroscopy technique with selective excitation of ZnPc at 680 nm or P3HT at 500 nm. Data analysis revealed that photoexcitation of ZnPc in the structure ZnO|ZnPc|P3HT results in a fast (1.8 ps) electron transfer from ZnPc to ZnO, which is followed by a hole transfer from the ZnPc cation to P3HT roughly in 30 ps. However, in the case of ZnO|ZnPc|Spiro-OMeTAD structure, the primary reaction upon excitation of ZnPc is a fast (0.5 ps) hole transfer from ZnPc to Spiro-OMeTAD, and the second step is electron injection from the ZnPc anion to ZnO in roughly 120 ps. Thus, we demonstrate two structurally very similar hybrid architectures that implement two different mechanisms for photoinduced charge separation found in dye-sensitized or in organic solar cells.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Contributors: Hakola, H., Sariola-Leikas, E., Efimov, A., Tkachenko, N. V.
Number of pages: 8
Pages: 7044-7051
Publication date: 21 Apr 2016
Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C
Volume: 120
Issue number: 13
ISSN (Print): 1932-7447
Ratings:
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.189
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)
DOIs:
10.1021/acs.jpcc.6b01583
Source: Scopus
Source ID: 84964529902
Research output: Contribution to journal > Article > Scientific > peer-review

Syntheses, Charge Separation, and Inverted Bulk Heterojunction Solar Cell Application of Phenothiazine-Fullerene Dyads

A series of phenothiazine-fulleropyrrolidine (PTZ-C₆₀) dyads having fullerene either at the C-3 aromatic ring position or at the N-position of phenothiazine macrocycle were newly synthesized and characterized. Photoinduced electron transfer leading to PTZ^{•+}-C₆₀^{•-} charge-separated species was established from studies involving femtosecond transient absorption spectroscopy. Because of the close proximity of the donor and acceptor entities, the C-3 ring substituted PTZ-C₆₀ dyads revealed faster charge separation and charge recombination processes than that observed in the dyad

functionalized through the N-position. Next, inverted organic bulk heterojunction (BHJ) solar cells were constructed using the dyads in place of traditionally used [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) and an additional electron donor material poly(3-hexylthiophene) (P3HT). The performance of the C-3 ring substituted PTZ-C₆₀ dyad having a polyethylene glycol substituent produced a power conversion efficiency of 3.5% under inverted bulk heterojunction (BHJ) configuration. This was attributed to optimal BHJ morphology between the polymer and the dyad, which was further promoted by the efficient intramolecular charge separation and relatively slow charge recombination promoted by the dyad within the BHJ structure. The present finding demonstrate PTZ-C₆₀ dyads as being good prospective materials for building organic photovoltaic devices.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, University of North Texas, VTT Technical Research Centre of Finland

Contributors: Blanco, G. D., Hiltunen, A. J., Lim, G. N., KC, C. B., Kaunisto, K. M., Vuorinen, T. K., Nesterov, V. N., Lemmetyinen, H. J., D'Souza, F.

Number of pages: 10

Pages: 8481-8490

Publication date: 20 Apr 2016

Peer-reviewed: Yes

Publication information

Journal: ACS Applied Materials and Interfaces

Volume: 8

Issue number: 13

ISSN (Print): 1944-8244

Ratings:

Scopus rating (2016): CiteScore 7.6 SJR 2.561 SNIP 1.536

Original language: English

ASJC Scopus subject areas: Materials Science(all)

Keywords: femtosecond transient spectroscopy, fullerene, inverted bulk heterojunction, organic photovoltaics, phenothiazine, photoinduced electron transfer

DOIs:

10.1021/acsami.6b00561

Bibliographical note

EXT="Vuorinen, Tommi K."

Source: Scopus

Source ID: 84964727703

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

Effect of temperature and concentration of precursors on morphology and photocatalytic activity of zinc oxide thin films prepared by hydrothermal route

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

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Materials Science, Department of Chemistry and Bioengineering, Research group: Ceramic materials, Research group: Surface Engineering, VTT Technical Research Centre of Finland

Contributors: Heinonen, S., Nikkanen, J. P., Hakola, H., Huttunen-Saarivirta, E., Kannisto, M., Hyvärinen, L., Järveläinen, M., Levänen, E.

Publication date: 15 Apr 2016

Host publication information

Title of host publication: 3rd International Conference on Competitive Materials and Technology Processes (IC-CMTP3)

Publication series

Name: IOP Conference Series: Materials Science and Engineering

Volume: 123

ISSN (Print): 1757-8981

ISSN (Electronic): 1757-899X

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

Electronic versions:

heinonen et al 2016

DOIs:

10.1088/1757-899X/123/1/012030

URLs:

<http://urn.fi/URN:NBN:fi:tty-201608154412>

Bibliographical note

JUFOID=76088

Source: Scopus

Source ID: 84977566121

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

Coordination networks incorporating halogen-bond donor sites and azobenzene groups

Two Zn coordination networks, $\{[Zn(1)(Py)_2]_2(2\text{-propanol})\}_n$ (3) and $\{[Zn(1)_2(Bipy)_2](DMF)_2\}_n$ (4), incorporating halogen-bond (XB) donor sites and azobenzene groups have been synthesized and fully characterized. Obtaining 3 and 4 confirms that it is possible to use a ligand wherein its coordination bond acceptor sites and XB donor sites are on the same molecular scaffold (i.e., an aromatic ring) without interfering with each other. We demonstrate that XBs play a fundamental role in the architectures and properties of the obtained coordination networks. In 3, XBs promote the formation of 2D supramolecular layers, which, by overlapping each other, allow the incorporation of 2-propanol as a guest molecule. In 4, XBs support the connection of the layers and are essential to firmly pin DMF solvent molecules through $I\cdots O$ contacts, thus increasing the stability of the solvated systems.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Fernandez-Palacio, F., Saccone, M., Priimägi, A., Terraneo, G., Pilati, T., Metrangolo, P., Resnati, G.

Number of pages: 7

Pages: 2251-2257

Publication date: 7 Apr 2016

Peer-reviewed: Yes

Publication information

Journal: CrystEngComm

Volume: 18

Issue number: 13

ISSN (Print): 1466-8033

Ratings:

Scopus rating (2016): CiteScore 3.37 SJR 1.053 SNIP 0.905

Original language: English

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

DOIs:

10.1039/c6ce00059b

Source: Scopus

Source ID: 84962331348

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

Arsenic removal from acidic solutions with biogenic ferric precipitates

Treatment of acidic solution containing 5 g/L of Fe(II) and 10 mg/L of As(III) was studied in a system consisting of a biological fluidized-bed reactor (FBR) for iron oxidation, and a gravity settler for iron precipitation and separation of the ferric precipitates. At pH 3.0 and FBR retention time of 5.7 h, 96–98% of the added Fe(II) precipitated (99.1% of which was jarosite). The highest iron oxidation and precipitation rates were 1070 and 28 mg/L/h, respectively, and were achieved at pH 3.0. Subsequently, the effect of pH on arsenic removal through sorption and/or co-precipitation was examined by gradually decreasing solution pH from 3.0 to 1.6 (feed pH). At pH 3.0, 2.4 and 1.6, the highest arsenic removal efficiencies obtained were 99.5%, 80.1% and 7.1%, respectively. As the system had ferric precipitates in excess, decreased arsenic

removal was likely due to reduced co-precipitation at $\text{pH} < 2.4$. As(III) was partially oxidized to As(V) in the system. In shake flask experiments, As(V) sorbed onto jarosite better than As(III). Moreover, the sorption capacity of biogenic jarosite was significantly higher than that of synthetic jarosite. The developed bioprocess simultaneously and efficiently removes iron and arsenic from acidic solutions, indicating potential for mining wastewater treatment.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Ahoranta, S. H., Kokko, M. E., Papirio, S., Özkaya, B., Puhakka, J.

Pages: 124-132

Publication date: 5 Apr 2016

Peer-reviewed: Yes

Publication information

Journal: Journal of Hazardous Materials

Volume: 306

ISSN (Print): 0304-3894

Ratings:

Scopus rating (2016): CiteScore 6.31 SJR 1.742 SNIP 2.077

Original language: English

DOIs:

10.1016/j.jhazmat.2015.12.012

Bibliographical note

INT=keb,"Özkaya, Bestamin"

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

Long-Lived Triplet Excited States of Bent-Shaped Pentacene Dimers by Intramolecular Singlet Fission

Intramolecular singlet fission (ISF) is a promising photophysical process to construct more efficient light energy conversion systems as one excited singlet state converts into two excited triplet states. Herein we synthesized and evaluated bent-shaped pentacene dimers as a prototype of ISF to reveal intrinsic characters of triplet states (e.g., lifetimes of triplet excited states). In this study, meta-phenylene-bridged TIPS-pentacene dimer (PcD-3Ph) and 2,2'-bipheynyl bridged TIPS-pentacene dimer (PcD-Biph) were newly synthesized as bent-shaped dimers. In the steady-state spectroscopy, absorption and emission bands of these dimers were fully characterized, suggesting the appropriate degree of electronic coupling between pentacene moieties in these dimers. In addition, the electrochemical measurements were also performed to check the electronic interaction between two pentacene moieties. Whereas the successive two oxidation peaks owing to the delocalization were observed in a directly linked-pentacene dimer (PcD) by a single bond, the cyclic voltammograms in PcD-Biph and PcD-3Ph implied the weaker interaction compared to that of p-phenylene-bridged TIPS-pentacene dimer (PcD-4Ph) and PcD. The femtosecond and nanosecond transient absorption spectra clearly revealed the slower ISF process in bent-shaped pentacene dimers (PcD-Biph and PcD-3Ph), more notably, the slower relaxation of the excited triplet states in PcD-Biph and PcD-3Ph. Namely, the quantum yields of triplet states (Φ_T) by ISF approximately remain constant (ca. 180-200%) in all dimer systems, whereas the lifetimes of the triplet excited states became much longer (up to 360 ns) in PcD-Biph as compared to PcD-4Ph (15 ns). Additionally, the lifetimes of the corresponding triplet states in PcD-Biph and PcD-3Ph were sufficiently affected by solvent viscosity. In particular, the lifetimes of PcD-Biph triplet state in THF/paraffin (1.0 μs) increased up to approximately three times as compared to that in THF (360 ns), whereas those of PcD-4Ph were quite similar in both solvent.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Sakuma, T., Sakai, H., Araki, Y., Mori, T., Wada, T., Tkachenko, N. V., Hasobe, T.

Number of pages: 9

Pages: 1867-1875

Publication date: 31 Mar 2016

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry A

Volume: 120

Issue number: 11

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.971
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry

DOIs:

10.1021/acs.jpca.6b00988

Source: Scopus

Source ID: 84962062610

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

Quenching nematicon fluctuations via photo-stabilization

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Optics, Research group: Nonlinear Optics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Karimi, N., Alberucci, A., Virkki, M., Priimägi, A., Kauranen, M., Assanto, G.

Number of pages: 3

Pages: 2-4

Publication date: 31 Mar 2016

Peer-reviewed: Yes

Publication information

Journal: Photonics Letters of Poland

Volume: 8

Issue number: 1

ISSN (Print): 2080-2242

Ratings:

Scopus rating (2016): CiteScore 0.37 SJR 0.197 SNIP 0.272

Original language: English

Electronic versions:

626-2449-1-PB

DOIs:

10.4302/plp.2016.1.02

URLs:

<http://urn.fi/URN:NBN:fi:tty-201604253877>

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

Agronomic characteristics of five different urban waste digestates

The use of digestate in agriculture is an efficient way to recycle materials and to decrease the use of mineral fertilizers. The agronomic characteristics of the digestates can promote plant growth and soil properties after digestate fertilization but also harmful effects can arise due to digestate quality, e.g. pH, organic matter and heavy metal content. The objective of this study was to evaluate the differences and similarities in agronomic characteristics and the value of five urban waste digestates from different biogas plants treating either food waste, organic fraction of organic solid waste or a mixture of waste-activated sludge and vegetable waste. The digestate agronomic characteristics were studied with chemical analyses and the availability of nutrients was also assessed with growth experiments and soil mineralization tests. All studied urban digestates produced 5-30% higher ryegrass yields compared to a control mineral fertilizer with a similar inorganic nitrogen concentration, while the feedstock source affected the agronomic value. Food waste and organic fraction of municipal solid waste digestates were characterized by high agronomic value due to the availability of nutrients and low heavy metal load. Waste-activated sludge as part of the feedstock mixture, however, increased the heavy metal content and reduced nitrogen availability to the plant, thus reducing the fertilizer value of the digestate.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Natural Resources Institute Finland (Luke)

Contributors: Tampio, E., Salo, T., Rintala, J.

Number of pages: 10

Pages: 293-302
Publication date: 15 Mar 2016
Peer-reviewed: Yes

Publication information

Journal: Journal of Environmental Management

Volume: 169

ISSN (Print): 0301-4797

Ratings:

Scopus rating (2016): CiteScore 4.28 SJR 1.161 SNIP 1.833

Original language: English

ASJC Scopus subject areas: Environmental Engineering, Waste Management and Disposal, Management, Monitoring, Policy and Law

Keywords: Anaerobic digestion, Digestate, Fertilizer value, Heavy metals, Nutrients, Plant growth

DOIs:

10.1016/j.jenvman.2016.01.001

Source: Scopus

Source ID: 84954489661

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

Phenothiazine and carbazole substituted pyrene based electroluminescent organic semiconductors for OLED devices

Due to their easy availability, low cost and opportunities for exploiting reactions of bromo substituents, 1,3,6,8-tetrabromopyrene has attracted major attention in the organic electronics community for designing and constructing novel classes of pyrene based organic semiconducting functional materials. In the present work, 1,3,6,8-tetrabromo pyrene was transformed into the corresponding tetrasubstituted carbazole and phenothiazine derivatives using the classical Suzuki coupling reaction. These newly synthesized materials with a carbazole substituent (PY-CA) and a phenothiazine substituent (PY-PH) were characterised thoroughly and were successfully used as an active light-emitting layer in organic light emitting diodes which resulted in blue and green emission with promising device performance. PY-CA exhibited the maximum brightness at around 2500 cd m^{-2} and the power efficiency of 1.5 lm W^{-1} while that of PY-PH exhibited 2116 cd m^{-2} and 0.45 lm W^{-1} respectively.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Polymer Science and Engineering Division, Council of Scientific and Industrial Research India, University of Hong Kong, CSIRO Energy Centre, National University of Singapore, Queensland University of Technology QUT

Contributors: Salunke, J. K., Wong, F. L., Feron, K., Manzhos, S., Lo, M. F., Shinde, D., Patil, A., Lee, C. S., Roy, V. A. L., Sonar, P., Wadgaonkar, P. P.

Number of pages: 10

Pages: 1009-1018

Publication date: 7 Feb 2016

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry C

Volume: 4

Issue number: 5

ISSN (Print): 2050-7534

Ratings:

Scopus rating (2016): CiteScore 5.14 SJR 1.825 SNIP 1.265

Original language: English

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

DOIs:

10.1039/c5tc03690a

Source: Scopus

Source ID: 84957013671

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

Intrinsic Properties of Two Benzodithiophene-Based Donor-Acceptor Copolymers Used in Organic Solar Cells: A Quantum-Chemical Approach

Conjugated donor-acceptor (D-A) copolymers show tremendous promise as active components in thin-film organic bulk heterojunction solar cells and transistors, as appropriate combinations of D-A units enable regulation of the intrinsic electronic and optical properties of the polymer. Here, the structural, electronic, and optical properties of two D-A copolymers that make use of thieno[3,4-c]pyrrole-4,6-dione as the acceptor and differ by their donor unit—benzo[1,2-

b:4,5-b']dithiophene (BDT) vs the ladder-type heptacyclic benzodi(cyclopentadithiophene)—are compared using density functional theory methods. Our calculations predict some general similarities, although the differences in the donor structures lead also to clear differences. The extended conjugation of the stiff ladder-type donor destabilizes both the highest occupied and lowest unoccupied molecular orbital energies of the ladder copolymer and results in smaller gap energies compared to its smaller counterpart. However, more significant charge transfer nature is predicted for the smaller BDT-based copolymer by natural transition orbitals than for the ladder copolymer. That is, the influence of the acceptor on the copolymer properties is “diluted” to some extent by the already extended conjugation of the ladder-type donor. Thus, the use of stronger acceptor units with the ladder-type donors would benefit the future design of new D–A copolymers.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Department of Physics, Research area: Computational Physics

Contributors: Kastinen, T., Niskanen, M., Risko, C., Cramariuc, O., Hukka, T. I.

Number of pages: 14

Pages: 1051-1064

Publication date: 3 Feb 2016

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry A

Volume: 120

Issue number: 7

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.971

Original language: English

Keywords: density functional theory, DFT, time-dependent DFT, donor-acceptor copolymer, benzodithiophene

DOIs:

10.1021/acs.jpca.5b08465

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

Cell-based bioreporter assay coupled to HPLC micro-fractionation in the evaluation of antimicrobial properties of the basidiomycete fungus *Pycnoporus cinnabarinus*

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, University of Helsinki, Universite de Geneve

Contributors: Järvinen, P., Nybond, S., Marcourt, L., Ferreira Queiroz, E., Wolfender, J. L., Mettälä, A., Karp, M., Vuorela, H., Vuorela, P., Hatakka, A., Tammela, P.

Number of pages: 8

Pages: 1-8

Publication date: 21 Jan 2016

Peer-reviewed: Yes

Publication information

Journal: Pharmaceutical Biology

Volume: 54

Issue number: 6

ISSN (Print): 1388-0209

Ratings:

Scopus rating (2016): CiteScore 1.88 SJR 0.575 SNIP 0.856

Original language: English

ASJC Scopus subject areas: Drug Discovery, Pharmacology, Pharmaceutical Science, Complementary and alternative medicine, Molecular Medicine

Keywords: Bioluminescent bacterial strain, Escherichia coli, Gram-negative bacteria, phlebiarubrone

DOIs:

10.3109/13880209.2015.1103754

Bibliographical note

OA kysytty 2.5.2016 / HO

Source: Scopus

Source ID: 84958036747

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

Advanced Solid Fuel Characterization for Reactivity and Physical Property Comparison

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

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

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

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

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology

Contributors: Tolvanen, H.

Number of pages: 66

Publication date: 19 Jan 2016

Publication information

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-3666-3

ISBN (Electronic): 978-952-15-3674-8

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Publisher: Tampere University of Technology

Volume: 1359

ISSN (Print): 1459-2045

Electronic versions:

tolvanen_1359

URLs:

<http://URN.fi/URN:ISBN:978-952-15-3674-8>

Bibliographical note

Awarding institution: Tampere University of Technology

tolvanen_1359 ok 8.1.2016 KK

Research output: Book/Report > Doctoral thesis > Collection of Articles

Synthesis of Benzothiadiazole Derivatives by Applying C–C Cross-Couplings

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Heiskanen, J. P., Vivo, P., Saari, N. M., Hukka, T. I., Kastinen, T., Kaunisto, K., Lemmetyinen, H. J., Hormi, O. E.

Number of pages: 12

Pages: 1535–1546

Publication date: 15 Jan 2016

Peer-reviewed: Yes

Publication information

Journal: Journal of Organic Chemistry

Volume: 81

Issue number: 4

ISSN (Print): 0022-3263

Ratings:

Scopus rating (2016): CiteScore 4.59 SJR 2.001 SNIP 1.048

Original language: English

DOIs:

[10.1021/acs.joc.5b02689](https://doi.org/10.1021/acs.joc.5b02689)

Bibliographical note

EXT="Heiskanen, Juha P."

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

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 chemo-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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

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

Number of pages: 10

Pages: 191-200

Publication date: 1 Jan 2016

Peer-reviewed: Yes

Early online date: 2015

Publication information

Journal: Plasma Processes and Polymers

Volume: 13

Issue number: 1

ISSN (Print): 1612-8869

Ratings:

Scopus rating (2016): CiteScore 2.69 SJR 0.881 SNIP 0.903

Original language: English

Keywords: Co₃O₄, Fe₂O₃, plasma-enhanced chemical vapor deposition (PE-CVD), sputtering, water splitting

DOIs:

10.1002/ppap.201500106

Source: Bibtext

Source ID: urn:fea2caf64465a2349fed5a21683d16de

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

Charge separation and charge recombination photophysical studies in a series of perylene-C₆₀ linear and cyclic dyads

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Pla, S., Niemi, M., Martí n-Gomis, L., Ferná ndez-La' zaro, F., Lemmetyinen, H., Tkachenko, N. V., Sastre-Santos, A.

Number of pages: 17

Pages: 3589-3606

Publication date: Jan 2016

Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 18

Issue number: 5

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.117

Original language: English

DOIs:

10.1039/c5cp06340j

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Optoelectronics Research Centre, Research group: Surface Science

Contributors: Sariola-Leikas, E., Ahmed, Z., Vivo, P., Ojanperä, A., Lahtonen, K., Saari, J., Valden, M., Lemmetyinen, H., Efimov, A.

Pages: 1501-1510

Publication date: Jan 2016

Peer-reviewed: Yes

Early online date: 3 Dec 2015

Publication information

Journal: Chemistry: A European Journal

Volume: 22

Issue number: 4

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.082

Original language: English

DOIs:

10.1002/chem.201503738

Bibliographical note

ORG=keb,0.5

ORG=orc,0.5

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

Toward the prediction of porous membrane permeability from morphological data

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Universitat Rovira i Virgili

Contributors: Nurra, C., Pitol, L., Carraud, R., Pertuz, S., Puig, D., Garcia, M. A., Salvado, J., Torras, C.

Pages: 118-124

Publication date: Jan 2016

Peer-reviewed: Yes

Publication information

Journal: Polymer Engineering and Science

Volume: 56

Issue number: 1

ISSN (Print): 0032-3888

Ratings:

Scopus rating (2016): CiteScore 1.61 SJR 0.575 SNIP 0.831

Original language: English

DOIs:

10.1002/pen.24198

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

Alginate microgels created by selective coalescence between core drops paired with an ultrathin shell

We report a highly biocompatible and practical protocol to create alginate microgels for bioactive encapsulation. Double-emulsion drops composed of dual cores enclosed by an ultrathin shell are prepared in a capillary microfluidic device, which exhibit selective coalescence between the cores. When the cores are laden with alginate precursors and divalent ions, respectively, coalescence leads to the formation of alginate microgels in the fused core of double-emulsion drops. The microgel can be rapidly released into a continuous water phase by rupturing the liquid shell. This method neither involves any toxic chemical cues for gelation nor long-term exposure to oil, thereby providing highly biocompatible

encapsulation.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Korea Institute of Energy Research, Chungnam National University

Contributors: Lee, T. Y., Ramasamy, P., Oh, Y. K., Lee, K., Kim, S. H.

Number of pages: 7

Pages: 3232-3238

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry B

Volume: 4

Issue number: 19

ISSN (Print): 2050-7518

Ratings:

Scopus rating (2016): CiteScore 4.8 SJR 1.468 SNIP 1.007

Original language: English

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

DOIs:

10.1039/c6tb00580b

Source: Scopus

Source ID: 84970955852

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

Anaerobes in bioelectrochemical systems

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

General information

Publication status: Published

MoE publication type: B2 Part of a book or another research book

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

Contributors: Kokko, M. E., Mäkinen, A. E., Puhakka, J. A.

Number of pages: 29

Pages: 263-292

Publication date: 2016

Host publication information

Title of host publication: Anaerobes in Biotechnology

Publisher: Springer Berlin Heidelberg

ISBN (Print): 978-3-319-45649-2

ISBN (Electronic): 978-3-319-45651-5

Publication series

Name: Advances in Biochemical Engineering/Biotechnology

Publisher: Springer Berlin Heidelberg

Volume: 156

ISSN (Print): 0724-6145

ISSN (Electronic): 1616-8542

DOIs:

10.1007/10_2015_5001

Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific

Are Sphagnum-species potential antagonists for pathogens?

General information

Publication status: Published

MoE publication type: D3 Professional conference proceedings

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Natural Resources Institute Finland, Natural Resources Institute Finland (Luke), Parkano Research Unit

Contributors: Kuovi, A., Karp, M., Franzén, R., Sarjala, T., Muilu-Mäkelä, R., Aro, T., Tienaho, J., Silvan, N.

Publication date: 2016

Host publication information

Title of host publication: XIV Meeting of the IOBC-WPRS Working Group Biological Control of Fungal and Bacterial Plant Pathogens Biocontrol and Microbial Ecology

Article number: 067

URLs:

<http://www.iobc-wprsberlin2016.de/> (Conference website)

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Professional

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology

Contributors: Tolvanen, H., Keipi, T., Raiko, R.

Pages: 153-164

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Fuel

Volume: 176

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2016): CiteScore 4.9 SJR 1.736 SNIP 2.185

Original language: English

Keywords: Combustion, Biomass, Chemical kinetics, Carbon dioxide, Drop-tube reactor

DOIs:

10.1016/j.fuel.2016.02.071

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

A Three-Component Assembly Promoted by Boronic Acids Delivers a Modular Fluorophore Platform (BASHY Dyes)

A multicomponent reaction, symbolized on the cover by a puzzle, was used to prepare a molecularly diverse series of boron-containing heterocyclic dyes [boronic acid salicylidenehydrazone (BASHY) dyes]. The dyes are strongly fluorescent in the green-yellow spectral range and were applied in cell-staining protocols to visualize lipid droplets (as shown in the background of the picture). More information can be found in the Full Paper by U.Pischel, et al. (DOI: 10.1002/chem.201503943).

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Urban circular bioeconomy (UrCirBio), Faculdade de Farmacia da Universidade de Lisboa, Universidad de Huelva

Contributors: Santos, F. M. F., Rosa, J. N., Candeias, N. R., Carvalho, C. P., Matos, A. I., Ventura, A. E., Florindo, H. F., Silva, L. C., Pischel, U., Gois, P. M. P.

Pages: 1631-1637

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Chemistry: A European Journal

Volume: 22

Issue number: 5

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.082

Original language: English

ASJC Scopus subject areas: Chemistry(all)

DOIs:

10.1002/chem.201503943

Source: Scopus

Source ID: 84958037809

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

Biological and Bioelectrochemical Recovery of Critical and Scarce Metals

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Biofouling and Biofilm Processes Section, Bhabha Atomic Research Centre, Council of Scientific and Industrial Research India, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education

Contributors: Nancharaiah, Y. V., Mohan, S. V., Lens, P. N. L.

Number of pages: 19

Pages: 137-155

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Trends in Biotechnology

Volume: 34

Issue number: 2

ISSN (Print): 0167-7799

Ratings:

Scopus rating (2016): CiteScore 9.97 SJR 4.203 SNIP 3.177

Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering

Keywords: Bioelectrochemical systems, Biomining, Bioprecipitation, Biorecovery, Critical metals, Microbial fuel cells, Platinum group metals, Rare earth elements

DOIs:

10.1016/j.tibtech.2015.11.003

Source: Scopus

Source ID: 84961085643

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

Biomass-Based and Oxidant-Free Preparation of Hydroquinone from Quinic Acid

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Supramolecular photochemistry, Inst Super Tecn, Instituto Superior Tecnico,

Universidade de Lisboa, CQE, Univ Lisbon, Universidade de Lisboa, Fac Pharm, Res Inst Med & Pharmaceut Sci iMed UL

Contributors: Assoah, B., Veiros, L. F., Afonso, C. A. M., R. Candeias, N.

Number of pages: 6

Pages: 3856-3861

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: European Journal of Organic Chemistry

Volume: 2016

Issue number: 22

ISSN (Print): 1434-193X

Ratings:

Scopus rating (2016): CiteScore 2.74 SJR 1.177 SNIP 0.69

Original language: English

Electronic versions:

eujoc

DOIs:

10.1002/ejoc.201600616

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

Chemical and bacterial leaching of metals from a smelter slag in acid solutions

The purpose of this study was to assess the dissolution of Si, Fe, Cu and Zn from a smelter slag sample under acidic chemical and bacterial leaching conditions. The Cu-containing solid phases were Cu-sulfides (57% distribution), fayalite (18%) and metallic Cu (16%). Zn was mostly associated with fayalite, magnetite and Na-silicate phases (Σ94%). Two mixed cultures (HB1 and HB2) were enriched from samples taken from the slag lagoon site at the smelter location. Comparable results of metal dissolution were obtained with the two mixed cultures. The enrichment culture HB1 was characterized further by denaturing gradient gel electrophoresis (DGGE) of polymerase chain reaction amplified 16S rRNA genes. Based on the 16S rRNA gene sequences, culture HB1 contained at least *Acidithiobacillus ferrivorans* and *Alicyclobacillus cycloheptanicus*, with sequences of three DGGE bands matching distantly with *Alicyclobacillus tolerans* and *Alicyclobacillus herbarium* in the database. *Alicyclobacillus* spp. have not been previously associated with slag lagoons or slag bioleaching. Approximately 80% Cu and 25% Zn were dissolved from the slag (10% pulp) in shake flasks when S^0 was provided for the bacteria to produce H_2SO_4 . Bioleaching in stirred tanks was conducted at controlled pH values and was practiced at pH levels promoting metal dissolution and suppressing iron and silicate solubilization from fayalite and Na-silicate. Chemical leaching at pH 2.3-4.0 did not yield substantial dissolution of valuable metals.

General information

Publication status: Published

MoE 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

Contributors: Kaksonen, A. H., Särkijärvi, S., Puhakka, J. A., Peuraniemi, E., Junnikkala, S., Tuovinen, O. H.

Pages: 46-53

Publication date: 2016

Peer-reviewed: Yes

Early online date: 2015

Publication information

Journal: Hydrometallurgy

Volume: 159

ISSN (Print): 0304-386X

Ratings:

Scopus rating (2016): CiteScore 2.8 SJR 1.154 SNIP 1.777

Original language: English

ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Materials Chemistry, Metals and Alloys

Keywords: Acidithiobacillus, Alicyclobacillus, Bacterial leaching, Bioleaching, Chemical leaching, Smelter slag

DOIs:

10.1016/j.hydromet.2015.10.032

Source: Scopus

Source ID: 84946882317

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

Compact hematite buffer layer as a promoter of nanorod photoanode performances

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Milan, R., Cattarin, S., Comisso, N., Baratto, C., Kaunisto, K., Tkachenko, N. V., Concina, I.

Number of pages: 10

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Scientific Reports

Volume: 6

Article number: 35049

ISSN (Print): 2045-2322

Ratings:

Scopus rating (2016): CiteScore 4.63 SJR 1.692 SNIP 1.364

Original language: English

Electronic versions:

srep35049

DOIs:

10.1038/srep35049

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201612094855>

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

Controllable Electronic Structures and Photoinduced Processes of Bay-Linked Perylenediimide Dimers and a Ferrocene-Linked Triad

A series of perylene-3,4,9,10-bis(dicarboximide) (PDI) dimers linked through the bay regions was systematically synthesized to examine the electronic structures and photophysical properties in dependence on the distance and orientation between the two PDI units. The spectroscopic and electrochemical measurements suggested that the coupling value of a directly linked PDI dimer (PDI)₂ is much larger than those of para- and meta-phenylene-bridged PDI dimers p-

(PDI)₂ and m-(PDI)₂. The width of Davydov splitting was quantitatively evaluated to compare the coupling values between the two PDI units in these dimers by absorption spectroscopy in frozen 2-methyl-THF. Excimer formation of PDI dimers induced the strong fluorescence quenching and large red-shifts. Femtosecond transient absorption revealed a broad absorption derived from an excimer in the range from about 600nm to the near-IR region. The rate constants of formation and decay of the excimer are strongly dependent on the coupling values. Time-resolved measurements on ferrocene-linked p-(PDI)₂ revealed a competition between the photoinduced processes of electron transfer and excimer formation in PhCN, which is in sharp contrast with the sole electron-transfer process in toluene.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Horinouchi, H., Sakai, H., Araki, Y., Sakanoue, T., Takenobu, T., Wada, T., Tkachenko, N. V., Hasobe, T.

Pages: 9631-9641

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Chemistry: A European Journal

Volume: 22

Issue number: 28

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.082

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Electron transfer, Electronic structure, Excimers, Perylenediimides, Photophysics

DOIs:

10.1002/chem.201601058

Source: Scopus

Source ID: 84973522054

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

Downstream integration of microalgae harvesting and cell disruption by means of cationic surfactant-decorated Fe₃O₄ nanoparticles

Microalgal biofuel, albeit an exciting potential fossil-fuel-replacement candidate, still requires the development of more advanced downstream processing technology for its price competitiveness. The major challenge in a microalgae-based biorefinery is the efficient separation of microalgae from low-concentration culture broth. The post-harvesting cell-disruption step necessary to render microalgae suitable for lipid extraction, moreover, further raises energy consumption and cost. For the mitigation of biorefinery complexity and costs, we suggest herein a new scheme that integrates the critical downstream processes (harvesting and cell disruption) by means of cationic surfactant-decorated Fe₃O₄ nanoparticles. The cationic surfactants' quaternary ammonium heads play an important role in not only flocculating negatively charged microalgae but also weakening thick cell walls. In the present study, the harvesting efficiency and cell-damaging effects of three cationic surfactants - cetrimonium bromide (CTAB), cetylpyridinium chloride (CPC), and cetylpyridinium bromide (CPB) - were evaluated. The CTAB-decorated Fe₃O₄ nanoparticles, which were found to be the most effective, achieved a 96.6% microalgae harvesting efficiency at a dosage of 0.46 g particle per g cell. Next, for the purposes of magnetic nanoparticle recycling and high-purity microalgal biomass obtainment, microalgae detachment from microalgae-Fe₃O₄ flocs was performed by addition of an anionic surfactant, sodium dodecyl sulfate (SDS). The detached CTAB-decorated Fe₃O₄ nanoparticles showed a steady reuse efficiency of about 80%. Furthermore, microalgae harvesting by CTAB-decorated Fe₃O₄ nanoparticles could contribute to a great improvement in the total extracted lipid content and greener wet extraction without the additional energy-intensive cell-disruption step, thus demonstrating the cell-disruption ability of CTAB-decorated Fe₃O₄ nanoparticles.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, National NanoFab Center, Korea Institute of Energy Research, Korea Advanced Institute of Science and Technology (KAIST), Chungnam National University

Contributors: Seo, J. Y., Ramasamy, P., Kim, B., Seo, J. C., Park, J. Y., Na, J. G., Jeon, S. G., Park, S. B., Lee, K., Oh, Y. K.

Number of pages: 9

Pages: 3981-3989

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Green Chemistry

Volume: 18

Issue number: 14

ISSN (Print): 1463-9262

Ratings:

Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021

Original language: English

ASJC Scopus subject areas: Environmental Chemistry, Pollution

DOIs:

10.1039/c6gc00904b

Source: Scopus

Source ID: 84978832811

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

Effect of source-separated urine storage on estrogenic activity detected using bioluminescent yeast *Saccharomyces cerevisiae*

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Jaatinen, S., Kivistö, A., Palmroth, M., Karp, M.

Pages: 2172-2182

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Environmental Technology

Volume: 37

Issue number: 17

ISSN (Print): 0959-3330

Ratings:

Scopus rating (2016): CiteScore 1.6 SJR 0.569 SNIP 0.818

Original language: English

DOIs:

10.1080/09593330.2016.1144797

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

Enhanced adsorption of orthophosphate and copper onto hydrochar derived from sewage sludge by KOH activation

Hydrothermal carbonization producing hydrochar from organic waste is increasingly gaining attention to deal with the challenge of excess waste activated sludge produced during centralized aerobic wastewater treatment. Hydrochar is used as an adsorbent for the removal of organics, metals and biotic contaminants. This study demonstrated the application of KOH activated hydrochar, called enhanced hydrochar (EHC) derived from sewage sludge, for the removal of orthophosphate from wastewater by means of batch adsorption, zetametry and infrared spectroscopy. The maximum Q_e - PO_4^{3-} of EHC was 14.3 mg orthophosphate adsorbed per g of EHC when the initial orthophosphate concentration was increased to 150 mg L^{-1} . The application of orthophosphate removal by EHC from the effluent of a constructed wetland was demonstrated by achieving more than 97% orthophosphate removal at an EHC dosage of 6.0 g L^{-1} and an initial orthophosphate concentration of 13.1 mg L^{-1} . pH dependent adsorption experiments and infrared spectroscopy showed the orthophosphate removal by EHC was due to the replacement of hydroxyl groups by orthophosphate in the EHC. Acid-base titration showed the KOH washing of the raw hydrochar (RHC) led to a 1.7 times increase in the hydroxyl groups in EHC compared to RHC. This study further confirmed the higher uptake capacity of EHC compared to RHC towards

copper as a model divalent cation. EHC can thus be applied for the removal of both anions (orthophosphate) and cations (copper) from wastewater.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education, Zurich University of Applied Sciences

Contributors: Spataru, A., Jain, R., Chung, J. W., Gerner, G., Krebs, R., Lens, P. N. L.

Number of pages: 8

Pages: 101827-101834

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: RSC Advances

Volume: 6

Issue number: 104

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757

Original language: English

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

DOIs:

10.1039/c6ra22327c

URLs:

<http://www.scopus.com/inward/record.url?scp=84994048409&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84994048409

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

Formation and stability of porphyrin and phthalocyanine self-assembled monolayers on ZnO surfaces

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Department of Chemistry and Bioengineering, Tampere University of Technology

Contributors: Hakola, H., Sariola-Leikas, E., Jääntti, P., Mokus, T., Stranius, K., Efimov, A., Tkachenko, N. V.

Number of pages: 8

Pages: 1264-1271

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Journal of Porphyrins and Phthalocyanines

Volume: 20

Issue number: 08n11

ISSN (Print): 1088-4246

Ratings:

Scopus rating (2016): CiteScore 1.05 SJR 0.354 SNIP 0.374

Original language: English

Keywords: self-assembled monolayer; porphyrin; phthalocyanine; TiO₂; nanorods

DOIs:

10.1142/S1088424616501029

Bibliographical note

INT=keb,"Jäntti, Paavo"

INT=keb,"Mokus, Thomas"

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

High Water-Splitting Efficiency through Intentional In and Sn Codoping in Hematite Photoanodes

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Kaouk, A., Ruoko, T., Pyeon, M., Gönüllü, Y., Kaunisto, K., Lemmetyinen, H., Mathur, S.

Number of pages: 9

Pages: 28345-28353

Publication date: 2016

Peer-reviewed: Yes

Early online date: 18 Nov 2016

Publication information

Journal: Journal of Physical Chemistry C

Volume: 120

Issue number: 49

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.189

Original language: English

DOIs:

10.1021/acs.jpcc.6b10432

Source: RIS

Source ID: urn:A8E794C0F0E1A8F34099ED3D227C7E26

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

High-Yield Excited Triplet States in Pentacene Self-Assembled Monolayers on Gold Nanoparticles through Singlet Exciton Fission

One of the major drawbacks of organic-dye-modified self-assembled monolayers on metal nanoparticles when employed for efficient use of light energy is the fact that singlet excited states on dye molecules can be easily deactivated by means of energy transfer to the metal surface. In this study, a series of 6,13-bis(triisopropylsilylethynyl)pentacene-alkanethiolate monolayer protected gold nanoparticles with different particle sizes and alkane chain lengths were successfully synthesized and were employed for the efficient generation of excited triplet states of the pentacene derivatives by singlet fission. Time-resolved transient absorption measurements revealed the formation of excited triplet states in high yield (172±26%) by suppressing energy transfer to the gold surface.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Keio University

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

Pages: 5230-5234

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Angewandte Chemie (International Edition)

Volume: 55

Issue number: 17

ISSN (Print): 1433-7851

Ratings:

Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.182

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis

Keywords: Gold, Nanoparticles, Pentacene, Self-assembled monolayers, Singlet fission

DOIs:

10.1002/anie.201601421

Source: Scopus

Source ID: 84961773531

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

Homologation Reaction of Ketones with Diazo Compounds

This review covers the addition of diazo compounds to ketones to afford homologated ketones, either in the presence or in the absence of promoters or catalysts. Reactions with diazoalkanes, aryldiazomethanes, trimethylsilyldiazomethane, α -diazo esters, and disubstituted diazo compounds are covered, commenting on the complex regiochemistry of the reaction and the nature of the catalysts and promoters. The recent reports on the enantioselective version of ketone homologation reactions are gathered in one section, followed by reports on the use of cyclic ketones ring expansion in total synthesis. Although the first reports of this reaction appeared in the literature almost one century ago, the recent achievements, in particular, for the asymmetric version, forecast the development of new breakthroughs in the synthetically valuable field of diazo chemistry.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

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

Contributors: Candeias, N. R., Paterna, R., Gois, P. M. P.

Number of pages: 45

Pages: 2937-2981

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Chemical Reviews

Volume: 116

Issue number: 5

ISSN (Print): 0009-2665

Ratings:

Scopus rating (2016): CiteScore 42.79 SJR 19.51 SNIP 10.419

Original language: English

DOIs:

10.1021/acs.chemrev.5b00381

Bibliographical note

PMID: 26854865

Source: Bibtex

Source ID: urn:23384934f13a3832c004ac95a6c56945

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

Metathesis Reactions on Solid-Phase: Towards New Synthesis Challenges

Today there are many types of transition-metal-catalyzed carbon-carbon bond-forming reactions. Of these, the olefin metathesis has made possible a wide range of transformations with commercially available and easily handled catalysts. Olefin metathesis is widely considered as one of the most powerful synthetic tool in organic chemistry. During the last 20

years many new catalysts with excellent selectivity and efficiency have been developed, also to be used in solid phase organic chemistry protocols. The understanding of the mechanisms and interactions between the catalyst and substrate has resulted that an increasing number of research groups have employed these reactions in multistep procedures and in the synthesis of active pharmaceutical ingredients and natural products. Although the olefin metathesis reaction still proceeds better in homogeneous phase, some structural modifications of the catalyst and new approaches for immobilization have provided interesting possibilities towards more efficient use also in heterogeneous phase. To celebrate 10 years since the Nobel Prize in Chemistry given to Yves Chauvin, Richard Schrock and Robert Grubbs for the "development of the metathesis method in organic synthesis" and to summarize recent results obtained in the field of solid phase metathesis chemistry this short review was written.

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

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

Contributors: Franzen, R. G.

Number of pages: 8

Pages: 1143-1150

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Topics in Catalysis

Volume: 59

Issue number: 13

ISSN (Print): 1022-5528

Ratings:

Scopus rating (2016): CiteScore 2.55 SJR 0.975 SNIP 0.811

Original language: English

DOIs:

10.1007/s11244-016-0635-6

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

On describing the optoelectronic characteristics of poly(benzodithiophene-: Co -quinoxaline)-fullerene complexes: The influence of optimally tuned density functionals

Here, we investigate the effects of both tuning the range-separation parameter of long-range corrected (LRC) density functionals and including dispersion corrections on describing the local optoelectronic properties of polymer-fullerene interfaces that are critical to the performance of polymer solar cells (PSCs). Focusing on recently studied (Chen, et al., Chem. Mater., 2012, 24, 4766-4772) PSC active layers derived from poly(benzodithiophene-co-quinoxaline) and substituted fullerene PC₇₁BM, we compare the performance of global hybrid functionals (B3LYP and B3LYP-D) alongside two LRC functionals (ω B97X and ω B97X-D) and their optimally tuned (OT) analogs (OT- ω B97X and OT- ω B97X-D). Our results confirm that OT-LRC functionals generally improve the description of the optical properties of the individual materials with respect to experiment. For electron-donor (eD)-electron-acceptor (eA) complexes used to describe the local optoelectronic properties of the material interface, PC₇₁BM is found to preferentially settle near the quinoxaline acceptor units on the copolymer backbone, regardless of the functional, though dispersion corrections have a strong influence on the intermolecular distances and, in turn, the nature of the excited states. All functionals yield very similar descriptions of the transition maxima for the complexes, i.e. predominant local excitations on the copolymer. Importantly, tuning the range-separation parameter of the LRC functional is shown to have a profound effect, as the OT functionals allow for the description of the charge transfer states of the eD-eA complexes, while the non-tuned LRC functionals predict only local intramolecular excitations. These results hold considerable importance for deriving the appropriate physical understanding of the interfacial structure-property-function relationships of PSCs.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Department of Physics, University of Kentucky

Contributors: Kastinen, T., Niskanen, M., Risko, C., Cramariuc, O., Hukka, T. I.

Number of pages: 17

Pages: 27654-27670

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 18

Issue number: 39
ISSN (Print): 1463-9076
Ratings:

Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.117
Original language: English
ASJC Scopus subject areas: Physics and Astronomy(all), Physical and Theoretical Chemistry
DOIs:

10.1039/c6cp04567g
Source: Scopus
Source ID: 84991045177
Research output: Contribution to journal > Article > Scientific > peer-review

Photoinduced nonlinear optical response in azobenzene-functionalized molecular glass

We show that mexylaminotriazine molecular glass functionalized with the azobenzene derivative Disperse Red 1 shows equally strong second-order nonlinear optical response as well-known polymers with the same photoactive component. Furthermore, even high chromophore loading does not adversely affect the nonlinear response. This suggests that chromophore-chromophore intermolecular interactions do not greatly limit the response of such molecular glasses, which therefore provide an excellent materials platform for nonlinear optical applications.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research area: Optics, Research group: Nonlinear Optics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Department of Physics, Tampere University of Technology
Contributors: Virkki, M., Tuominen, O., Kauranen, M., Priimägi, A.
Number of pages: 8
Pages: 4964-4971
Publication date: 2016
Peer-reviewed: Yes

Publication information

Journal: Optics Express
Volume: 24
Issue number: 5
ISSN (Print): 1094-4087
Ratings:
Scopus rating (2016): CiteScore 3.48 SJR 1.532 SNIP 1.528
Original language: English
DOIs:
10.1364/OE.24.004964
Research output: Contribution to journal > Article > Scientific > peer-review

Photoresponsive liquid-crystalline polymer films bilayered with an inverse opal structure

An inverse opal film was layered to a photodeformable film, and its photoresponsive behavior was investigated. This bilayer films composed of colorless photonic crystal using inverse opal structures and colored photoresponsive layers with azobenzene-containing CLCP.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tokyo Institute of Technology, Japan Science and Technology Agency
Contributors: Akamatsu, N., Aizawa, M., Tatsumi, R., Hisano, K., Priimägi, A., Shishido, A.
Number of pages: 4
Pages: 145-148
Publication date: 2016
Peer-reviewed: Yes

Publication information

Journal: JOURNAL OF PHOTOPOLYMER SCIENCE AND TECHNOLOGY
Volume: 29
Issue number: 1
ISSN (Print): 0914-9244

Ratings:

Scopus rating (2016): CiteScore 0.88 SJR 0.3 SNIP 0.558

Original language: English

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

Keywords: Bragg diffraction, Inverse opal structure, Photoresponsive film

DOIs:

10.2494/photopolymer.29.145

Source: Scopus

Source ID: 84981200985

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

Porphyrin-Based Donor-Acceptor Dyads: Engineering the Linker and Tuning the Photoinduced Electron Transfer

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Tkachenko, N. V., Efimov, A., Lemmetyinen, H.

Number of pages: 51

Pages: 121-171

Publication date: 2016

Host publication information

Title of host publication: Handbook of Porphyrin Science : With Applications to Chemistry, Physics, Materials Science, Engineering, Biology and Medicine — Volume 42: Towards Tuned Properties of Porphyrinoids

Volume: 42

Publisher: World Scientific Publishing

Editors: Kadish, K. M., Smith, K. M., Guillard, R.

ISBN (Print): 9789813143524

ISBN (Electronic): 978-981-3149-62-5

DOIs:

10.1142/9789813149625_0002

Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific › peer-review

Sorption of zinc onto elemental selenium nanoparticles immobilized in *Phanerochaete chrysosporium* pellets

The use of a novel hybrid biosorbent, elemental selenium nanoparticles ($n\text{Se}^0$) immobilized in pellets of *Phanerochaete chrysosporium*, to remove Zn from aqueous solutions was investigated. Fungal pellets containing $n\text{Se}^0$ ($n\text{Se}^0$ -pellets) showed to be better biosorbents as they removed more Zn ($88.1 \pm 5.3\%$) compared to Se-free fungal pellets ($56.2 \pm 2.8\%$) at pH 4.5 and an initial Zn concentration of 10 mg L^{-1} . The enhanced sorption capacity of $n\text{Se}^0$ -pellets was attributed to a higher concentration of sorption sites resulting in a more negative surface charge density, as determined by analysis of the potentiometric titration data. Fourier transform infrared spectroscopy (FT-IR) analysis of fungal pellets prior to and after being loaded with Zn showed the functional groups, including hydroxyl and carboxyl groups, involved in the sorption process. The experimental data indicated that the sorption rate of the $n\text{Se}^0$ -pellets fitted well to the pseudo-second order kinetic model ($R^2 = 0.99$), and the sorption isotherm was best represented by the Sips model (Langmuir-Freundlich) with heterogeneous factor $n = 1$ ($R^2 = 0.99$), which is equivalent to the Langmuir model. Operational advantages of fungal pelleted reactors and the Zn removal efficiencies achieved by $n\text{Se}^0$ -pellets under mild acidic conditions make $n\text{Se}^0$ -pellet based bioreactors an efficient biosorption process.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Hydraulic and Environmental Engineering (IHE) Inst. for Water Education, Environmental Engineering and Water Technology Department, Université Paris-Est

Contributors: Espinosa-Ortiz, E. J., Shakya, M., Jain, R., Rene, E. R., van Hullebusch, E. D., Lens, P. N. L.

Number of pages: 12

Pages: 21619–21630

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Environmental Science and Pollution Research

Volume: 23

Issue number: 21

ISSN (Print): 0944-1344

Ratings:

Scopus rating (2016): CiteScore 2.66 SJR 0.891 SNIP 1.127

Original language: English

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

Keywords: Fungal pellets, Hybrid biosorbent, Phanerochaete chrysosporium, Selenium nanoparticles, Zinc biosorption
DOIs:

10.1007/s11356-016-7333-6

Source: Scopus

Source ID: 84982179903

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

Superfluorinated Ionic Liquid Crystals Based on Supramolecular, Halogen-Bonded Anions

Unconventional ionic liquid crystals in which the liquid crystallinity is enabled by halogen-bonded supramolecular anions $[C_nF_{2n+1}-I \cdots I \cdots I-C_nF_{2n+1}]^-$ are reported. The material system is unique in many ways, demonstrating for the first time 1) ionic, halogen-bonded liquid crystals, and 2) imidazolium-based ionic liquid crystals in which the occurrence of liquid crystallinity is not driven by the alkyl chains of the cation.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Cavallo, G., Terraneo, G., Monfredini, A., Saccone, M., Priimägi, A., Pilati, T., Resnati, G., Metrangolo, P., Bruce, D. W.

Pages: 6300-6304

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Angewandte Chemie (International Edition)

Volume: 55

Issue number: 21

ISSN (Print): 1433-7851

Ratings:

Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.182

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis

Keywords: Fluorophobic effect, Halogen bonding, Ionic liquid crystals, Self-assembly, Supramolecular chemistry

Electronic versions:

Superfluorinated Ionic Liquid Crystals Based on Supramolecular, Halogen-Bonded Anions

DOIs:

10.1002/anie.201601278

URLs:

<http://urn.fi/URN:NBN:fi:tty-201605033937>

Source: Scopus

Source ID: 84979722901

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

The effect of urine storage on antiviral and antibiotic compounds in the liquid phase of source-separated urine

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Jaatinen, S. T., Palmroth, M. R., Rintala, J. A., Tuhkanen, T. A.

Pages: 2189-2198

Publication date: 2016

Peer-reviewed: Yes

Early online date: 2016

Publication information

Journal: Environmental Technology

Volume: 37

Issue number: 17

ISSN (Print): 0959-3330

Ratings:

Scopus rating (2016): CiteScore 1.6 SJR 0.569 SNIP 0.818

Original language: English

DOIs:

10.1080/09593330.2016.1144799

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

The Halogen Bond

General information

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Politecnico di Milano, VTT Tech Res Ctr Finland, VTT Technical Research Center Finland

Contributors: Cavallo, G., Metrangolo, P., Milani, R., Pilati, T., Priimägi, A., Resnati, G., Terraneo, G.

Number of pages: 123

Pages: 2478-2601

Publication date: 2016

Peer-reviewed: Yes

Publication information

Journal: Chemical Reviews

Volume: 116

Issue number: 4

ISSN (Print): 0009-2665

Ratings:

Scopus rating (2016): CiteScore 42.79 SJR 19.51 SNIP 10.419

Original language: English

DOIs:

10.1021/acs.chemrev.5b00484

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

Use of laboratory anaerobic digesters to simulate the increase of treatment rate in full-scale high nitrogen content sewage sludge and co-digestion biogas plants

The aim of this study was to assess the effect of increasing feedstock treatment rate on the performance of full-scale anaerobic digestion using laboratory-scale reactors with digestate and feedstock from full-scale digesters. The studied nitrogen-containing feedstocks were i) a mixture of industrial by-products and pig slurry, and ii) municipal sewage sludge, which digestion was studied at 41 and 52 degrees C, respectively. This study showed the successful reduction of hydraulic retention times from 25 and 20 days to around 15 days, which increased organic loading rates from 2 to 3.5 kg volatile solids (VS)/m³ d and 4 to 6 kg VS/m³ d. As a result, the optimum retention time in terms of methane production and VS removal was 10-15% lower than the initial in the full-scale digesters. Accumulation of acids during start-up of the co-digestion reactor was suggested to be connected to the high ammonium nitrogen concentration and intermediate temperature of 41 degrees C. (C) 2016 Elsevier Ltd. All rights reserved.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Gasum Biovacka Ltd, Natural Resources Institute Finland (Luke)

Contributors: Tampio, E., Ervasti, S., Paavola, T., Rintala, J.
Number of pages: 8
Pages: 47-54
Publication date: 2016
Peer-reviewed: Yes

Publication information

Journal: Bioresource Technology

Volume: 220

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2016): CiteScore 5.94 SJR 2.215 SNIP 1.932

Original language: English

Keywords: Anaerobic digestion, Nitrogen, Co-digestion, Sewage sludge, Hydraulic retention time, MICROBIAL COMMUNITY STRUCTURE, FOOD WASTE, SUBSTRATE RATIO, AMMONIA, INOCULUM, TEMPERATURE, PERFORMANCE, MANURE

DOIs:

10.1016/j.biortech.2016.08.058

Bibliographical note

EXT="Tampio, Elina"

Source: WOS

Source ID: 000384712900007

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

Preparation and antimicrobial characterization of silver-containing packaging materials for meat

In food technology, antimicrobial packaging materials could inhibit or limit the growth of spoilage bacteria and thus improve the shelf life of packaged products. The present study provides new insights into the preparation and antimicrobial characterization of silver-containing packaging materials and their efficacy against typical meat spoilage bacteria. Antimicrobial efficacy of packaging films produced by coextrusion or liquid flame spray process was determined by bioluminescence imaging and conventional antimicrobial assay. Fresh pork sirloin was packaged in selected films and composition of meat microbiota was analyzed by 16S rRNA amplicon sequencing. Shelf life of meat was not affected by any of the silver-containing packaging films, even though meat microbiota mostly consisted of bacteria that were inhibited or retarded in vitro by nanoscale silver coating. This may be due to different release dynamics of silver ions on meat surfaces compared to the circumstances in the antimicrobial assay or interactions between silver and amino acids.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Paper Converting and Packaging, Department of Chemistry and Bioengineering, Engineering materials science and solutions (EMASS), Urban circular bioeconomy (UrCirBio), University of Helsinki, Department of Food Hygiene and Environmental Health

Contributors: Kuuliala, L., Pippuri, T., Hultman, J., Auvinen, S., Kolppo, K., Nieminen, T., Karp, M., Björkroth, J., Kuusipalo, J., Jääskeläinen, E.

Number of pages: 8

Pages: 53-60

Publication date: 1 Dec 2015

Peer-reviewed: Yes

Publication information

Journal: Food Packaging and Shelf Life

Volume: 6

Article number: 67

ISSN (Print): 2214-2894

Ratings:

Scopus rating (2015): CiteScore 2.21 SJR 0.695 SNIP 0.947

Original language: English

ASJC Scopus subject areas: Food Science, Safety, Risk, Reliability and Quality, Biomaterials, Polymers and Plastics, Microbiology (medical)

Keywords: Active packaging, Antimicrobial film, Bioluminescence, Lactic acid bacteria, Liquid flame spray, Silver nanoparticle

DOIs:

10.1016/j.fpsl.2015.09.004

URLs:

<http://www.scopus.com/inward/record.url?scp=84945244937&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

ORG=mol,0.5

ORG=keb,0.5

Source: Scopus

Source ID: 84945244937

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

Graphene-intercalated Fe₂O₃/TiO₂ heterojunctions for efficient photoelectrolysis of water

Interfacial modification of α -Fe₂O₃/TiO₂ multilayer photoanodes by intercalating few-layer graphene (FLG) was found to improve water splitting efficiency due to superior transport properties, when compared to individual iron and titanium oxides and heterojunctions thereof. Both metal oxides and graphene sheets were grown by plasma-enhanced chemical vapor deposition. Compared to the onset potential achieved for α -Fe₂O₃ films (1 V vs. RHE), the α -Fe₂O₃/TiO₂ bilayer structure yielded a better onset potential (0.3 V vs. RHE). Heterojunctioned bilayers exhibited a higher photocurrent density (0.32 mA cm⁻² at 1.23 V vs. RHE) than the single α -Fe₂O₃ layer (0.22 mA cm⁻² at 1.23 V vs. RHE), indicating more efficient light harvesting and higher concentration of photogenerated charge carriers. For more efficient charge transport at the interface, a few layer graphene sheet was intercalated into the α -Fe₂O₃/TiO₂ interface, which substantially increased the photocurrent density to 0.85 mA cm⁻² (1.23 V vs. RHE) and shifted the onset potential (0.25 V vs. RHE). Ultrafast transient absorption spectroscopy studies indicated that the incorporation of FLG between the α -Fe₂O₃ and TiO₂ layers resulted in reduced recombination in the α -Fe₂O₃ layer. The results showed that graphene intercalation improved the charge separation and the photocurrent density of the FTO/ α -Fe₂O₃/FLG/TiO₂ system.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Universitat zu Koln, Institute of Inorganic Chemistry, Ruhr-Universität Bochum

Contributors: Kaouk, A., Ruoko, T. P., Gönüllü, Y., Kaunisto, K., Mettenbörger, A., Gurevich, E., Lemmetyinen, H., Ostendorf, A., Mathur, S.

Number of pages: 7

Pages: 101401-101407

Publication date: 13 Nov 2015

Peer-reviewed: Yes

Publication information

Journal: RSC Advances

Volume: 5

Issue number: 123

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2015): CiteScore 3.42 SJR 0.947 SNIP 0.834

Original language: English

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

Electronic versions:

Manuscript_FGT

DOIs:

10.1039/c5ra18330h

URLs:

<http://urn.fi/URN:NBN:fi:tty-201611254802>

URLs:

<http://www.scopus.com/inward/record.url?scp=84948652698&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84948652698

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

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

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

light–molecule interaction as well as their application in optical components.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications, Augmented Human Activities (AHA), Frontier Photonics, Institute of Physical Chemistry, University of Hamburg

Contributors: Kietzmann, S., Strelow, C., Tavares, L., Penttinen, J., Hakkarainen, T. V., Schramm, A., Osadnik, A., Lützen, A., Kjelstrup-Hansen, J., Mews, A., Kipp, T.

Number of pages: 7

Pages: 1532-1538

Publication date: 27 Oct 2015

Peer-reviewed: Yes

Publication information

Journal: ACS Photonics

Volume: 2

Issue number: 11

ISSN (Print): 2330-4022

Ratings:

Scopus rating (2015): CiteScore 5.71 SJR 2.975 SNIP 1.477

Original language: English

DOIs:

[10.1021/acsphotonics.5b00349](https://doi.org/10.1021/acsphotonics.5b00349)

URLs:

<http://pubs.acs.org/doi/abs/10.1021/acsphotonics.5b00349>

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

Photomechanical Energy Transfer to Photopassive Polymers through Hydrogen and Halogen Bonds

The supramolecular assembly of photoactive azobenzenes with passive polymers via halogen or hydrogen bonding is a cost-effective way to design materials for various photomechanical applications that convert light energy directly into macroscopic motion, for instance, in all-optical surface patterning and photochemical imaging of plasmonic structures. To elucidate the molecular-level origins of this motion, we show, by coupling dynamic infrared spectroscopy to a photo-orientation setup, that supramolecular bonds above a certain interaction strength threshold are photostable under vigorous photoisomerization cycling and capable of translating the photo-orientation of azobenzenes into the orientation of nonabsorbing host polymer side chains. A correlation is found between azobenzene photoinduced molecular orientation and macroscopic all-optical surface patterning efficiency. The improved performance of halogen-bonded systems in photopatterning applications can be related to the absence of a plasticizing effect on the polymer matrix, which may enable the material to retain an optimal glass transition temperature, in contrast to hydrogen-bonded and nonbonded references. Thus, our results provide design guidelines in terms of the nature and strength of the supramolecular interaction and of the degree of azo functionalization needed to optimize the motion transfer to passive polymers.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Département de Chimie, Succ. Centre-Ville, Aalto University, Politecnico di Milano, Royal Military College of Canada

Contributors: Vapaavuori, J., Heikkinen, I. T. S., Dichiarante, V., Resnati, G., Metrangolo, P., Sabat, R. G., Bazuin, C. G., Priimagi, A., Pellerin, C.

Number of pages: 8

Pages: 7535-7542

Publication date: 27 Oct 2015

Peer-reviewed: Yes

Publication information

Journal: Macromolecules

Volume: 48

Issue number: 20

ISSN (Print): 0024-9297

Ratings:

Scopus rating (2015): CiteScore 5.82 SJR 2.357 SNIP 1.58

Original language: English

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

DOIs:

10.1021/acs.macromol.5b01813

URLs:

<http://www.scopus.com/inward/record.url?scp=84945400553&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

EXT="Vapaavuori, Jaana"

Source: Scopus

Source ID: 84945400553

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

Changes in global gene expression of *Vibrio parahaemolyticus* induced by cold- and heat-stress

Background: *Vibrio* (*V.*) *parahaemolyticus* causes seafood-borne gastro-intestinal bacterial infections in humans worldwide. It is widely found in marine environments and is isolated frequently from seawater, estuarine waters, sediments and raw or insufficiently cooked seafood. Throughout the food chain, *V. parahaemolyticus* encounters different temperature conditions that might alter metabolism and pathogenicity of the bacterium. In this study, we performed gene expression profiling of *V. parahaemolyticus* RIMD 2210633 after exposure to 4, 15, 20, 37 and 42°C to describe the cold and heat shock response. **Methods:** Gene expression profiles of *V. parahaemolyticus* RIMD 2210633 after exposure to 4, 15, 20, 37 and 42°C were investigated via microarray. Gene expression values and RT-qPCR experiments were compared by plotting the log₂ values. Moreover, volcano plots of microarray data were calculated to visualize the distribution of differentially expressed genes at individual temperatures and to assess hybridization qualities and comparability of data. Finally, enriched terms were searched in annotations as well as functional-related gene categories using the Database for Annotation, Visualization and Integrated Discovery. **Results:** Analysis of 37°C normalised transcriptomics data resulted in differential expression of 19 genes at 20°C, 193 genes at 4°C, 625 genes at 42°C and 638 genes at 15°C. Thus, the largest number of significantly expressed genes was observed at 15 and 42°C with 13.3 and 13 %, respectively. Genes of many functional categories were highly regulated even at lower temperatures. Virulence associated genes (*tdh1*, *tdh2*, *toxR*, *toxS*, *vopC*, *T6SS-1*, *T6SS-2*) remained mostly unaffected by heat or cold stress. **Conclusion:** Along with folding and temperature shock depending systems, an overall temperature-dependent regulation of expression could be shown. Particularly the energy metabolism was affected by changed temperatures. Whole-genome gene expression studies of food related pathogens such as *V. parahaemolyticus* reveal how these pathogens react to stress impacts to predict its behaviour under conditions like storage and transport.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Department of Signal Processing, Freie Universität Berlin, University of Tampere

Contributors: Urmersbach, S., Aho, T., Alter, T., Hassan, S. S., Autio, R., Huehn, S.

Publication date: 23 Oct 2015

Peer-reviewed: Yes

Publication information

Journal: BMC Microbiology

Volume: 15

Issue number: 1

Article number: 229

ISSN (Print): 1471-2180

Ratings:

Scopus rating (2015): CiteScore 2.93 SJR 1.42 SNIP 1.007

Original language: English

ASJC Scopus subject areas: Microbiology, Microbiology (medical)

Keywords: Gene expression, Thermal shock, *Vibrio parahaemolyticus*

DOIs:

10.1186/s12866-015-0565-7

URLs:

<http://www.scopus.com/inward/record.url?scp=84944883751&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

ORG=keb,0.5

ORG=sgn,0.5

Source: Scopus

Source ID: 84944883751

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

Regenerative Astaxanthin Extraction from a Single Microalgal (*Haematococcus pluvialis*) Cell Using a Gold Nano-Scalpel

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), KAIST, Ajou University, Korea Institute of Energy Research

Contributors: Ramasamy, P., Gwak, R., Kang, M., Shim, T. S., Cho, S., Lee, J., Oh, Y. K., Lee, K., Kim, B.

Number of pages: 7

Pages: 22702-22708

Publication date: 14 Oct 2015

Peer-reviewed: Yes

Publication information

Journal: ACS Applied Materials and Interfaces

Volume: 7

Issue number: 40

ISSN (Print): 1944-8244

Ratings:

Scopus rating (2015): CiteScore 7.38 SJR 2.262 SNIP 1.548

Original language: English

ASJC Scopus subject areas: Materials Science(all)

Keywords: astaxanthin, mechanotransduction, microalgae, nanoscalpel, regenerative extraction, wound-healing

DOIs:

10.1021/acsami.5b07651

URLs:

<http://www.scopus.com/inward/record.url?scp=84944350823&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84944350823

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Engineering materials science and solutions (EMASS)

Contributors: Mylläri, V., Ruoko, T., Vuorinen, J., Lemmetyinen, H.

Number of pages: 8

Pages: 419-426

Publication date: 1 Oct 2015
Peer-reviewed: Yes
Early online date: 6 Aug 2015

Publication information

Journal: Polymer Degradation and Stability

Volume: 120

ISSN (Print): 0141-3910

Ratings:

Scopus rating (2015): CiteScore 3.48 SJR 1.209 SNIP 1.61

Original language: English

ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry, Mechanics of Materials, Condensed Matter Physics

Keywords: Fibre, PEEK, Thermal degradation

Electronic versions:

Characterization of thermally aged polyetheretherketone fibres_pre-print

DOIs:

[10.1016/j.polymdegradstab.2015.08.003](https://doi.org/10.1016/j.polymdegradstab.2015.08.003)

URLs:

<http://urn.fi/URN:NBN:fi:tty-201612024835>

URLs:

<http://www.scopus.com/inward/record.url?scp=84942433318&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

ORG=mol,0.75

ORG=keb,0.25

24 kk embargo (post-print)

Source: Scopus

Source ID: 84942433318

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Urban circular bioeconomy (UrCirBio), University of Turku, Department of Biochemistry/Molecular Plant Biology, Department of Biochemistry/Food Chemistry and Food Development

Contributors: Polishchuk, A., Valev, D., Tarvainen, M., Mishra, S., Kinnunen, V., Antal, T., Yang, B., Rintala, J., Tyystjärvi, E.

Number of pages: 8

Pages: 469-476

Publication date: 1 Oct 2015

Peer-reviewed: Yes

Early online date: 2 Jul 2015

Publication information

Journal: Bioresource Technology

Volume: 193

ISSN (Print): 0960-8524

Ratings:

Scopus rating (2015): CiteScore 5.47 SJR 2.243 SNIP 1.887

Original language: English

ASJC Scopus subject areas: Bioengineering, Environmental Engineering, Waste Management and Disposal

Keywords: Eicosapentaenoic acid, *Nannochloropsis*, Paper mill, Pulp mill, Wastewater

DOIs:

10.1016/j.biortech.2015.06.135

URLs:

<http://www.scopus.com/inward/record.url?scp=84936059366&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84936059366

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

Measuring the green color of vegetables from digital images using image analysis

When analyzing the color of foods, a measurement device consisting of a digital camera and image analysis software is an attractive alternative to traditional instruments such as spectrophotometers, colorimeters and sensory evaluations. The device enables the measuring of the surface of a sample pixel-by-pixel and offers versatile possibilities for new imaging-based analysis strategies for food research. Our objective was to evaluate if this apparatus could detect differences in colors existing in green vegetables. We showed that the device separated batches of green vegetables and detected color differences that existed in vegetables with different degrees of green color. We demonstrated that this device could measure the color change of green vegetables during heat treatments. We conclude that this experimental setup has the potential to evaluate the healthiness of a diet by analyzing the proportion and quality of green vegetables for use in a serving at a buffet table or dinner plate.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Turun Yliopisto/Turun Biomateriaalikeskus, University of Oslo, Faculty of Medicine, 22.10.2010, University of Turku, Functional Foods Forum

Contributors: Manninen, H., Paakki, M., Hopia, A., Franzén, R.

Number of pages: 7

Pages: 1184-1190

Publication date: 1 Oct 2015

Peer-reviewed: Yes

Early online date: 14 Apr 2015

Publication information

Journal: LWT: Food Science and Technology

Volume: 63

Issue number: 2

ISSN (Print): 0023-6438

Ratings:

Scopus rating (2015): CiteScore 3.11 SJR 1.29 SNIP 1.563

Original language: English

ASJC Scopus subject areas: Food Science

Keywords: a, b, Digital camera, Green vegetables, L, Thermal degradation

DOIs:

10.1016/j.lwt.2015.04.005

URLs:

<http://www.scopus.com/inward/record.url?scp=84930380290&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84930380290

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

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 $1.5 \pm 0.2 \text{ A/m}^2$ and $62 \pm 11\%$, 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 hafnience*, that has been reported to use mediated electron transfer, were detected. This study shows that the anode potential has a substantial effect on microbial communities and on xylose metabolism.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Urban circular bioeconomy (UrCirBio)

Contributors: Kokko, M. E., Mäkinen, A. E., Sulonen, M. L. K., Puhakka, J. A.

Number of pages: 5

Pages: 248-252

Publication date: 5 Sep 2015

Peer-reviewed: Yes

Early online date: 24 Jun 2015

Publication information

Journal: Biochemical Engineering Journal

Volume: 101

ISSN (Print): 1369-703X

Ratings:

Scopus rating (2015): CiteScore 2.75 SJR 0.952 SNIP 1.075

Original language: English

ASJC Scopus subject areas: Biotechnology, Bioengineering, Biomedical Engineering, Environmental Engineering

Keywords: Anaerobic processes, Anode potential, Batch processing, Biocatalysis, Bioconversion, Microbial fuel cell

DOIs:

10.1016/j.bej.2015.06.007

URLs:

<http://www.scopus.com/inward/record.url?scp=84936752873&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84936752873

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

Measuring synthesis yield in graphene oxide synthesis by modified hummers method

Synthesis of graphene oxide by the modified Hummers method and measuring the synthesis yield were investigated.

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Ceramic materials, Tampere University of Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group:

Materials Characterization, Engineering materials science and solutions (EMASS), University of Helsinki

Contributors: Frankberg, E. J., George, L., Efimov, A., Honkanen, M., Pessi, J., Levänen, E.

Number of pages: 5

Pages: 755-759

Publication date: 2 Sep 2015

Peer-reviewed: Yes

Publication information

Journal: Fullerenes Nanotubes and Carbon Nanostructures

Volume: 23

Issue number: 9

ISSN (Print): 1536-383X

Ratings:

Scopus rating (2015): CiteScore 1.62 SJR 0.278 SNIP 0.596

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Physical and Theoretical Chemistry, Materials Science(all), Atomic and Molecular Physics, and Optics

Keywords: Concentration, Graphene oxide, Hummers method, Synthesis, Yield

Electronic versions:

Frankberg_revised_text_print

DOIs:

10.1080/1536383X.2014.993754

URLs:

<http://urn.fi/URN:NBN:fi:tty-201603173654>

Bibliographical note

Versio ja lupa ok 26.1.2016 KK

Source: Scopus

Source ID: 84929598253

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

Gene expression profiles of *Vibrio parahaemolyticus* in the early stationary phase

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 7

Pages: 231-237

Publication date: 1 Sep 2015

Peer-reviewed: Yes

Early online date: 2 Aug 2015

Publication information

Journal: Letters in Applied Microbiology

Volume: 61

Issue number: 3

ISSN (Print): 0266-8254

Ratings:

Scopus rating (2015): CiteScore 1.66 SJR 0.653 SNIP 0.756

Original language: English

ASJC Scopus subject areas: Applied Microbiology and Biotechnology

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

DOIs:

10.1111/lam.12452

URLs:

<http://www.scopus.com/inward/record.url?scp=84939267412&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84939267412

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

Searching for a robust strategy for minimizing alkali chlorides in fluidized bed boilers during burning of high SRF-energy-share fuel

To meet the increasing volume of waste to be treated via energy recovery, high SRF-energy-share fuel is being fired in conventional waste-to-energy facilities. In this work, corrosion related risk during firing of 70 e-% share (target fuel) is studied and compared against the base case fuel containing 50 e-% share. Cl and S concentration is highest in the target fuel as a direct result of increasing the proportion of SRF in the fuel mixture. Br, Zn and Pb showed the same trend. Meanwhile, the concentration of Na, K, Al and Si are highly dependent on the type of the SRF fired. The corrosion risk of the base and target fuels are analyzed using the composition of the fine aerosol fraction and deposit samples measured near the vicinity of the superheater. Surprisingly aerosols for the target fuel are less risky - having less Cl and more S, than that of the base fuel. The effects of sulfur based additives - elemental sulfur and sulfate injection, and fuel substitution on the risk of superheater corrosion are likewise analyzed. All these strategies can reduce the concentration of Cl in the aerosols, however it is concluded that sulfate injection is considered as a robust strategy for mitigating alkali chloride

formation. Sulfate injection is able to reduce Cl in the aerosols and deposits regardless of the quality of the fuel mixture. Robust strategies are important in ensuring the boiler performance during high SRF-energy share firing. An attempt of linking the quality of the deposits and the properties of the flue gas and aerosols around the superheater using partial least squares regression is also presented.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), University of Jyväskylä, Valmet Technologies Oy, VTT Technical Research Centre of Finland, Department of Chemistry, Renewable Natural Resources and Chemistry of Living Environment, Stora Enso

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

Number of pages: 12

Pages: 25-36

Publication date: 1 Sep 2015

Peer-reviewed: Yes

Publication information

Journal: Fuel

Volume: 155

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2015): CiteScore 4.46 SJR 1.781 SNIP 2.091

Original language: English

ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all),

Organic Chemistry

Keywords: Alkali chloride mitigation, Corrosion, SRF, Waste-to-energy

DOIs:

10.1016/j.fuel.2015.03.087

URLs:

<http://www.scopus.com/inward/record.url?scp=84928243284&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84928243284

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

Fe₂O₃-TiO₂ nanosystems by a hybrid PE-CVD/ALD approach: controllable synthesis, growth mechanism, and photocatalytic properties

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Padova University, Padova University and INSTM, Department of Physics and Astronomy, University of Turku, Univ Antwerp, University of Antwerp, EMAT, CNR-IENI and INSTM, Department of Chemistry, Department of Chemical and Pharmaceutical Sciences, ICCOM-CNR Trieste Research Unit - INSTM Research Unit, Trieste University

Contributors: Barreca, D., Carraro, G., Warwick, M. E. A., Kaunisto, K., Gasparotto, A., Gombac, V., Sada, C., Turner, S., Van Tendeloo, G., Maccato, C., Fornasiero, P.

Number of pages: 8

Pages: 6219-6226

Publication date: 28 Aug 2015

Peer-reviewed: Yes

Publication information

Journal: CrystEngComm

Volume: 17
Issue number: 32
ISSN (Print): 1466-8033
Ratings:

Scopus rating (2015): CiteScore 3.83 SJR 1.04 SNIP 0.98

Original language: English

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

DOIs:

10.1039/c5ce00883b

URLs:

<http://www.scopus.com/inward/record.url?scp=84938522112&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84938522112

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Industrial Bioengineering and Applied Organic Chemistry, Frontier Photonics, Urban circular bioeconomy (UrCirBio)

Contributors: George Abraham, B., Sarkisyan, K. S., Mishin, A. S., Santala, V., Tkachenko, N. V., Karp, M.

Number of pages: 15

Publication date: 3 Aug 2015

Peer-reviewed: Yes

Publication information

Journal: PLoS ONE

Volume: 10

Issue number: 8

Article number: e0134436

ISSN (Print): 1932-6203

Ratings:

Scopus rating (2015): CiteScore 3.32 SJR 1.427 SNIP 1.149

Original language: English

Keywords: RESONANCE ENERGY-TRANSFER, IMAGING MICROSCOPY, FORSTER DISTANCES, MONOMERIC RED , LIVING CELLS, LIVE CELLS, BIOSENSORS, SENSOR, FLIM, ENVIRONMENT

DOIs:

10.1371/journal.pone.0134436

Source: WOS

Source ID: 000358942400027

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

Photoinduced Electron Transfer in CdSe/ZnS Quantum Dot-Fullerene Hybrids

Photoinduced electron transfer (ET) in CdSe/ZnS core-shell quantum dot (QD) - fullerene (COOH-C₆₀) hybrids was studied by the means of time-resolved emission and absorption spectroscopy techniques. A series of four QDs with emission in the range 540-630 nm was employed to investigate the dependence of the electron transfer rate on the QD size. Emission of the QDs is quenched upon hybrid formation, and the quenching mechanism is identified as photoinduced electron transfer from the QD to the fullerene moiety due to the fullerene anion signature observed in transient absorption. In order to obtain quantitative information on the ET reaction, several kinetic data analysis techniques were used, including a conventional multiexponential fitting and a maximum entropy method for emission decay analysis, as well as a

distributed decay model based on the Poisson distribution of fullerenes in the hybrids. The latter gradually simplifies the interpretation of the transient absorption spectra and indicates that the spectra of QD cations are essentially similar to those of neutral QDs, differing only by a minor decrease in the intensity and broadening. Furthermore, only a minor decrease in the ET rate with the increasing QD size was observed, the time constants being in the range 100-200 ps for all studied QDs. The charge recombination is extended to 10 ns or longer for all hybrids.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Virkki, K., Demir, S., Lemmetyinen, H., Tkachenko, N. V.

Number of pages: 12

Pages: 17561-17572

Publication date: 23 Jul 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 119

Issue number: 31

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.24

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

DOIs:

10.1021/acs.jpcc.5b04251

Bibliographical note

INT=keb,"Demir, Sinem"

Source: Scopus

Source ID: 84938703282

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

Subpicosecond to Second Time-Scale Charge Carrier Kinetics in Hematite-Titania Nanocomposite Photoanodes

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology, ETH Zürich, Laboratory for Multifunctional Materials

Contributors: Ruoko, T. P., Kaunisto, K., Bärtsch, M., Pohjola, J., Hiltunen, A., Niederberger, M., Tkachenko, N. V., Lemmetyinen, H.

Number of pages: 6

Pages: 2859-2864

Publication date: 8 Jul 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry Letters

Volume: 6

Issue number: 15

ISSN (Print): 1948-7185

Ratings:

Scopus rating (2015): CiteScore 8.04 SJR 4.143 SNIP 1.719

Original language: English

ASJC Scopus subject areas: Materials Science(all)

Keywords: FILM ELECTRODES, IRON-OXIDE, SEMICONDUCTOR ELECTRODES, WATER OXIDATION, VISIBLE-LIGHT, ALPHA-Fe₂O₃, PHOTOELECTRODES, TiO₂, RECOMBINATION, ELECTROLYSIS

Electronic versions:

Subpicosecond_post-print

DOIs:

10.1021/acs.jpcclett.5b01128

URLs:

<http://urn.fi/URN:NBN:fi:tty-201612024836>

Bibliographical note

AUX=mol,"Pohjola, Juuso"

Source: Scopus

Source ID: 84938694613

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

Synthesis and study of electrochemical and optical properties of substituted perylenemonoimides in solutions and on solid surfaces

A new and efficient methodology towards the synthesis of 7-pyrrolidinyl and 7,12-bispyrrolidinyl perylenemonoimide monoanhydrides (PMI monoanhydrides) and their corresponding dicarboxylic acids is devised. The high yields (70-96%) and facile synthesis of PMI monoanhydrides, as compared to traditional methodologies, make the method attractive and versatile. The reported 7,12-bispyrrolidinyl PMI monoanhydrides are a new family of peryleneimides, where both the bay-substituents are located towards the anhydride cycle. The electrochemical and optical properties of target molecules and their precursors were investigated using UV-Vis spectroscopy and differential pulse voltammetry. Atomic charges and electronic properties were calculated using density functional theory (DFT). In addition, self-assembling monolayers of the PMI monoanhydrides and their corresponding diacids were successfully formed over ZnO and TiO₂ films. The results of the current study indicate that these molecules are potentially good candidates for various applications in the fields of organic electronics and solar cells.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Ahmed, Z., George, L., Hiltunen, A., Lemmetyinen, H., Hukka, T., Efimov, A.

Number of pages: 8

Pages: 13332-13339

Publication date: 7 Jul 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry A

Volume: 3

Issue number: 25

ISSN (Print): 2050-7488

Ratings:

Scopus rating (2015): CiteScore 8.36 SJR 2.62 SNIP 1.63

Original language: English

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

DOIs:

10.1039/c5ta02241j

URLs:

<http://www.scopus.com/inward/record.url?scp=84934958229&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84934958229

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

A comparison of rheology and FTIR in the study of polypropylene and polystyrene photodegradation

Rheology and FTIR spectroscopy are compared as methods to study the degree of photodegradation in polypropylene (PP) and polystyrene (PS) sheets. The materials are hot pressed, artificially photo-aged with fluorescent lights for 4-2048 h and then measured with a rotational rheometer and FTIR. Both materials show a tendency for chain scission which can

be seen as a reduction in viscosity. Changes in PP can be observed with both methods after 256 h of irradiation. Changes in PS become significant in rheology after 64 h but in FTIR only after 1024 h of irradiation. Due to the different chemical nature of the materials, the degradation of PS is rather linear with exposure, whereas the degradation of PP is more exponential. Using the zero shear viscosities obtained through extrapolations of the Cole-Cole and Carreau-Yasuda models, relative molecular weights are estimated with the aid of the power-law relationship between these two. These results are compared with the carbonyl indices determined from the FTIR spectra. Rheology is found to be a viable alternative for FTIR in certain situations.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research area: Sustainable Machine Systems, Department of Mechanical Engineering and Industrial Systems, Tampere Univ Technol, Tampere University of Technology, Dept Chem & Bioengn

Contributors: Mylläri, V., Ruoko, T., Syrjäälä, S.

Number of pages: 6

Publication date: 1 Jul 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Applied Polymer Science

Volume: 132

Issue number: 28

Article number: 42246

ISSN (Print): 0021-8995

Ratings:

Scopus rating (2015): CiteScore 1.74 SJR 0.587 SNIP 0.846

Original language: English

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

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

Electronic versions:

[comparison_of_rheology_and_ftir_post-print](#)

DOIs:

[10.1002/app.42246](https://doi.org/10.1002/app.42246)

URLs:

<http://urn.fi/URN:NBN:fi:tty-201612024837>

URLs:

<http://www.scopus.com/inward/record.url?scp=84928363110&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

ORG=mol,0.7

ORG=keb,0.2

ORG=mei,0.1

Source: Scopus

Source ID: 84928363110

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Kyoto Univ, Kyoto University, Grad Sch Engn, Dept Mol Engr, Nishikyo Ku, Natl Inst Adv Ind Sci & Technol, National Institute of Advanced Industrial Science & Technology (AIST), Nanomat Res Inst, Kyoto Univ, Kyoto University, Inst Integrated Cell Mat Sci WPI iCeMS, Nishikyo Ku

Contributors: Umeyama, T., Baek, J., Sato, Y., Suenaga, K., Abou-Chahine, F., Tkachenko, N. V., Lemmetyinen, H., Imahori, H.

Number of pages: 9

Publication date: Jul 2015

Peer-reviewed: Yes

Publication information

Journal: Nature Communications

Volume: 6

Article number: 7732

ISSN (Print): 2041-1723

Ratings:

Scopus rating (2015): CiteScore 11.23 SJR 6.287 SNIP 2.815

Original language: English

Keywords: FUNCTIONALIZATION, POTENTIALS, PERFORMANCE, DEPENDENCE, PORPHYRIN, VOLTAGE, C-60, N,M

DOIs:

10.1038/ncomms8732

Source: WOS

Source ID: 000358858500038

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

Synthesis and Photophysical Properties of Two Diazaporphyrin-Porphyrin Hetero Dimers in Polar and Nonpolar Solutions

Two diazaporphyrin (DAP)-porphyrin hetero dimers, in β -meso and β - β configurations, were prepared to study their photoinduced intramolecular electron transfer properties. The two meso nitrogen atoms in the porphyrin ring of DAP change its redox potential, making DAP more easily reduced, compared to its porphyrin counterpart. A charge-transfer from porphyrin to DAP in both hetero dimers was verified by versatile optical spectroscopic methods. The steady-state fluorescence spectra indicated an efficient intramolecular exciplex formation for both dimers. For the β -meso dimer, ultrafast time-resolved spectroscopic methods revealed the subpicosecond formation of two types of primary short-living (1-18 ps) intramolecular exciplexes, which relaxed in toluene to form a long-living final exciplex (1.4 ns) followed by a longer-living charge transfer complex (>5 ns). However, in benzonitrile, the lifetime of the final exciplex was longer (660 ps) as was that of the charge transfer complex (180 ps). The β - β analogue formed similar short-living exciplexes in both solvents, but the final exciplex and the charge transfer state had significantly shorter lifetimes. The electrochemical redox potential measurements and density functional theory calculations supported the proposed mechanism.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Tampere Graduate School in Information Science and Engineering (TISE), Kyoto Women's University, Department of Molecular Engineering, Graduate School of Engineering, Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto University, Kyushu University, Niigata University

Contributors: Abou-Chahine, F., Fujii, D., Imahori, H., Nakano, H., Tkachenko, N. V., Matano, Y., Lemmetyinen, H.

Number of pages: 10

Pages: 7328-7337

Publication date: 18 Jun 2015

Peer-reviewed: Yes

Early online date: 30 Jan 2015

Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 119

Issue number: 24

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.058

Original language: English

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

DOIs:

10.1021/jp510903a

URLs:

<http://www.scopus.com/inward/record.url?scp=84934905262&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84934905262

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

Catalytic effect of Ca and K on 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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio), Abo Akademi University, Åbo Akademi University, University of Jyväskylä, Process Chemistry Center, VTT Technical Research Centre of Finland

Contributors: Perander, M., DeMartini, N., Brink, A., Kramb, J., Karlström, O., Hemming, J., Moilanen, A., Konttinen, J., Hupa, M.

Number of pages: 9

Pages: 464-472

Publication date: 15 Jun 2015

Peer-reviewed: Yes

Publication information

Journal: Fuel

Volume: 150

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2015): CiteScore 4.46 SJR 1.781 SNIP 2.091

Original language: English

ASJC Scopus subject areas: Fuel Technology, Energy Engineering and Power Technology, Chemical Engineering(all), Organic Chemistry

Keywords: Biomass, Calcium, Char reactivity, CO, Gasification, Potassium

DOIs:

10.1016/j.fuel.2015.02.062

URLs:

<http://www.scopus.com/inward/record.url?scp=84924100908&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

EXT="Kramb, J."

Source: Scopus

Source ID: 84924100908

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

Polymorph crystal packing effects on charge transfer emission in the solid state

Condensation of 1,8-naphthalic anhydride with N,N-(dimethylamino)aniline produced the donor-acceptor compound DMIM, which crystallised from a chloroform-diethyl ether mixture to afford two different coloured crystal polymorphs. Crystals for one polymorph are small and green, whereas the other crystals are orange and needle-like. X-ray crystal structures for both polymorphs were determined. The donor N,N-dimethylaniline and acceptor naphthalimide groups are twisted with respect to each other; the degree of twist is marginally different for the two structures. The orange crystal polymorph crystallises in the monoclinic space group C2/c and contains two slightly different molecular conformers in the unit cell (calculated density is 1.410 g cm⁻³). The green crystal polymorph crystallises in the triclinic space group P1 and contains only one type of molecule in the unit cell (calculated density is 1.401 g cm⁻³). The crystal packing motifs for the two polymorphs are subtly different, explaining the small variance in the observed densities. Very weak room temperature emission was observed for DMIM in a CHCl₃ solution, but crystals deposited on a glass slide glowed when irradiated at 488 nm using a fluorescence microscope. Disparate solid-state emission spectra and lifetimes for the two polymorphic crystal forms are observed for the dyad. The emission is assigned to charge recombination fluorescence from a charge transfer state. This journal is

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 8

Pages: 3525-3532

Publication date: 1 Jun 2015

Peer-reviewed: Yes

Publication information

Journal: Chemical Science

Volume: 6

Issue number: 6

ISSN (Print): 2041-6520

Ratings:

Scopus rating (2015): CiteScore 9.13 SJR 4.647 SNIP 1.718

Original language: English

ASJC Scopus subject areas: Chemistry(all)

DOIs:

10.1039/c5sc01151e

URLs:

<http://www.scopus.com/inward/record.url?scp=84929589670&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84929589670

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

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

Publication status: Published

MoE 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

Contributors: Wang, J., Aihara, Y., Kinoshita, M., Mamiya, J., Priimagi, A., Shishido, A.

Number of pages: 7

Publication date: 6 May 2015

Peer-reviewed: Yes

Publication information

Journal: Scientific Reports

Volume: 5

Article number: 9890

ISSN (Print): 2045-2322

Ratings:

Scopus rating (2015): CiteScore 5.3 SJR 2.034 SNIP 1.588

Original language: English

Keywords: ORIENTATIONAL OPTICAL NONLINEARITY, GENERATION, STORAGE, LIGHT

DOIs:

10.1038/srep09890

Source: WOS

Source ID: 000354060200001

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Sorkio, A. E., Vuorimaa-Laukkanen, E. P., Hakola, H. M., Liang, H., Ujula, T. A., Valle-Delgado, J. J., Österberg, M., Yliperttula, M. L., Skottman, H.

Number of pages: 13

Pages: 257-269

Publication date: 1 May 2015

Peer-reviewed: Yes

Publication information

Journal: Biomaterials

Volume: 51

ISSN (Print): 0142-9612

Ratings:

Scopus rating (2015): CiteScore 9.35 SJR 3.404 SNIP 2.013

Original language: English

ASJC Scopus subject areas: Biomaterials, Bioengineering, Ceramics and Composites, Mechanics of Materials, Biophysics

Keywords: Biomimetic material, Collagen structure, Human embryonic stem cell, Langmuir Blodgett film, Retina, Retinal pigment epithelial cell

DOIs:

10.1016/j.biomaterials.2015.02.005

URLs:

<http://www.scopus.com/inward/record.url?scp=84924859980&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: WOS

Source ID: 000351796700025

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Free Univ Berlin, Free University of Berlin, Inst Food Hyg

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

Number of pages: 12

Publication date: May 2015

Peer-reviewed: Yes

Publication information

Journal: FEMS Microbiology Ecology

Volume: 91

Issue number: 5

Article number: 035

ISSN (Print): 0168-6496

Ratings:

Scopus rating (2015): CiteScore 3.77 SJR 1.698 SNIP 1.128

Original language: English

Keywords: *Vibrio parahaemolyticus*, whole genome gene expression, microarray, viable but not culturable state, VBNC, exponential phase, early stationary phase, *ESCHERICHIA-COLI* O157-H7, REAL-TIME PCR, NONCULTURABLE STATE, BIOFILM FORMATION, ADAPTIVE MUTAGENESIS, MESSENGER-RNA, *CHOLERA* O1, IN-SITU, BACTERIA, *VULNIFICUS*

DOIs:

10.1093/femsec/fiv035

Source: WOS

Source ID: 000355328100010

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

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

Publication status: Published

MoE 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

Contributors: Lajunen, T., Viitala, L., Kontturi, L., Laaksonen, T., Liang, H., Vuorimaa-Laukkanen, E., Viitala, T., Le Guevel, X., Yliperttula, M., Murtomaki, L., Urtti, A.

Number of pages: 14

Pages: 85-98

Publication date: 10 Apr 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Controlled Release

Volume: 203

ISSN (Print): 0168-3659

Ratings:

Scopus rating (2015): CiteScore 8.11 SJR 2.738 SNIP 2.062

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

DOIs:

10.1016/j.jconrel.2015.02.028

Bibliographical note

EXT="Laaksonen, Timo"

Source: WOS

Source ID: 000351696600010

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

Crystal structure of 2-methylpiperazine-1,4-dium bis(hydrogen maleate)

In the title salt,

$C_5H_{14}N_2^{2+} \cdot 2C_4H_3O_4^{2-}$, the asymmetric unit contains two independent 2-methylpiperazinium dications, which comprise a racemic pair, and four hydrogen maleate monoanions. In the roughly planar hydrogen maleate anions, intramolecular O-H \cdots O hydrogen bonds generate S(7) rings. In the crystal, the four independent anions are linked to the 2-methylpiperazinium cations through N-H \cdots O hydrogen bonds, forming two-dimensional layered structures lying parallel to (001).

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Laboratoire de chimie des Matériaux, Faculté des Sciences de Bizerte, Université de Carthage, Queensland University of Technology QUT

Contributors: Wecharine, I., Valkonen, A., Rzaigui, M., Sta, W. S., Smith, G.

Pages: o193-o194

Publication date: 1 Mar 2015

Peer-reviewed: Yes

Publication information

Journal: Acta Crystallographica Section E : Structure Reports Online

Volume: 71

Issue number: 3

ISSN (Print): 1600-5368

Ratings:

Scopus rating (2015): CiteScore 0.17 SJR 0.186 SNIP 0.118

Original language: English

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

Keywords: 2-methylpiperazine-1,4-dium, Crystal structure, Hydrogen bonding, Hydrogen maleate

DOIs:

10.1107/S2056989015003102

URLs:

<http://www.scopus.com/inward/record.url?scp=84928116257&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84928116257

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

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 (perylene diimide, PDI), and covalently linked porphyrin-fullerene donor acceptor dyad (D-A) layer (free base or Zn-porphyrin-fullerene dyad) were studied in this work by using a transient photocurrent method to monitor the electrical response in millisecond and second time scales. The active layers were in between two electrodes, which were insulated from them by several non-conductive octadecylamine films. Kinetics of charge generation, transport, and recombination was studied by monitoring light intensity dependent lifetimes of photocurrent signals. Both the signal intensities and lifetimes were increased by two orders of magnitude in the complete devices, H-(D-A)-E (or H vertical bar D-A vertical bar E), compared to the reference structures, H-(D-A) or (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.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Russian Acad Sci, Russian Academy of Sciences, Inst Gen Phys

Contributors: Alekseev, A. S., Lemmetyinen, H., Tolkki, A.

Number of pages: 9

Pages: 741-749

Publication date: Mar 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Nanoelectronics and Optoelectronics

Volume: 9

Issue number: 6

ISSN (Print): 1555-130X

Ratings:

Scopus rating (2015): CiteScore 0.56 SJR 0.192 SNIP 0.35

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

DOIs:

10.1166/jno.2014.1665

Bibliographical note

EXT="Alekseev, A. S."

Source: WOS

Source ID: 000353610000006

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

Encapsulation of secondary and tertiary ammonium salts by resorcinarenes and pyrogallarenes: The effect of size and charge concentration

The binding of different categories of alkyl ammonium (secondary and tertiary mono- and di-ammonium) salts with resorcinarenes and a pyrogallarene through weak interactions was analysed in all phases. 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.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, University of Jyväskylä

Contributors: Beyeh, N. K., Pan, F., Valkonen, A., Rissanen, K.

Number of pages: 7

Pages: 1182-1188

Publication date: 7 Feb 2015

Peer-reviewed: Yes

Publication information

Journal: CrystEngComm

Volume: 17

Issue number: 5

ISSN (Print): 1466-8033

Ratings:

Scopus rating (2015): CiteScore 3.83 SJR 1.04 SNIP 0.98

Original language: English

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

DOIs:

10.1039/c4ce01927j

URLs:

<http://www.scopus.com/inward/record.url?scp=84921648549&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84921648549

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, Tampere University of Technology, Urban circular bioeconomy (UrCirBio), Centre for Drug Research, Division of Pharmaceutical Biosciences, Helsinki University, Division of Pharmaceutical Chemistry and Technology

Contributors: Nybond, S., Ghemtio, L., Nawrot, D. A., Karp, M., Xhaard, H., Tammela, P.

Number of pages: 9

Pages: 25-33

Publication date: 1 Feb 2015

Peer-reviewed: Yes

Publication information

Journal: Assay and Drug Development Technologies

Volume: 13

Issue number: 1

ISSN (Print): 1540-658X

Ratings:

Scopus rating (2015): CiteScore 1.05 SJR 0.843 SNIP 0.643

Original language: English

ASJC Scopus subject areas: Drug Discovery, Molecular Medicine

DOIs:

10.1089/adt.2014.625

URLs:

<http://www.scopus.com/inward/record.url?scp=84923872765&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84923872765

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

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, Tampere Univ Technol, Tampere University of Technology, Dept Chem & Bioengn

Contributors: Rosholm, T., Gois, P. M. P., Franzen, R., R. Candeias, N.

Number of pages: 8

Pages: 39-46

Publication date: Feb 2015

Peer-reviewed: Yes

Publication information

Journal: Chemistryopen

Volume: 4

Issue number: 1

ISSN (Print): 2191-1363

Ratings:

Scopus rating (2015): CiteScore 3.23 SJR 1.266 SNIP 0.73

Original language: English

Keywords: amines, boron, glycerol, multicomponent reactions, sustainable chemistry, CROSS-COUPLING REACTIONS, ALPHA-AMINO-ACIDS, ONE-POT, ORGANOBORONIC ACIDS, SOLVENT, DERIVATIVES, ALDEHYDES, HYDROGEN , SALICYLALDEHYDES, 2H-CHROMENES

DOIs:

10.1002/open.201402066

Bibliographical note

AUX=orc,"Rosholm, Tomi"

Source: WOS

Source ID: 000349953300006

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

Supramolecular hierarchy among halogen and hydrogen bond donors in light-induced surface patterning

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Aalto University, VTT Technical Research Centre of Finland, Politecn Milan, Polytechnic University of Milan, NFMLab, DCMIC Giulio Natta, ISTM-CNR, Institute of Molecular Sciences and Technologies of CNR, Università Degli Studi di Milano, McGill University, Politecnico di Milano

Contributors: Saccone, M., Dichiarante, V., Forni, A., Goulet-Hanssens, A., Cavallo, G., Vapaavuori, J., Terraneo, G., Barrett, C. J., Resnati, G., Metrangolo, P., Priimägi, A.

Number of pages: 10

Pages: 759-768

Publication date: 28 Jan 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry C

Volume: 3

ISSN (Print): 2050-7534

Ratings:

Scopus rating (2015): CiteScore 5.32 SJR 1.713 SNIP 1.477

Original language: English

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

DOIs:

10.1039/c4tc02315c

URLs:

<http://www.scopus.com/inward/record.url?scp=84925407935&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

EXT="Saccone, Marco"

EXT="Vapaavuori, Jaana"

Source: Scopus

Source ID: 84925407935

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

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Tampere Univ Technol, Tampere University of Technology, Dept Chem & Bioengn

Contributors: Stranius, K., George, L., Efimov, A., Ruoko, T., Pohjola, J., Tkachenko, N. V.

Number of pages: 9

Pages: 944-952

Publication date: 27 Jan 2015

Peer-reviewed: Yes

Publication information

Journal: Langmuir

Volume: 31

Issue number: 3

ISSN (Print): 0743-7463

Ratings:

Scopus rating (2015): CiteScore 4.33 SJR 1.65 SNIP 1.271

Original language: English

Keywords: PHOTOINDUCED ELECTRON-TRANSFER, PORPHYRIN-FULLERENE DYADS, SOLAR-CELLS, CHARGE-SEPARATION, STATE, MONOLAYERS, DYNAMICS, ENERGY, PERFORMANCE, GENERATION

Electronic versions:

Photophysical_study_post-print

DOIs:

10.1021/la5025873

URLs:

<http://urn.fi/URN:NBN:fi:tty-201612094852>

Bibliographical note

AUX=mol,"Pohjola, Juuso"

Source: WOS

Source ID: 000348689700008

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

Controlled Regioselective Amination of Peryleneimides

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: George, L., Ahmed, Z., Lemmetyinen, H., Efimov, A.

Number of pages: 7

Pages: 584-590

Publication date: 14 Jan 2015

Peer-reviewed: Yes

Early online date: 12 Dec 2014

Publication information

Journal: European Journal of Organic Chemistry

Volume: 2015

Issue number: 3

ISSN (Print): 1434-193X

Ratings:

Scopus rating (2015): CiteScore 2.88 SJR 1.225 SNIP 0.785

Original language: English

DOIs:

10.1002/ejoc.201403299

URLs:

<http://onlinelibrary.wiley.com/doi/10.1002/ejoc.201403299/abstract>

Bibliographical note

Article first published online: 12 DEC 2014
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-12-30
Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA

Source: researchoutputwizard

Source ID: 337

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

Aryl end-capped quaterthiophenes applied as anode interfacial layers in inverted organic solar cells

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, University of Oulu, Department of Chemistry and Mathematics, Faculty of Petroleum and Mining Engineering, Suez University

Contributors: Heiskanen, J. P., Manninen, V. M., Pankov, D., Omar, W. A. E., Kastinen, T., Hukka, T. I., Lemmetyinen, H. J., Hormi, O. E. O.

Number of pages: 11

Pages: 196-206

Publication date: 1 Jan 2015

Peer-reviewed: Yes

Publication information

Journal: Thin Solid Films

Volume: 574

ISSN (Print): 0040-6090

Ratings:

Scopus rating (2015): CiteScore 1.84 SJR 0.68 SNIP 0.923

Original language: English

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

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

DOIs:

10.1016/j.tsf.2014.12.007

URLs:

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

Bibliographical note

EXT="Heiskanen, J. P."

Source: Scopus

Source ID: 84921286591

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

Photophysical properties of Sn (IV)tetraphenylporphyrin-pyrene dyad with a β -vinyl linker

A Sn(IV)tetraphenylporphyrin (T) has been functionalized with a β -vinyl pyrene (P) and the photophysical properties of the formed dyad (T-P) with its corresponding precursors were studied in three solvents with different polarities using steady-state and time-resolved measurements in ps and fs timescales. When the pyrene moiety is excited at $\lambda_{ex} = 340$ nm, the fluorescence spectroscopy experiments indicate in all the studied solvents, an efficient quenching of the pyrene emission. When excited at either $\lambda_{ex} = 340$ nm or $\lambda_{ex} = 405$ nm, where porphyrin absorbs, a new emissive excited state complex (T-P)* is observed at wavelengths close to the parent porphyrin emission. The emission is more pronounced in nonpolar hexane showing a mono-exponential decay, but bi-exponential decays are observed in more polar dichloromethane and acetonitrile. When the porphyrin moiety is excited at $\lambda_{ex} = 425$ 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 ν (T-P)*state, with a lifetime of 80-100 ps.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 13

Pages: 288-300

Publication date: 1 Jan 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Porphyrins and Phthalocyanines

Volume: 19

Issue number: 1-3

ISSN (Print): 1088-4246

Ratings:

Scopus rating (2015): CiteScore 1.17 SJR 0.413 SNIP 0.457

Original language: English

ASJC Scopus subject areas: Chemistry(all)

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

DOIs:

10.1142/S1088424615500108

URLs:

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

Source: Scopus

Source ID: 84928483683

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

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-1,2-(5,5"-Dimethyl-(2,2':3',2"-terthiophene) vinylene (BSTV) and octathienylene vinylene (BOTV) (E)-Bis-1,2-(5,5"-Dimethyl-(2,2':5',2":3',2"-tetrathiophene) vinylene oligomers, have been synthesized and used as electron donor or dopant in a bulk heterojunction poly(3-hexylthiophene) (P3HT), [6,6]-phenyl C61-butyric acid methylester (PCBM), Organic Photovoltaic cell.

General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Universidad de Chile

Contributors: Martinez, F., Neculqueo, G., Vasquez, S. O., Lemmetyinen, H., Efimov, A., Vivo, P.

Number of pages: 7

Pages: 19-25

Publication date: 2015

Host publication information

Title of host publication: Materials Research Society Symposium Proceedings

Volume: 1737

Publisher: MATERIALS RESEARCH SOCIETY

ISBN (Print): 9781510806177

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

DOIs:

10.1557/opl.2015.529

URLs:

<http://www.scopus.com/inward/record.url?scp=84938866855&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84938866855

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

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/m^2 . Optimal mediator concentrations with respect to the achieved maximum power output for MB, NR and HNQ were 300 μM , 200 μM and 50 μM , respectively. The results demonstrate that tin-coated copper mesh showed a higher biocompatibility and electrical conductivity.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Firat University

Contributors: Taskan, E., Özkaya, B., Hasar, H.

Number of pages: 9

Pages: 320-328

Publication date: 2015

Peer-reviewed: Yes

Publication information

Journal: Water Science and Technology

Volume: 71

Issue number: 3

ISSN (Print): 0273-1223

Ratings:

Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.596

Original language: English

ASJC Scopus subject areas: Environmental Engineering, Water Science and Technology

Keywords: Internal resistance, Mediator, Microbial fuel cell, Power output

DOIs:

10.2166/wst.2014.487

URLs:

<http://www.scopus.com/inward/record.url?scp=84925246339&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84925246339

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

$\text{Fe}_2\text{O}_3\text{-TiO}_2$ Nano-heterostructure Photoanodes for Highly Efficient Solar Water Oxidation

Harnessing solar energy for the production of clean hydrogen by photo-electrochemical water splitting represents a very attractive, but challenging approach for sustainable energy generation. In this regard, the fabrication of $\text{Fe}_2\text{O}_3\text{-TiO}_2$

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 Fe_2O_3 , is achieved by atomic layer deposition of TiO_2 over hematite ($\alpha\text{-Fe}_2\text{O}_3$) nanostructures fabricated by plasma enhanced-chemical vapor deposition and final annealing at 650 °C. The adopted approach enables an intimate $\text{Fe}_2\text{O}_3\text{-TiO}_2$ coupling, resulting in an electronic interplay at the $\text{Fe}_2\text{O}_3/\text{TiO}_2$ interface. The reasons for the photocurrent enhancement determined by TiO_2 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

Publication status: Published

MoE 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

Contributors: Barreca, D., Carraro, G., Gasparotto, A., Maccato, C., Warwick, M. E. A., Kaunisto, K., Sada, C., Turner, S., Gönüllü, Y., Ruoko, T., Borgese, L., Bontempi, E., Van Tendeloo, G., Lemmetyinen, H., Mathur, S.

Publication date: 2015

Peer-reviewed: Yes

Publication information

Journal: Advanced Materials Interfaces

Volume: 2

Issue number: 17

ISSN (Print): 2196-7350

Ratings:

Scopus rating (2015): CiteScore 2.47 SJR 1.193 SNIP 0.738

Original language: English

ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials

Keywords: FeO, Nano-heterostructures, Photoelectrochemistry, TiO, Water splitting

Electronic versions:

Fe2O3-TiO2_post-print

DOIs:

10.1002/admi.201500313

URLs:

<http://urn.fi/URN:NBN:fi:tty-201612024841>

Source: Scopus

Source ID: 84955180397

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

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

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, VTT Technical Research Centre of Finland, Politecnico di Milano, Aalto University

Contributors: Saccone, M., Cavallo, G., Metrangolo, P., Resnati, G., Priimägi, A.

Number of pages: 20

Pages: 147-166

Publication date: 2015

Host publication information

Title of host publication: Halogen Bonding II : Impact on Materials Chemistry and Life Sciences

Publisher: Springer International Publishing

ISBN (Print): 978-3-319-15731-3

ISBN (Electronic): 978-3-319-15732-0

Publication series

Name: Topics in Current Chemistry

Volume: 359

ISSN (Print): 0340-1022

ASJC Scopus subject areas: Chemistry(all)

Keywords: Azobenzene, Halogen bonding, Liquid crystals, Photoresponsive materials, Polymers

DOIs:

10.1007/128_2014_615

URLs:

<http://www.scopus.com/inward/record.url?scp=84930627375&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

JUFOID=68510

EXT="Saccone, Marco"

Source: Scopus

Source ID: 84930627375

Research output: Chapter in Book/Report/Conference proceeding > Chapter > Scientific > peer-review

Halogen bonding enhances nonlinear optical response in poled supramolecular polymers

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Optics, Research group: Nonlinear Optics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Tampere Univ Technol, Tampere University of Technology, Dept Phys, Univ Milan, Consiglio Nazionale delle Ricerche (CNR), University of Milan, Inst Mol Sci & Technol, CNR, ISTM, Politecn Milan, Polytechnic University of Milan, NFMLab, DCMIC Giulio Natta, Aalto University

Contributors: Virkki, M., Tuominen, O., Forni, A., Saccone, M., Metrangolo, P., Resnati, G., Kauranen, M., Priimägi, A.

Number of pages: 4

Pages: 3003-3006

Publication date: 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry C

Volume: 3

ISSN (Print): 2050-7534

Ratings:

Scopus rating (2015): CiteScore 5.32 SJR 1.713 SNIP 1.477

Original language: English

Keywords: FILMS

DOIs:

10.1039/c5tc00484e

Bibliographical note

AUX=orc,"Tuominen, Ossi"

EXT="Saccone, Marco"

ORG=fys,0.5

ORG=keb,0.5

Source: WOS

Source ID: 000351601200002

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

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

Background Extracellular vesicles (EVs) are naturally occurring membrane particles that mediate intercellular communication by delivering molecular information between cells. In this study, we investigated the effectiveness of two different populations of EVs (microvesicle- and exosome-enriched) as carriers of Paclitaxel to autologous prostate cancer cells. Methods EVs were isolated from LNCaP- and PC-3 prostate cancer cell cultures using differential centrifugation and characterized by electron microscopy, nanoparticle tracking analysis, and Western blot. The uptake of microvesicles and

exosomes by the autologous prostate cancer cells was assessed by flow cytometry and confocal microscopy. The EVs were loaded with Paclitaxel and the effectiveness of EV-mediated drug delivery was assessed with viability assays. The distribution of EVs and EV-delivered Paclitaxel in cells was inspected by confocal microscopy. Results Our main finding was that the loading of Paclitaxel to autologous prostate cancer cell-derived EVs increased its cytotoxic effect. This capacity was independent of the EV population and the cell line tested. Although the EVs without the drug increased cancer cell viability, the net effect of enhanced cytotoxicity remained. Both EV populations delivered Paclitaxel to the recipient cells through endocytosis, leading to the release of the drug from within the cells. The removal of EV surface proteins did not affect exosomes, while the drug delivery mediated by microvesicles was partially inhibited. Conclusions Cancer cell-derived EVs can be used as effective carriers of Paclitaxel to their parental cells, bringing the drug into the cells through an endocytic pathway and increasing its cytotoxicity. However, due to the increased cell viability, the use of cancer cell-derived EVs must be further investigated before any clinical applications can be designed.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Saari, H., Lázaro-Ibáñez, E., Viitala, T., Vuorimaa-Laukkanen, E., Siljander, P., Yliperttula, M.

Number of pages: 11

Pages: 727-737

Publication date: 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Controlled Release

Volume: 220

ISSN (Print): 0168-3659

Ratings:

Scopus rating (2015): CiteScore 8.11 SJR 2.738 SNIP 2.062

Original language: English

Keywords: Extracellular vesicles, Microvesicles, Exosomes, Paclitaxel, Drug delivery, Prostate cancer

DOIs:

10.1016/j.jconrel.2015.09.031

Source: RIS

Source ID: urn:1C9EE295CFC4CF9BEC0AB2A50515AF77

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

Nano-graphite cold cathodes for electric solar wind sail

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Kleshch, V. I., Smolnikova, E. A., Orekhov, A. S., Kalvas, T., Tarvainen, O., Kauppinen, J., Nuottajärvi, A., Koivisto, H., Janhunen, P., Obraztsov, A. N.

Number of pages: 5

Pages: 132-136

Publication date: 2015

Peer-reviewed: Yes

Publication information

Journal: Carbon

Volume: 81

ISSN (Print): 0008-6223

Ratings:

Scopus rating (2015): CiteScore 6.53 SJR 1.988 SNIP 1.739

Original language: English

DOIs:

10.1016/j.carbon.2014.09.038

Bibliographical note

siirretään portfolio15
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2015-01-15
Publisher name: Pergamon; American Carbon Society

Source: researchoutputwizard

Source ID: 13

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-ethylenedioxythienylvinylene (EDOTV) unit into the conjugated bridge, which increases the distance between D and A, but, at the same time, provides increased electronic communication between them. Two essential outcomes that result from the introduction of the EDOTV unit in the bridge are as follows: 1) faster charge recombination, which indicates enhanced electronic coupling between the charge-separated and ground electronic states; and 2) the disappearance of the intramolecular exciplex, which mediates photoinduced charge separation in the ZnP-Ph-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.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Universitat Politècnica de Valencia, Spain, Universidad de Castilla-La Mancha

Contributors: Pelado, B., Abou-Chahine, F., Calbo, J., Caballero, R., delaCruz, P., Junquera-Hernández, J. M., Ortí, E., Tkachenko, N. V., Langa, F.

Number of pages: 12

Pages: 5814-5825

Publication date: 2015

Peer-reviewed: Yes

Publication information

Journal: Chemistry: A European Journal

Volume: 21

Issue number: 15

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2015): CiteScore 4.99 SJR 2.461 SNIP 1.195

Original language: English

ASJC Scopus subject areas: Chemistry(all)

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

DOIs:

10.1002/chem.201406514

URLs:

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

Source: Scopus

Source ID: 84925396738

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Institute of Organic Chemistry of the Polish Academy of Sciences, Politechnika Warszawska, Warsaw Univ Technol, Warsaw University of Technology, Fac Phys, Opt Div, Department of Laboratory Diagnostics and Clinical Immunology of Developmental Age, Medical University of Warsaw, Department of Chemistry and Bioengineering, Tampere University of Technology

Contributors: Stasyuk, A. J., Smoleń, S., Glodkowska-Mrowka, E., Brutkowski, W., Cyrański, M. K., Tkachenko, N., Gryko, D. T.

Number of pages: 6
Pages: 553-558
Publication date: 2015
Peer-reviewed: Yes

Publication information

Journal: Chemistry - An Asian Journal

Volume: 10

Issue number: 3

ISSN (Print): 1861-4728

Ratings:

Scopus rating (2015): CiteScore 4.41 SJR 1.742 SNIP 0.906

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Cyclization, Fluorescence, Heterocycles, Pyrenes, Quinolines

DOIs:

10.1002/asia.201403339

URLs:

<http://www.scopus.com/inward/record.url?scp=84923364824&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84923364824

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

Van der Waals interactions are critical in Car-Parrinello molecular dynamics simulations of porphyrin-fullerene dyads

The interplay between electrostatic and van der Waals (vdW) interactions in porphyrin-C₆₀ dyads is still under debate despite its importance in influencing the structural characteristics of such complexes considered for various applications in molecular photovoltaics. In this article, we sample the conformational space of a porphyrin-C₆₀ dyad using Car-Parrinello molecular dynamics simulations with and without empirical vdW corrections. Long-range vdW interactions, which are poorly described by the commonly used density functional theory functionals, prove to be essential for a proper dynamics of the dyad moieties. Inclusion of vdW corrections brings porphyrin and C₆₀ close together in an orientation that is in agreement with experimental observations. The structural differences arising from the vdW corrections are shown to be significant for several properties and potentially less important for others. Additionally, our Mulliken population analysis reveals that contrary to the common belief, porphyrin is not the primary electron donating moiety for C₆₀. In the considered dyad, fullerene's affinity for electrons is primarily satisfied by charge transfer from the amide group of the linker. However, we show that in the absence of another suitable bound donor, C₆₀ can withdraw electrons from porphyrin if it is sufficiently close.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Computational Science X (CompX), Frontier Photonics, VTT Technical Research Centre of Finland

Contributors: Karilainen, T., Cramariuc, O., Kuisma, M., Tappura, K., Hukka, T. I.

Number of pages: 10

Pages: 612-621

Publication date: 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Computational Chemistry

Volume: 36

Issue number: 9

ISSN (Print): 0192-8651

Ratings:

Scopus rating (2015): CiteScore 3.81 SJR 1.382 SNIP 1.368

Original language: English

ASJC Scopus subject areas: Chemistry(all), Computational Mathematics

Keywords: Car-Parrinello molecular dynamics, Fullerene, Porphyrin, Time-dependent-density functional theory

DOIs:

10.1002/jcc.23834

URLs:

<http://www.scopus.com/inward/record.url?scp=84923259668&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

ORG=fys,0.5

ORG=keb,0.5

Source: Scopus

Source ID: 84923259668

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

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.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology, Frontier Photonics, Politechnika Warszawska, Foundation for Research and Technology-Hellas, Institute of Electronic Structure and Laser, Institute of Organic Chemistry of the Polish Academy of Sciences

Contributors: Nazir, R., Bourquard, F., Balčiūnas, E., Smoleń, S., Gray, D., Tkachenko, N. V., Farsari, M., Gryko, D. T.

Number of pages: 9

Pages: 682-690

Publication date: 2015

Peer-reviewed: Yes

Publication information

Journal: ChemPhysChem

Volume: 16

Issue number: 3

ISSN (Print): 1439-4235

Ratings:

Scopus rating (2015): CiteScore 3.21 SJR 1.303 SNIP 0.889

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Atomic and Molecular Physics, and Optics

Keywords: Aldol reaction, Ketones, Photosensitizers, Polymerization, Two-photon absorption

DOIs:

10.1002/cphc.201402646

URLs:

<http://www.scopus.com/inward/record.url?scp=84920105777&partnerID=8YFLogxK> (Link to publication in Scopus)

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere Univ Technol, Tampere University of Technology, Dept Chem & Bioengn

Contributors: 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 (2014): CiteScore 1.39 SJR 0.486 SNIP 0.549

Original language: English

Keywords: phthalocyanine, phthalocyanine-fullerene dyad, photovoltage, molecular modeling, solar cell, Langmuir-Schafer, PHOTOINDUCED ELECTRON-TRANSFER, MOLECULAR-FORCE FIELD, PORPHYRIN-FULLERENE, CHARGE SEPARATION, DENSITY, MMFF94, C-60, BISADDUCTS, ISOMERS, FILMS

DOIs:

10.1142/S1088424614500928

Bibliographical note

AUX=keb,"Mundy, M. Elizabeth"

Source: WOS

Source ID: 000349121200004

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

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

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Department of Chemistry and Bioengineering

Contributors: Stranius, K.

Number of pages: 147

Publication date: 26 Nov 2014

Publication information

Place of publication: Tampere

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-3412-6

ISBN (Electronic): 978-952-15-3424-9

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Publisher: Tampere University of Technology

Volume: 1269

ISSN (Print): 1459-2045

Electronic versions:

stranius.pdf

URLs:

<http://urn.fi/URN:ISBN:978-952-15-3424-9>

Bibliographical note

Awarding institution: Tampere University of Technology

Source: researchoutputwizard

Source ID: 1553

Research output: Book/Report > Doctoral thesis > Collection of Articles

Molecular modifications of active and anode buffer layers of bulk heterojunction solar cell

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

General information

Publication status: Published
MoE publication type: G5 Doctoral dissertation (article)
Organisations: Department of Chemistry and Bioengineering
Contributors: Manninen, V.
Publication date: 23 May 2014

Publication information

Publisher: Tampere University of Technology
ISBN (Print): 978-952-15-3293-1
ISBN (Electronic): 978-952-15-3299-3
Original language: English

Publication series

Name: Tampere University of Technology. Publication
Publisher: Tampere University of Technology
Volume: 1214
ISSN (Print): 1459-2045
ISSN (Electronic): 1459-2045
Electronic versions:
manninen.pdf
URLs:
<http://urn.fi/URN:ISBN:978-952-15-3299-3>

Bibliographical note

Awarding institution: Tampere University of Technology
Source: researchoutputwizzard
Source ID: 1024
Research output: Book/Report > Doctoral thesis > Collection of Articles

Binding Affinity and Mechanism of Polymer-DNA Polyplexes for Gene Delivery

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

General information

Publication status: Published
MoE publication type: G5 Doctoral dissertation (article)
Organisations: Department of Chemistry and Bioengineering
Contributors: Ketola, T. C.

Number of pages: 64
Publication date: 31 Jan 2014

Publication information

Publisher: Tampere University of Technology
ISBN (Print): 978-952-15-3216-0
Original language: English

Publication series

Name: Tampere University of Technology. Publication
Publisher: Tampere University of Technology
No.: 1187
ISSN (Print): 1459-2045
Electronic versions:
ketola.pdf
URLs:
<http://urn.fi/URN:ISBN:978-952-15-3223-8>

Bibliographical note

Awarding institution: Tampere University of Technology
Source: researchoutputwizard
Source ID: 705
Research output: Book/Report > Doctoral thesis > Collection of Articles

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Contributors: 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 (2014): CiteScore 8.89 SJR 3.595 SNIP 2.204
Original language: English
DOIs:
[10.1021/cm5023129](https://doi.org/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: Contribution to journal > Article > Scientific > peer-review

Charge-Transfer Dynamics in Poly(3-hexylthiophene):Perylenediimide-C-60 Blend Films Studied by Ultrafast Transient Absorption

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Kaunisto, K. M., Vivo, P., Dubey, R. K., Chukharev, V. I., Efimov, A., Tkachenko, N. V., Lemmetyinen, H. J.
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 (2014): CiteScore 5.08 SJR 2.032 SNIP 1.435
Original language: English
DOIs:
10.1021/jp501605k

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-08-27
Publisher name: American Chemical Society
Source: researchoutputwizard
Source ID: 689
Research output: Contribution to journal > Article > Scientific > peer-review

Deprotonation of resorcinarenes by mono- and diamine bases: complexation and intermolecular interactions in the solid state

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Contributors: 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 (2014): CiteScore 3.97 SJR 1.128 SNIP 1.094
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
Research output: Contribution to journal > Article > Scientific > peer-review

Dynamics of time-resolved photoluminescence in GaInNAs and GaNAsSb solar cells

General information

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

Publication information

Journal: Nanoscale Research Letters

Volume: 9

Article number: 80

ISSN (Print): 1931-7573

Ratings:

Scopus rating (2014): CiteScore 2.15 SJR 0.762 SNIP 1.064

Original language: English

DOIs:

10.1186/1556-276X-9-80

Bibliographical note

Contribution: organisation=orc,FACT1=0.7
Contribution: organisation=keb,FACT2=0.3
Portfolio EDEND: 2014-04-29
Publisher name: SpringerOpen

Source: researchoutputwizard

Source ID: 371

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

Effect of mutual position of electron donor and acceptor on photoinduced electron transfer in supramolecular chlorophyll-fullerene dyads

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2014): CiteScore 2.65 SJR 1.159 SNIP 1.061

Original language: English

DOIs:

10.1021/jp412442t

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-04-29
Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 1554

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

Electricity generating capacity and performance deterioration of a microbial fuel cell fed with beer brewery wastewater

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Köroglu, 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 (2014): CiteScore 2.05 SJR 0.745 SNIP 0.932
Original language: English
DOIs:
10.1016/j.jbiosc.2014.05.006

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2015-03-02
Publisher name: Society for Biotechnology, Japan
Source: researchoutputwizard
Source ID: 762
Research output: Contribution to journal > Article > Scientific > peer-review

Excited State Intramolecular Proton Transfer in pi-Expanded Phenazine-Derived Phenols

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: 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 (2014): CiteScore 2.65 SJR 1.159 SNIP 1.061
Original language: English
DOIs:
10.1021/jp411395c

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-05-08
Publisher name: American Chemical Society
Source: researchoutputwizard
Source ID: 1275
Research output: Contribution to journal > Article > Scientific > peer-review

Femtosecond spectroscopy of the dithiolate Cu(II) and Ni(II) complexes

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: 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 (2014): CiteScore 4.06 SJR 1.389 SNIP 1.064
Original language: English
DOIs:
10.1039/C4DT01407C

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2015-01-12
Publisher name: R S C Publications
Source: researchoutputwizard
Source ID: 1281
Research output: Contribution to journal > Article > Scientific > peer-review

Formation of a stable polymer blue phase under UV irradiation of Langmuir-Schaefer films of diin N-arylcarbamate derivative

General information

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

Publication information

Journal: Bulletin of the Lebedev Physics Institute
Volume: 41
Issue number: 6
ISSN (Print): 1068-3356
Ratings:
Scopus rating (2014): CiteScore 0.13 SJR 0.127 SNIP 0.201
Original language: English
DOIs:
10.3103/S1068335614060025

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-08-27
Publisher name: Allerton Press, Inc.; Rossiiskaya Akademiya Nauk
Source: researchoutputwizard
Source ID: 86
Research output: Contribution to journal > Article > Scientific > peer-review

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Contributors: 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 (2014): CiteScore 5.08 SJR 2.032 SNIP 1.435

Original language: English

DOIs:

10.1021/jp507486x

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-11-20
Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 1526

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Frontier Photonics

Contributors: Koskela, J. E., Vapaavuori, J., Ras, R. H. A., Priimagi, A.

Number of pages: 5

Pages: 1196-1200

Publication date: 2014

Peer-reviewed: Yes

Publication information

Journal: ACS Macro Letters

Volume: 3

ISSN (Print): 2161-1653

Ratings:

Scopus rating (2014): CiteScore 5.66 SJR 2.515 SNIP 1.611

Original language: English

DOIs:

10.1021/mz500616q

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-11-20
Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 787

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2014): CiteScore 4.29 SJR 1.771 SNIP 1.231

Original language: English

DOIs:

10.1039/c4cp01165a

Additional files:

MNiskanen_TIHukka_PCCP_2014_16_13294_13305

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-06-27
Publisher name: R S C Publications

Source: researchoutputwizard

Source ID: 1150

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

Monoisomeric phthalocyanines and phthalocyanine-fullerene dyads with polar side chains: synthesis, modeling, and photovoltage

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2014): CiteScore 5.08 SJR 2.032 SNIP 1.435

Original language: English

DOIs:

10.1021/jp4096002

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-06-27
Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 1344

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

Organic-inorganic azafullerene-gold C59N-Au nanohybrid: Synthesis, characterization, and properties

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Rotas, G., Niemi, M., Tkachenko, N. V., Zhao, S., Shinohara, H., Tagmatarchis, 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 (2014): CiteScore 5.51 SJR 2.526 SNIP 1.222

Original language: English

DOIs:

10.1002/chem.201403517

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-11-20
Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA

Source: researchoutputwizard

Source ID: 1407

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Hakola, H., Pyymaki Perros, A., Myllyperkiö, P., Kurotobi, K., Lipsanen, H., Imahori, H., Lemmetyinen, H., Tkachenko, N. V.

Number of pages: 5

Pages: 47-51

Publication date: 2014

Peer-reviewed: Yes

Publication information

Journal: Chemical Physics Letters

Volume: 592

ISSN (Print): 0009-2614

Ratings:

Scopus rating (2014): CiteScore 1.83 SJR 0.755 SNIP 0.762

Original language: English

DOIs:

10.1016/j.cplett.2013.11.028

Bibliographical note

poistettu tupla r=123, r=357, r=523 portfolio14
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: Elsevier

Source: researchoutputwizard

Source ID: 397

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Beyeh, N. K., Ala-Korpi, A., Cetina, M., Valkonen, A., Rissanen, K.

Number of pages: 7

Pages: 15144-15150

Publication date: 2014

Peer-reviewed: Yes

Publication information

Journal: Chemistry: A European Journal

Volume: 20

Issue number: 46

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2014): CiteScore 5.51 SJR 2.526 SNIP 1.222

Original language: English

DOIs:

10.1002/chem.201402533

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-11-20
Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA
Source: researchoutputwizard
Source ID: 166
Research output: Contribution to journal > Article > Scientific > peer-review

ROFRET: A Molecular-Scale Fluorescent Probe Displaying Viscosity-Enhanced Intramolecular Förster Energy Transfer

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: 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 (2014): CiteScore 3.12 SJR 1.37 SNIP 0.9
Original language: English
DOIs:
10.1002/cphc.201402320

Bibliographical note

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

Slow charge recombination and enhanced photoelectrochemical properties of Diazaporphyrin-Fullerene linked dyad

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: 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 (2014): CiteScore 5.08 SJR 2.032 SNIP 1.435
Original language: English
DOIs:
10.1021/jp410436f

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-05-28
Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 1813

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

Solid state anion-pi interactions involving polyhalides

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: 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 (2014): CiteScore 4.06 SJR 1.389 SNIP 1.064

Original language: English

DOIs:

10.1039/c3dt52960f

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2015-01-13
Publisher name: R S C Publications

Source: researchoutputwizard

Source ID: 346

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

Spectroscopic study of a synthesized Alq3 end-capped oligothiophene applied in organic solar cells

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Manninen, V. M., Heiskanen, J. P., Kaunisto, K. M., Hormi, O. E. O., Lemmetyinen, H. J.

Number of pages: 10

Pages: 8846-8855

Publication date: 2014

Peer-reviewed: Yes

Publication information

Journal: RSC Advances

Volume: 4

Issue number: 17

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2014): CiteScore 3.87 SJR 1.113 SNIP 0.962

Original language: English

DOIs:

10.1039/c3ra47367h

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-09-30
Publisher name: R S C Publications

Source: researchoutputwizard

Source ID: 1025

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

Subcellular localization of bacteriophage PRD1 proteins in Escherichia coli

General information

Publication status: Published

MoE 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)

Contributors: Karttunen, J., Mäntynen, S., Ihalainen, T. O., Lehtivuori, H., Tkachenko, N. V., Vihinen-Ranta, M., Ihalainen, J. A., Bamford, J. K., Oksanen, H. M.

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 (2014): CiteScore 2.63 SJR 1.213 SNIP 0.923

Original language: English

DOIs:

10.1016/j.virusres.2013.11.015

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-05-28
Publisher name: Elsevier BV

Source: researchoutputwizard

Source ID: 669

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

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

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Department of Chemistry and Bioengineering

Contributors: Ranta, J.

Number of pages: 160

Publication date: 2014

Publication information

Place of publication: Tampere

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-3389-1

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Publisher: Tampere University of Technology

Volume: 1254

ISSN (Print): 1459-2045

Bibliographical note

Awarding institution: Tampere University of Technology

Source: researchoutputwizard

Source ID: 1343

Research output: Book/Report > Doctoral thesis > Collection of Articles

Synthesis and properties of a meso- tris-ferrocene appended zinc(II) porphyrin and a critical evaluation of its dye sensitised solar cell (DSSC) performance

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Sirbu, D., Turta, C., Benniston, A., Abou-Chahine, F., Lemmetyinen, H., Tkachenko, N., Wood, C., Gibson, E.

Number of pages: 10

Pages: 22733-22742

Publication date: 2014

Peer-reviewed: Yes

Publication information

Journal: RSC Advances

Volume: 4

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2014): CiteScore 3.87 SJR 1.113 SNIP 0.962

Original language: English

DOIs:

10.1039/c4ra03105a

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-06-29
Publisher name: R S C Publications

Source: researchoutputwizard

Source ID: 1521

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

Tetraiodoethynyl resorcinarene cavitands as multivalent halogen bond donors

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: 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 (2014): CiteScore 6.83 SJR 2.692 SNIP 1.427

Original language: English

DOIs:

10.1039/c4cc07771g

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-12-12
Publisher name: R S C Publications

Source: researchoutputwizard

Source ID: 1661

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

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2014): CiteScore 2.55 SJR 0.885 SNIP 0.95
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: Contribution to journal > Article > Scientific > peer-review

The effect of thiophene substituents of fulleropyrrolidine acceptors on the performance of inverted organic solar cells

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Kaunisto, K. M., Subbaiyan, N. K., Bikram K.C., C., Chukharev, V. I., Hakola, H. M., Vuorinen, T. K., Manninen, V. M., Tkachenko, N. V., Lemmetyinen, H. J., D'Souza, F.
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 (2014): CiteScore 2.42 SJR 0.709 SNIP 0.936
Original language: English
DOIs:
10.1016/j.synthmet.2014.06.007

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-09-12
Publisher name: Elsevier S.A.
Source: researchoutputwizard
Source ID: 688
Research output: Contribution to journal > Article > Scientific > peer-review

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.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology
Contributors: Mylläri, V., Ruoko, T. P., Järvelä, P.
Number of pages: 7
Pages: 278-284
Publication date: 2014
Peer-reviewed: Yes

Publication information

Journal: Polymer Degradation and Stability
Volume: 109
ISSN (Print): 0141-3910
Ratings:
Scopus rating (2014): CiteScore 3.37 SJR 1.282 SNIP 1.879
Original language: English
ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry, Mechanics of Materials, Condensed Matter Physics
Keywords: PEEK, Fibre, Ultraviolet, Rheology, POLY(ETHER ETHER KETONE), STRUCTURE/DEGRADABILITY RELATIONSHIPS, SCANNING CALORIMETRY, THERMAL-DEGRADATION, POLYPROPYLENE, PHOTODEGRADATION, POLYMERS, PHOTOOXIDATION, CRYSTALLINITY
Electronic versions:
The_effects_of_UV_irradiation_pre-print
DOIs:
10.1016/j.polymdegradstab.2014.08.003
URLs:
<http://urn.fi/URN:NBN:fi:tty-201612024839>
URLs:
<http://www.scopus.com/inward/record.url?scp=84907310748&partnerID=8YFLogxK> (Link to publication in Scopus)

Bibliographical note

Contribution: organisation=mol,FACT1=0.8
Contribution: organisation=keb,FACT2=0.2
Portfolio EDEND: 2014-09-10
Publisher name: Elsevier Ltd
Source: researchoutputwizzard
Source ID: 1117
Research output: Contribution to journal › Article › Scientific › peer-review

The Wolff Rearrangement

General information

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

Host publication information

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

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-09-30
Source: researchoutputwizzard
Source ID: 205
Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific › peer-review

Ultrafast photophysical processes for Fe(III)-carboxylates

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Pozdnyakov, I. P., Melnikov, A. A., Tkachenko, N., Chekalin, S. V., Lemmetyinen, H., Plyusnin, V. F.

Number of pages: 6

Pages: 17590-17595

Publication date: 2014

Peer-reviewed: Yes

Publication information

Journal: DALTON TRANSACTIONS

Volume: 43

Issue number: 47

ISSN (Print): 1477-9234

Ratings:

Scopus rating (2014): CiteScore 4.06 SJR 1.389 SNIP 1.064

Original language: English

DOIs:

10.1039/c4dt01419g

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-12-11
Publisher name: R S C Publications

Source: researchoutputwizzard

Source ID: 1302

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

Porphyrin adsorbed on the (1010) surface of the wurtzite structure of ZnO-conformation induced effects on the electron transfer characteristics

Electron transfer at the adsorbate-surface interface is crucial in many applications but the steps taking place prior to and during the electron transfer are not always thoroughly understood. In this work a model system of 4-(porphyrin-5-yl)benzoic acid adsorbed as a corresponding benzoate on the ZnO wurtzite (1010) surface is studied using density functional theory (DFT) and time-dependent DFT. Emphasis is on the initial photoexcitation of porphyrin and on the strength of coupling between the porphyrin LUMO or LUMO + 1 and the ZnO conduction band that plays a role in the electron transfer. Firstly, ZnO wurtzite bulk is optimized to minimum energy geometry and the properties of the isolated ZnO (1010) surface model and the porphyrin model are discussed to gain insight into the combined system. Secondly, various orientations of the model porphyrin on the ZnO surface are studied: the porphyrin model standing perpendicularly to the surface and gradually brought close to the surface by tilting the linker in a few steps. The porphyrin model approaches the surface either sideways with hydrogen atoms of the porphyrin ring coming down first or twisted in a ca. 45° angle, giving rise to π -interactions of the porphyrin ring with ZnO. Because porphyrins are closely packed and near the surface, emerging van der Waals (vdW) interactions are examined using Grimme's D2 method. While the orientation affects the initial excitation of porphyrin only slightly, the coupling between the LUMO and LUMO + 1 of porphyrin and the conduction band of ZnO increases considerably if porphyrin is close to the surface, especially if the π -electrons are interacting with the surface. Based on the results of coupling studies, not only the distance between porphyrin and the ZnO surface but also the orientation of porphyrin can greatly affect the electron transfer. © 2013 the Owner Societies.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Supramolecular photochemistry, Department of Chemistry and Bioengineering, Tampere University of Technology, Department of Physics, Department of Physics, Research area: Computational Physics, Research group: Electronic Structure Theory, Computational Science X (CompX), Frontier Photonics

Contributors: Niskanen, M., Kuisma, M., Cramariuc, O., Golovanov, V., Hukka, T. I., Tkachenko, N., Rantala, T. T.

Number of pages: 11

Pages: 17408-17418

Publication date: 28 Oct 2013

Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 15

Issue number: 40

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.196

Original language: English

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

DOIs:

10.1039/c3cp51685g

URLs:

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

Bibliographical note

poistettu tuplat r=2454 ja r=3218
Contribution: organisation=keb,FACT1=0.5
Contribution: organisation=fys,FACT2=0.5
Portfolio EDEND: 2013-10-29
Publisher name: R S C Publications

Source: researchoutputwizard

Source ID: 2999

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

Bis(aryl)acenaphthenequinonediimine substituent effect on the properties and coordination environment of ligands and their bis-chelate AgI complexes

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Papanikolaou, P., Gdaniec, M., Wicher, B., Akrivos, P. D., Tkachenko, N.

Number of pages: 10

Pages: 5196-5205

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: European Journal of Inorganic Chemistry

Volume: 2013

Issue number: 29

ISSN (Print): 1434-1948

Ratings:

Scopus rating (2013): CiteScore 2.82 SJR 1.067 SNIP 0.823

Original language: English

DOIs:

10.1002/ejic.201300828

Bibliographical note

poistettu tupla r=122 portfolio14
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: Wiley - VCH Verlag

Source: researchoutputwizard

Source ID: 3095

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

Chain processes in the photochemistry of Pt(IV) halide complexes in aqueous solutions

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Glebov, E. M., Kolomeets, A. V., Pozdnyakov, I. P., Grivin, V. P., Plyusnin, V. F., Tkachenko, N. V., Lemmetyinen, H.

Number of pages: 9

Pages: 1540-1548

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: Russian Chemical Bulletin
Volume: 62
Issue number: 7
ISSN (Print): 1066-5285
Ratings:
Scopus rating (2013): CiteScore 0.45 SJR 0.225 SNIP 0.415
Original language: English
DOIs:
10.1007/s11172-013-0221-z
URLs:
<http://link.springer.com/article/10.1007/s11172-013-0221-z>

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-04-29
Publisher name: Springer New York LLC
Source: researchoutputwizard
Source ID: 2177
Research output: Contribution to journal > Article > Scientific > peer-review

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: 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 (2013): CiteScore 3.74 SJR 1.119 SNIP 0.905
Original language: English
DOIs:
10.1039/c3ra22813d

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: RSC Publishing
Source: researchoutputwizard
Source ID: 1988
Research output: Contribution to journal > Article > Scientific > peer-review

Chlorophyll tailored 20-trifluoroacetamide and its azacrown derivative as pH sensitive colorimetric sensor probe with response to AcO⁻, F⁻ and CN⁻ ions

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Contributors: 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 (2013): CiteScore 3.74 SJR 1.119 SNIP 0.905
Original language: English
DOIs:
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: Contribution to journal > Article > Scientific > peer-review

Complexation enhanced excited-state deactivation by lithium ion coordination to a borondipyromethene (Bodipy) donor-bridge-acceptor dyad

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: 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

Journal: European Journal of Organic Chemistry
Volume: 2013
Issue number: 30
ISSN (Print): 1434-193X
Ratings:
Scopus rating (2013): CiteScore 2.96 SJR 1.336 SNIP 0.827
Original language: English
DOIs:
10.1002/ejoc.201300867

Bibliographical note

Article first published online: 4 SEP 2013
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-11-29
Publisher name: WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
Source: researchoutputwizard
Source ID: 1989
Research output: Contribution to journal > Article > Scientific > peer-review

Conjugated donor-acceptor (D-A) copolymers in inverted organic solar cells - a combined experimental and modelling study

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Manninen, V., Niskanen, M., Hukka, T. I., Pasker, F., Claus, S., Höger, S., Baek, J., Umeyama, T., Imahori, H., Lemmetyinen, H.
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
Original language: English
DOIs:
10.1039/c3ta10686a

Bibliographical note

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

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Electronics and Communications Engineering, Department of Chemistry and Bioengineering , Research group: Supramolecular photochemistry, Frontier Photonics, Integrated Technologies for Tissue Engineering Research (ITTE)
Contributors: 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 (2013): CiteScore 1.71 SJR 0.629 SNIP 1.095
Original language: English
DOIs:
10.1002/app.39513

Bibliographical note

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

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

General information

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

Publication information

Journal: Crystallography Reports
Volume: 58
Issue number: 6

ISSN (Print): 1063-7745

Ratings:

Scopus rating (2013): CiteScore 0.4 SJR 0.318 SNIP 0.638

Original language: English

DOIs:

10.1134/S1063774513060205

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: MAIK Nauka - Interperiodica

Source: researchoutputwizard

Source ID: 3402

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2013): CiteScore 2 SJR 0.814 SNIP 1.183

Original language: English

DOIs:

10.1016/j.tsf.2013.08.106

Bibliographical note

Available online 7 September 2013
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-11-29
Publisher name: Elsevier

Source: researchoutputwizard

Source ID: 3716

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

Direct evidence of significantly different chemical behavior and excited-state dynamics of 1,7- and 1,6-regioisomers of pyrroldinyl-substituted perylene diimide

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2013): CiteScore 5.68 SJR 2.643 SNIP 1.239

Original language: English

DOIs:

10.1002/chem.201203387

Bibliographical note

poistettu tupla r=2208
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-06-29
Publisher name: WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

Source: researchoutputwizard

Source ID: 2089

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

Effect of anion coordination on electron transfer in double-linked zinc phthalocyanine-fullerene dyad

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2013): CiteScore 2.07 SJR 0.858 SNIP 0.831

Original language: English

DOIs:

10.1016/j.cplett.2013.04.035

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: Elsevier

Source: researchoutputwizard

Source ID: 1896

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

Excited-state interaction of red and green perylene diimides with luminescent Ru(II) polypyridine complex

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2013): CiteScore 4.9 SJR 1.821 SNIP 1.368

Original language: English

DOIs:

10.1021/ic400474b

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 2088

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

Fluorescence properties of the chromophore-binding domain of bacteriophytochrome from Deinococcus radiodurans

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Lehtivuori, H., Rissanen, I., Takala, H., Bamford, J., Tkachenko, N. V., Ihalainen, J. A.

Pages: 11049-11057

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 117

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2013): CiteScore 3.53 SJR 1.504 SNIP 1.194

Original language: English

DOIs:

10.1021/jp312061b

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 2752

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

Homoleptic Bis(aryl)acenaphthenequinonediimine-CuI complexes - synthesis and characterization of a family of compounds with improved light-gathering characteristics

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Papanikolaou, P., Akrivos, P. D., Czapiak, A., Wicher, B., Gdaniec, M., Tkachenko, N.

Number of pages: 14

Pages: 2418-2431

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: European Journal of Inorganic Chemistry

Volume: 2013

Issue number: 13

ISSN (Print): 1434-1948

Ratings:

Scopus rating (2013): CiteScore 2.82 SJR 1.067 SNIP 0.823

Original language: English

DOIs:

10.1002/ejic.201201507

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA

Source: researchoutputwizard

Source ID: 3094

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

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.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Biomedical Engineering, Department of Chemistry and Bioengineering, Frontier Photonics, Integrated Technologies for Tissue Engineering Research (ITTE)

Contributors: Ahola, N., Veiranto, M., Rich, J., Efimov, A., Hannula, M., Seppälä, J., Kellomäki, M.

Pages: 529-543

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: Journal of Biomaterials Applications

Volume: 28

Issue number: 4

ISSN (Print): 0885-3282

Ratings:

Scopus rating (2013): CiteScore 2.35 SJR 0.733 SNIP 1.004

Original language: English

Electronic versions:

ahola_hydrolytic_degradation_of_composites.pdf

DOIs:

10.1177/0885328212462258

URLs:

<http://jba.sagepub.com/content/early/2012/10/09/0885328212462258>

<http://urn.fi/URN:NBN:fi:ty-201401291066>

Bibliographical note

Online First : Published online before print October 9, 2012, doi: 10.1177/0885328212462258 : J Biomater Appl October 9, 2012 0885328212462258
Contribution: organisation=bme,FACT1=0.5
Contribution: organisation=keb

kem,FACT2=0.5
Publisher name: Sage

Source: researchoutputwizard

Source ID: 1887

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

Independent versus cooperative binding in polyethylenimine-DNA and poly(L-lysine)-DNA polyplexes

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Ketola, T., Hanzlikova, M., Leppänen, L., Ravina, M., Bishop, C. J., Green, J. J., Urtti, A., Lemmetyinen, H., Yliperttula, M., Vuorimaa-Laukkanen, E.

Number of pages: 9

Pages: 10405-10413

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 117
Issue number: 36
ISSN (Print): 1520-6106
Ratings:

Scopus rating (2013): CiteScore 3.53 SJR 1.504 SNIP 1.194

Original language: English

DOIs:

10.1021/jp404812a

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 2551

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

Influence of plasma chemistry on impurity incorporation in AlN prepared by plasma enhanced atomic layer deposition

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Frontier Photonics

Contributors: Pymaki Perros, A., Hakola, H., Sajavaara, T., Huhtio, T., Lipsanen, H.

Number of pages: 8

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: Journal of Physics D: Applied Physics

Volume: 46

Issue number: 50

Article number: 505502

ISSN (Print): 0022-3727

Ratings:

Scopus rating (2013): CiteScore 2.6 SJR 1.194 SNIP 1.462

Original language: English

DOIs:

10.1088/0022-3727/46/50/505502

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2014-02-15
Publisher name: Institute of Physics Publishing Ltd.

Source: researchoutputwizard

Source ID: 3204

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

Molecular dipole effects on tuning electron transfer in a porphine-quinone complex: A DFT and TDDFT study

General information

Publication status: Published

MoE 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

Contributors: 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 (2013): CiteScore 1.94 SJR 0.525 SNIP 0.727

Original language: English

DOIs:

10.1007/s00894-012-1595-9

Bibliographical note

Contribution: organisation=fys,FACT1=0.5
Contribution: organisation=keb kem,FACT2=0.5
Publisher name: Springer

Source: researchoutputwizard

Source ID: 2053

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

Molecular weight distribution of a full-scale landfill leachate treatment by membrane bioreactor and nanofiltration membrane

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Campagna, M., Cakmakci, M., Busra Yaman, F., Özkaya, B.

Number of pages: 5

Pages: 866-870

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: Waste Management

Volume: 33

Issue number: 4

ISSN (Print): 0956-053X

Ratings:

Scopus rating (2013): CiteScore 3.39 SJR 1.815 SNIP 2.419

Original language: English

DOIs:

10.1016/j.wasman.2012.12.010

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: Pergamon

Source: researchoutputwizard

Source ID: 2028

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

Photophysics of bis(ethylxanthato)nickel(II) [Ni(EtOCS₂)₂] complex studied by femtosecond pump-probe spectroscopy

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2013): CiteScore 2.5 SJR 0.835 SNIP 1.013

Original language: English
DOIs:
10.1016/j.jphotochem.2012.08.005

Bibliographical note

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

Plasma-assisted chemical vapor deposition of Fe:TiO₂ films for photoelectrochemical hydrogen production

General information

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

Host publication information

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

Publication series

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

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: American Ceramic Society
Source: researchoutputwizard
Source ID: 2921
Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

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

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Frontier Photonics
Contributors: Papanikolaou, P., Tkachenko, N.
Number of pages: 9
Pages: 13128-13136
Publication date: 2013
Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics
Volume: 15
Issue number: 31
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.196
Original language: English
DOIs:

10.1039/c3cp50838b

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: R S C Publications

Source: researchoutputwizard

Source ID: 3093

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

Ring-expansion reaction of isatins with ethyl diazoacetate catalyzed by dirhodium(II)/DBU metal-organic system: En route to viridicatin alkaloids

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio)

Contributors: Paterna, R., Andre, V., Duarte, M. T., Veiros, L. F., Rafael Candeias, N., Gois, P. M.

Number of pages: 11

Pages: 6280-6290

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: European Journal of Organic Chemistry

Volume: 2013

Issue number: 28

ISSN (Print): 1434-193X

Ratings:

Scopus rating (2013): CiteScore 2.96 SJR 1.336 SNIP 0.827

Original language: English

DOIs:

10.1002/ejoc.201300796

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: Wiley

Source: researchoutputwizard

Source ID: 3106

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

Sequential photoinduced energy and electron transfer directed improved performance of the supramolecular solar cell of a zinc porphyrin - zinc phthalocyanine conjugate modified TiO₂ surface

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: KC, C. B., Stranius, K., D'Souza, P., Subbaiyan, N. K., Lemmetyinen, H., Tkachenko, N. V., D'Souza, F.

Number of pages: 11

Pages: 763-773

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 117

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.432

Original language: English

DOIs:

10.1021/jp308923e

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29

Source: researchoutputwizard

Source ID: 2538

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

Short synthesis of the natural product 3 β -hydroxy-labd-8(17)-en-15-oic acid via microbial transformation of labdanolic acid

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), Former organisation of the author

Contributors: Frija, L. M., Garcia, H., Rodrigues, C., Martins, I., Rafael Candeias, N., Andre, V., Duarte, M. T., Pereira, S. C., Afonso, C. A.

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 (2013): CiteScore 1.57 SJR 0.647 SNIP 0.983

Original language: English

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-06-29
Publisher name: Elsevier

Source: researchoutputwizard

Source ID: 2147

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Wondraczek, H., Kotiaho, A., Niemi, M., Fardim, P., Heinze, T.

Number of pages: 7

Pages: 45-51

Publication date: 2013

Peer-reviewed: Yes

Publication information

Journal: Carbohydrate Polymers

Volume: 97

Issue number: 1

ISSN (Print): 0144-8617

Ratings:

Scopus rating (2013): CiteScore 4.39 SJR 1.346 SNIP 1.945

Original language: English

DOIs:

10.1016/j.carbpol.2013.04.040

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: Pergamon

Source: researchoutputwizard

Source ID: 3748

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

Study of structural order in porphyrin-fullerene dyad ZnDHD6ee monolayers by electron diffraction and atomic force microscopy

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: D'yakova, Y. A., Suvorova, E., Orekhov, A. S., Orekhov, A. S., Alekseev, A., Gainutdinov, R. V., Klechkovskaya, V., Tereschenko, E., Tkachenko, N., Lemmetyinen, H., Feigin, L., Kovalchuk, M.

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 (2013): CiteScore 0.4 SJR 0.318 SNIP 0.638

Original language: English

DOIs:

10.1134/S1063774513060096

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: MAIK Nauka - Interperiodica

Source: researchoutputwizard

Source ID: 2064

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

Supramolecular assemblies of bay-substituted perylene diimides in solution and on a solid substrate

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2013): CiteScore 3.55 SJR 1.492 SNIP 0.892

Original language: English

DOIs:

10.1039/c3ob41058g

Bibliographical note

ei vielä UT 2013-09-19
Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-09-29
Publisher name: R S C Publications

Source: researchoutputwizard

Source ID: 3370

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: 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 (2013): CiteScore 11.38 SJR 5.993 SNIP 2.446

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

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

Triarylamine-substituted imidazole- and quinoxaline-fused push-pull porphyrins for dye-sensitized solar cells

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Supramolecular photochemistry, Department of Chemistry and Bioengineering, Frontier Photonics

Contributors: 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 (2013): CiteScore 6.79 SJR 2.561 SNIP 1.452

Original language: English

DOIs:

10.1002/cssc.201200869

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-11-29
Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA

Source: researchoutputwizard

Source ID: 2255

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

Tuning the Förster overlap integral: energy transfer over 20 Ångstroms from a pyrene-based donor to borondipyrromethene (Bodipy)

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Bai, D., Benniston, A., Hagon, J., Lemmetyinen, H., Tkachenko, N., Harrington, R.
Number of pages: 8
Pages: 9854-9861
Publication date: 2013
Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics
Volume: 15
Issue number: 24
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.196
Original language: English
DOIs:
10.1039/c3cp50173f

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-10-29
Publisher name: R S C Publications
Source: researchoutputwizard
Source ID: 1958
Research output: Contribution to journal > Article > Scientific > peer-review

Algorithm for In Silico Optimization of Production Strains

General information

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

Host publication information

Title of host publication: Proceedings of Ninth International Workshop on Computational Systems Biology, WCSB 2012, 4-6 June, Ulm, Germany. TICSP Series
Place of publication: Tampere
Publisher: Tampere University of Technology
Editors: Larjo, A., Schober, S., Farhan, M., Bossert, M., Yli-Harja, O.
ISBN (Print): 978-952-15-2853-8

Publication series

Name: International Workshop on Computational Systems Biology
Volume: 61
ISSN (Print): 1456-2774

Bibliographical note

ei ut-numeroa 13.8.2013
Contribution: organisation=sgn,FACT1=0.8
Contribution: organisation=keb,FACT2=0.2
Publisher name: Tampere University of Technology
Source: researchoutputwizard
Source ID: 4181
Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

A Photoconductive, Thiophene-Fullerene Double-Cable Polymer, Nanorod Device

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Imahori, H., Kitaura, S., Kira, A., Hayashi, H., Nishi, M., Hirao, K., Isoda, S., Tsujimoto, M., Takano, M., Zhe, Z., Miyato, Y., Noda, K., Matsushige, K., Stranius, K., Tkachenko, N. V., Lemmetyinen, H., Qin, L., Hurst, S. J., Mirkin, C. A.

Pages: 478-481

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry Letters

Volume: 3

Issue number: 4

ISSN (Print): 1948-7185

Ratings:

Scopus rating (2012): CiteScore 6.3 SJR 3.965 SNIP 1.72

Original language: English

DOIs:

10.1021/jz300015e

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society - ACS

Source: researchoutputwizard

Source ID: 4305

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

Asymmetric Intramolecular C-H Insertion of alpha-Diazoacetamides in Water by Dirhodium(II) Catalysts Derived from Natural Amino Acids

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Urban circular bioeconomy (UrCirBio)

Contributors: Rafael Candeias, N., Carias, C., Gomes, L. F., Andre, V., Teresa Duarte, M., Gois, P. M., Afonso, C. A.

Pages: 2921-2927

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Advanced Synthesis and Catalysis

Volume: 354

Issue number: 16

ISSN (Print): 1615-4150

Ratings:

Scopus rating (2012): CiteScore 5.33 SJR 2.796 SNIP 1.146

Original language: English

DOIs:

10.1002/adsc.201200101

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA

Source: researchoutputwizard

Source ID: 5130

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

Azafullerene C59N-Phthalocyanine Dyad: Synthesis, Characterisation and Photoinduced Electron Transfer

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Rotas, G., Ranta, J., Efimov, A., Niemi, M., Lemmetyinen, H., Tkachenko, N., Tagmatarchis, N.

Pages: 1246-1254

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: ChemPhysChem

Volume: 13

Issue number: 5

ISSN (Print): 1439-4235

Ratings:

Scopus rating (2012): CiteScore 3.24 SJR 1.769 SNIP 0.954

Original language: English

DOIs:

10.1002/cphc.201101029

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: ChemPubSoc Europe; Wiley - VCH Verlag GmbH & Co. KGaA

Source: researchoutputwizard

Source ID: 5198

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

Car-parrinello molecular dynamics study of a porphyrin-fullerene electron donor-acceptor dyad

General information

Publication status: Published

MoE publication type: B3 Non-refereed article in conference proceedings

Organisations: Research area: Computational Physics, Department of Chemistry and Bioengineering, Department of Physics

Contributors: Karilainen, T., Cramariuc, O., Tappura, K., Hukka, T.

Number of pages: 1

Pages: 1-1

Publication date: 2012

Host publication information

Title of host publication: Physics Days 2012, the 46th annual meeting of the Finnish Physical Society, 13.-15.3.2012, Joensuu, Finland

Place of publication: Joensuu

Publisher: University of Eastern Finland; Suomen fyysikkoseura

Publication series

Name: Physics Days / Fysiikan päivät : Annual Meeting of the Finnish Physical Society

URLs:

http://www.uef.fi/c/document_library/get_file?uuid=41e478a5-dda0-49bf-90e0-e4013cc1196d&groupId=1326215&p_l_id=1326219

Bibliographical note

poistettu tupla r=2996. ei ut-numeroa 19.8.2013
Contribution: organisation=fys,FACT1=0.5
Contribution: organisation=keb kem,FACT2=0.5
Publisher name: University of Eastern Finland; Suomen fyysikkoseura

Source: researchoutputwizard

Source ID: 4424

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific

Diaryl-Substituted Perylene Bis(imides): Synthesis, Separation, Characterization and Comparison of Electrochemical and Optical Properties of 1,7- and 1,6-Regioisomer

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Dey, S., Efimov, A., Lemmetyinen, H.

Pages: 2367-2374

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: European Journal of Organic Chemistry

ISSN (Print): 1434-193X

Ratings:

Scopus rating (2012): CiteScore 2.93 SJR 1.54 SNIP 0.87

Original language: English

DOIs:

10.1002/ejoc.201101825

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

Source: researchoutputwizard

Source ID: 4005

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

Directed electron transfer in Langmuir-Schäfer layers of porphyrin-fullerene and phthalocyanine-fullerene dyads in inverted organic solar cells

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Tolkki, A., Kaunisto, K., Efimov, A., Kivistö, H., Storbacka, L., Savikoski, R., Huttunen, K., Lehtimäki, S., Lemmetyinen, H.

Pages: 3498-3504

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 14

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.164

Original language: English

DOIs:

10.1039/c2cp24022j

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: RSC Publications

Source: researchoutputwizard

Source ID: 5434

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

Donor-acceptor alternating copolymer based on thermally converted isothianaphthene dimer and thiazolothiazole subunits

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Umeyama, T., Hirose, K., Noda, K., Matsushige, K., Shishido, T., Saarenpää, H., Tkachenko, N. V., Lemmetyinen, H., Ono, N., Imahori, H.

Pages: 17414-17423

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 116

Issue number: 33

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461

Original language: English

DOIs:

10.1021/jp305001p

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 5471

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Al-Subi, A. H., Niemi, M., Ranta, J., Tkachenko, N. V., Lemmetyinen, H.

Pages: 164-168

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Chemical Physics Letters

Volume: 531

ISSN (Print): 0009-2614

Ratings:

Scopus rating (2012): CiteScore 2.2 SJR 1.104 SNIP 0.901

Original language: English

DOIs:

10.1016/j.cplett.2012.02.026

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Elsevier

Source: researchoutputwizard

Source ID: 3834

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

Effect on Charge Transfer and Charge Recombination by Insertion of a Naphthalene-Based Bridge in Molecular Dyads Based on Borondipyrromethene (Bodipy)

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Benniston, A., Clift, S., Hagon, J., Lemmetyinen, H., Tkachenko, N., Clegg, W., Harrington, R.

Pages: 3672-3681

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: ChemPhysChem

Volume: 13

Issue number: 16

ISSN (Print): 1439-4235

Ratings:

Scopus rating (2012): CiteScore 3.24 SJR 1.769 SNIP 0.954

Original language: English

DOIs:

10.1002/cphc.201200510

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

Source: researchoutputwizard

Source ID: 3906

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

Effects of Carbon-Metal-Carbon Linkages on the Optical, Photophysical, and Electrochemical Properties of Phosphametallacycle-Linked Coplanar Porphyrin Dimers

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Matano, Y., Matsumoto, K., Hayashi, H., Nakao, Y., Kumpulainen, T., Chukharev, V., Tkachenko, N. V., Lemmetyinen, H., Shimizu, S., Kobayashi, N., Sakamaki, D., Ito, A., Tanaka, K., Imahori, H.

Pages: 1825-1839

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Journal of the American Chemical Society

Volume: 134

Issue number: 3

ISSN (Print): 0002-7863

Ratings:

Scopus rating (2012): CiteScore 10.37 SJR 6.211 SNIP 2.374

Original language: English

DOIs:

10.1021/ja210205v

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society - ACS

Source: researchoutputwizard

Source ID: 4827

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

Excited State Intramolecular Proton Transfer in Electron-Rich and Electron-Poor Derivatives of 10-Hydroxybenzo[h]quinoline

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Piechowska, J., Huttunen, K., Wrobel, Z., Lemmetyinen, H., Tkachenko, N. V., Gryko, D.

Pages: 9614-9620

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry A

Volume: 116

Issue number: 39

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.119

Original language: English

DOIs:

10.1021/jp305459r

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society, ACS

Source: researchoutputwizard

Source ID: 5067

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

Exploring Förster electronic energy transfer in a decoupled anthracenyl-based borondipyrromethene (bodipy) dyad

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Bai, D., Benniston, A., Hagon, J., Lemmetyinen, H., Tkachenko, N. V., Clegg, W., Harrington, R.

Pages: 4447-4456

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 14

Issue number: 13

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.164

Original language: English

DOIs:

10.1039/c2cp23868c

URLs:

<http://www.rsc.org/pccp>

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: RSC Publications

Source: researchoutputwizard

Source ID: 3887

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

Hydrogen-Bonding Effects on the Formation and Lifetimes of Charge-Separated States in Molecular Triads

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Hankache, J., Niemi, M., Lemmetyinen, H., Wenger, O. S.

Pages: 8159-8168

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry A

Volume: 116

Issue number: 31

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.119

Original language: English

DOIs:

10.1021/jp302790j

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society, ACS

Source: researchoutputwizard

Source ID: 4142

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

Intramolecular C-H insertion catalyzed by dirhodium(II) complexes using CO₂ as the reaction media

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.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), Univ Lisbon, Universidade de Lisboa, Fac Pharm, Res Inst Med & Pharmaceut Sci iMed UL, Univ Nova Lisboa, Universidade Nova de Lisboa, REQUIMTE, Dept Quim, Fac Ciencias & Tecnol, Lab Nacl Energia Geol, Laboratorio Nacional de Energia e Geologia IP (LNEG), Unit Bioenergy

Contributors: Zakrzewska, M. E., Cal, P. M. S. D., Candeias, N. R., Bogel-Lukasik, R., Afonso, C. A. M., Ponte, M. N., Gois, P. M. P.

Number of pages: 30

Pages: 211-240

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Green Chemistry Letters and Reviews

Volume: 5

Issue number: 2

ISSN (Print): 1751-8253

Ratings:

Scopus rating (2012): CiteScore 1.48 SJR 0.374 SNIP 0.594

Original language: English

Keywords: diazoacetamides, C-H insertion, dirhodium(II), lactams, scCO(2), ASYMMETRIC CYCLOPROPANATION, ALPHA-DIAZOACETAMIDES, HOMOGENEOUS CATALYSIS, SUPERCRITICAL FLUIDS, CARBOXYLATES, ENANTIOSELECTIVITY, TRANSFORMATIONS, IMMOBILIZATION, ACTIVATION, STRATEGY

DOIs:

10.1080/17518253.2011.620009

Source: WOS

Source ID: 000310597800014

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

Large Stokes Shift Fluorescent Dyes Based on a Highly Substituted Terephthalic Acid Core

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Benniston, A. C., Winstanley, T. P., Lemmetyinen, H., Tkachenko, N. V., Harrington, R. W., Wills, C.

Pages: 1374-1377

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Organic Letters

Volume: 14

Issue number: 6

ISSN (Print): 1523-7060

Ratings:

Scopus rating (2012): CiteScore 5.7 SJR 3.338 SNIP 1.353

Original language: English

DOIs:

10.1021/ol300038e

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society - ACS

Source: researchoutputwizard

Source ID: 3908

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

Making expensive dirhodium(II) catalysts cheaper: Rh(II) recycling methods

Dirhodium(II) catalysts have been widely used as a remarkable tool in organic synthesis, ultimately resulting in a myriad of transformations and formation of a wide variety of compounds, every so often intermediaries in drug synthesis. Aiming at a

more sustainable chemistry, several methods suitable for the reutilisation of expensive dirhodium complexes have been developed. Herein, we provide a combined overview of the available methods for recovering and reusing dirhodium(II) metal complexes in catalysis, covering homogeneous catalysis as well as heterogenisation methods.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), Univ Lisbon, Universidade de Lisboa, Fac Pharm, Res Inst Med & Pharmaceut Sci iMed UL

Contributors: Candeias, N. R., Afonso, C. A. M., Gois, P. M. P.

Number of pages: 22

Pages: 3357-3378

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Organic and Biomolecular Chemistry

Volume: 10

Issue number: 17

ISSN (Print): 1477-0520

Ratings:

Scopus rating (2012): CiteScore 3.47 SJR 1.653 SNIP 0.939

Original language: English

Keywords: C-H INSERTION, ACTIVE PHARMACEUTICAL INGREDIENTS, ALPHA-DIAZOCARBONYL COMPOUNDS, CHIRAL LEWIS-ACID, CYCLOPROPANATION REACTIONS, ASYMMETRIC-SYNTHESIS, RHODIUM CARBENOIDES, IONIC LIQUID, HOMOGENEOUS CATALYSIS, SUPERCRITICAL FLUIDS

DOIs:

10.1039/c2ob06731e

Source: WOS

Source ID: 000302420700001

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

Meteorological parameters as an important factor on the energy recovery of landfill gas in landfills

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Uyanik, I., Özkaya, B., Demir, S., Cakmakci, M.

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Journal of Renewable and Sustainable Energy

Volume: 4

Issue number: 6

Article number: 063135

ISSN (Print): 1941-7012

Ratings:

Scopus rating (2012): CiteScore 1.77 SJR 0.578 SNIP 1.266

Original language: English

DOIs:

10.1063/1.4769202

Bibliographical note

Contribution: organisation=keb,FACT1=1
Portfolio EDEND: 2013-12-29
Publisher name: American Institute of Physics AIP

Source: researchoutputwizard

Source ID: 5478

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

Modulation of visible room temperature phosphorescence by weak magnetic fields

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Mani, T., Tanabe, M., Yamauchi, S., Tkachenko, N. V., Vinogradov, S. A.
Pages: 3115-3119
Publication date: 2012
Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry Letters
Volume: 3
Issue number: 21
ISSN (Print): 1948-7185
Ratings:
Scopus rating (2012): CiteScore 6.3 SJR 3.965 SNIP 1.72
Original language: English
DOIs:
10.1021/jz301166e

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society ACS
Source: researchoutputwizard
Source ID: 4806
Research output: Contribution to journal > Article > Scientific > peer-review

N-1-Functionalized Indole-Phosphane Oxazoline (IndPHOX) Ligands in Asymmetric Allylic Substitution Reactions

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Contributors: Wang, Y., Vaismaa, M. J., Rissanen, K., Franzen, R.
Pages: 1569-1576
Publication date: 2012
Peer-reviewed: Yes

Publication information

Journal: European Journal of Organic Chemistry
Volume: 2012
Issue number: 8
ISSN (Print): 1434-193X
Ratings:
Scopus rating (2012): CiteScore 2.93 SJR 1.54 SNIP 0.87
Original language: English
DOIs:
10.1002/ejoc.201101540

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
Source: researchoutputwizard
Source ID: 5586
Research output: Contribution to journal > Article > Scientific > peer-review

Nature's Nonlinear Optical Antennas

General information

Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: Research group: Nonlinear Optics, Research area: Optics, Department of Chemistry and Bioengineering, Department of Physics, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Huttunen, M. J., Virkki, M., Bautista, G., Vuorimaa-Laukkanen, E., Der, A., Lemmetyinen, H., Kauranen, M.
Number of pages: 2
Pages: 1-2

Publication date: 2012

Host publication information

Title of host publication: CLEO 2012, San Jose, California, USA, 6-11 May 2012. Technical Digest

Publisher: OSA

Article number: QM4F.8

ISBN (Print): 978-1-55752-943-5

ISBN (Electronic): 978-146731839-6

Publication series

Name: Conference on Lasers and Electro-Optics

Bibliographical note

Contribution: organisation=fys,FACT1=0.5
Contribution: organisation=keb kem,FACT2=0.5
Publisher name: OSA

Source: researchoutputwizard

Source ID: 4265

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

Organometallic tris(8-hydroxyquinoline)aluminum complexes as buffer layers and dopants in inverted organic solar cells

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Tolkki, A., Kaunisto, K., Heiskanen, J. P., Omar Walaa, A., Huttunen, K., Lehtimäki, S., Hormi, O. E., Lemmetyinen, H.

Pages: 4475-4481

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Thin Solid Films

Volume: 520

Issue number: 13

ISSN (Print): 0040-6090

Ratings:

Scopus rating (2012): CiteScore 1.86 SJR 0.897 SNIP 1.153

Original language: English

DOIs:

10.1016/j.tsf.2012.02.084

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Elsevier

Source: researchoutputwizard

Source ID: 5435

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Urban circular bioeconomy (UrCirBio)

Contributors: Veselov, A. A., George Abraham, B., Lemmetyinen, H., Karp, M. T., Tkachenko, N. V.

Pages: 1149-1158

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Analytical and Bioanalytical Chemistry

Volume: 402

Issue number: 3

ISSN (Print): 1618-2642

Ratings:

Scopus rating (2012): CiteScore 3.51 SJR 1.354 SNIP 1.279

Original language: English

DOIs:

10.1007/s00216-011-5564-4

Bibliographical note

Poistettu tupla r=3716, online first
Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 5533

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

Photoinduced charge shift and charge recombination through an alkynyl spacer for an expanded acridinium-based dyad

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Benniston, A., Hagon, J., He, X., Clegg, W., Harrington, R., Tkachenko, N., Lemmetyinen, H.

Pages: 3194-3199

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics

Volume: 14

Issue number: 9

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.164

Original language: English

DOIs:

10.1039/C2CP23273A

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: RSC Publishing

Source: researchoutputwizard

Source ID: 3907

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Hankache, J., Niemi, M., Lemmetyinen, H., Wenger, O. S.

Pages: 6333-6344

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Inorganic Chemistry

Volume: 51

Issue number: 11

ISSN (Print): 0020-1669

Ratings:

Scopus rating (2012): CiteScore 4.72 SJR 2.094 SNIP 1.332

Original language: English

DOIs:

10.1021/ic300558s

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society - ACS

Source: researchoutputwizard

Source ID: 4141

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

Photolysis and Quantum-Chemical Calculations of the Nalidixic Acid Radical States

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Department of Physics, Computational Science X (CompX)

Contributors: Polischuk, A., Emelina, T., Cramariuc, O., Chukharev, V., Karaseva, T., Karasev, V.

Pages: 323-328

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Russian Journal of General Chemistry

Volume: 82

Issue number: 2

ISSN (Print): 1070-3632

Ratings:

Scopus rating (2012): CiteScore 0.24 SJR 0.203 SNIP 0.283

Original language: English

DOIs:

10.1134/S1070363212020247

Bibliographical note

Contribution: organisation=fys,FACT1=0.5
Contribution: organisation=keb kem,FACT2=0.5
Publisher name: M A

I K Nauka - Interperiodica : Pleiades Publishing

Source: researchoutputwizard

Source ID: 5080

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

Photophysics of Fe(III)-tartrate and Fe(III)-citrate complexes in aqueous solutions

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Pozdnyakov, I. P., Kolomeets, A. V., Plyusnin, V. F., Melnikov, A. A., Kompanets, V. O., Chekalin, S. V., Tkachenko, N. V., Lemmetyinen, H.

Pages: 45-48

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Chemical Physics Letters

Volume: 530

ISSN (Print): 0009-2614

Ratings:

Scopus rating (2012): CiteScore 2.2 SJR 1.104 SNIP 0.901

Original language: English

DOIs:

10.1016/j.cplett.2012.01.051

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Elsevier

Source: researchoutputwizard

Source ID: 5103

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

Preparation and Photophysical and Photoelectrochemical Properties of a Covalently Fixed Porphyrin–Chemically Converted Graphene Composite

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Umeyama, T., Mihara, J., Tezuka, N., Matano, Y., Stranius, K., Chukharev, V., Tkachenko, N., Lemmetyinen, H., Noda, K., Matsushige, K., Shishido, T., Liu, Z., Hirose-Takai, K., Suenaga, K., Imahori, H.

Pages: 4250-4257

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Chemistry: A European Journal

Volume: 18

Issue number: 14

ISSN (Print): 0947-6539

Ratings:

Scopus rating (2012): CiteScore 5.55 SJR 2.935 SNIP 1.291

Original language: English

DOIs:

10.1002/chem.201103843

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Wiley - V C H Verlag GmbH & Co. KGaA

Source: researchoutputwizard

Source ID: 5470

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

Processing and sustained in vitro release of rifampicin containing composites to enhance the treatment of osteomyelitis

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Biomedical Engineering, Department of Chemistry and Bioengineering, Frontier Photonics, Integrated Technologies for Tissue Engineering Research (ITTE), Urban circular bioeconomy (UrCirBio)

Contributors: Ahola, N., Veiranto, M., Männistö, N., Karp, M., Rich, J., Efimov, A., Seppälä, J., Kellomäki, M.

Number of pages: 13

Pages: 1-13

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Biomatter

Volume: 2

Issue number: 4

ISSN (Print): 2159-2527

Ratings:

Scopus rating (2012): SJR 0.149 SNIP 0.335

Original language: English

Electronic versions:

ahola_processing_and_sustained_in_vitro_release.pdf

DOIs:

10.4161/biom.22793

URLs:

<http://www.landesbioscience.com/journals/biomatter/>

<http://urn.fi/URN:NBN:fi:ty-201401301068>

Bibliographical note

ei ut-numeroa 9.8.2013
Contribution: organisation=bme,FACT1=0.8
Contribution: organisation=keb bio,FACT2=0.1
Contribution: organisation=keb kem,FACT3=0.1
Publisher name: Landes Bioscience

Source: researchoutputwizard

Source ID: 3813

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

Quantitative Analysis of Intramolecular Exciplex and Electron Transfer in a Double-Linked Zinc Porphyrin-Fullerene Dyad

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Al-Subi, A., Niemi, M., Tkachenko, N., Lemmetyinen, H.

Pages: 9653-9661

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry A

Volume: 116

Issue number: 39

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.119

Original language: English

DOIs:

10.1021/jp306953n

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society, ACS

Source: researchoutputwizard

Source ID: 3835

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

Redox processes in photochemistry of Pt(IV) hexahaloid complexes

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Glebov, E., Kolomeets, A., Pozdnyakov, I., Plyusnin, V., Grivin, V., Tkachenko, N., Lemmetyinen, H.

Pages: 5768-5778

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: RSC Advances

Volume: 2

Issue number: 13

ISSN (Print): 2046-2069

Ratings:

Scopus rating (2012): CiteScore 2.4 SJR 0.872 SNIP 0.619

Original language: English

DOIs:

10.1039/c2ra20715j

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: RSC Publications

Source: researchoutputwizard

Source ID: 4091

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

Rh-IndOleF_{ox} catalyzed conjugate addition/Heck-type coupling of organoboronics to a lactam or a lactone

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Kuuloja, N., Vaismaa, M., Franzen, R.

Pages: 2313-2318

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Tetrahedron

Volume: 68

Issue number: 10

ISSN (Print): 0040-4020

Ratings:

Scopus rating (2012): CiteScore 2.89 SJR 1.329 SNIP 0.984

Original language: English

DOIs:

10.1016/j.tet.2012.01.040

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Elsevier Ltd.

Source: researchoutputwizard

Source ID: 4578

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Department of Chemistry and Bioengineering, Research group:

Supramolecular photochemistry, Frontier Photonics

Contributors: Saarenpää, H., Sariola-Leikas, E., Pymaki Perros, A., Kontio, J. M., Efimov, A., Hayashi, H., Lipsanen, H., Imahori, H., Lemmetyinen, H., Tkachenko, N. V.

Pages: 2336-2343

Publication date: 2012

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 116

Issue number: 3

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461

Original language: English

DOIs:

10.1021/jp2104769

Bibliographical note

Contribution: organisation=keb kem,FACT1=0.5
Contribution: organisation=orc,FACT2=0.5
Publisher name: American Chemical Society
Source: researchoutputwizard
Source ID: 5225
Research output: Contribution to journal > Article > Scientific > peer-review

Syntheses and Excitation Transfer Studies of Near-Orthogonal Free-Base Porphyrin – Ruthenium Phthalocyanine Dyads and Pentad

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Jacobs, R., Stranius, K., Maligaspe, E., Lemmetyinen, H., Tkachenko, N. V., Zandler, M. E., D'Souza, F.
Pages: 3656-3665
Publication date: 2012
Peer-reviewed: Yes

Publication information

Journal: Inorganic Chemistry
Volume: 51
Issue number: 6
ISSN (Print): 0020-1669
Ratings:
Scopus rating (2012): CiteScore 4.72 SJR 2.094 SNIP 1.332
Original language: English
DOIs:
10.1021/ic202574q

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: American Chemical Society - ACS
Source: researchoutputwizard
Source ID: 4325
Research output: Contribution to journal > Article > Scientific > peer-review

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Manninen, V. M., Omar, W. A., Heiskanen, J. P., Lemmetyinen, H. J., Hormi, O. E.
Pages: 22971-22982
Publication date: 2012
Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry
Volume: 22
Issue number: 43
ISSN (Print): 0959-9428
Ratings:
Scopus rating (2012): SJR 2.773 SNIP 1.5
Original language: English
DOIs:
10.1039/C2JM35292C

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Royal Society of Chemistry, RSC
Source: researchoutputwizard
Source ID: 4807
Research output: Contribution to journal > Article > Scientific > peer-review

Synthesis of 2-Aryl-Substituted Chromans by Intramolecular C-O Bond Formation

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Contributors: Wang, Y., Franzen, R.
Pages: 925-929
Publication date: 2012
Peer-reviewed: Yes

Publication information

Journal: Synlett
Issue number: 6
ISSN (Print): 0936-5214
Ratings:
Scopus rating (2012): CiteScore 2.1 SJR 1.17 SNIP 0.64
Original language: English
DOIs:
10.1055/s-0031-1290607

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Georg Thieme Verlag
Source: researchoutputwizard
Source ID: 5585
Research output: Contribution to journal > Article > Scientific > peer-review

Synthesis of porphyrinoids with silane anchors and their covalent self-assembling and metallation on solid surface

General information

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

Publication information

Journal: Journal of Colloid and Interface Science
Volume: 369
Issue number: 1
ISSN (Print): 0021-9797
Ratings:
Scopus rating (2012): CiteScore 3.4 SJR 1.304 SNIP 1.463
Original language: English
DOIs:
10.1016/j.jcis.2011.12.044

Bibliographical note

Contribution: organisation=keb kem,FACT1=0.5
Contribution: organisation=orc,FACT2=0.5
Publisher name: Academic Press Inc.; Elsevier Science
Source: researchoutputwizard
Source ID: 5279
Research output: Contribution to journal > Article > Scientific > peer-review

Synthesis of titanate nanostructures using amorphous precursor material and their adsorption/photocatalytic properties

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Contributors: Ylhäinen, E. K., Nunes, M., Silvestre, A., Monteiro, O.
Pages: 4305-4312
Publication date: 2012
Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Science
Volume: 47
Issue number: 10
ISSN (Print): 0022-2461
Ratings:
Scopus rating (2012): CiteScore 2.2 SJR 0.988 SNIP 1.383
Original language: English
DOIs:
10.1007/s10853-012-6281-x

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Springer
Source: researchoutputwizard
Source ID: 5609
Research output: Contribution to journal › Article › Scientific › peer-review

The fluorine effect: photophysical properties of borondipyrromethene (bodipy) dyes appended at the meso position with fluorinated aryl groups

General information

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

Publication information

Journal: RSC Advances
Volume: 2
Issue number: 11
ISSN (Print): 2046-2069
Ratings:
Scopus rating (2012): CiteScore 2.4 SJR 0.872 SNIP 0.619
Original language: English
DOIs:
10.1039/c2ra20219k

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: The Royal Society of Chemistry - RSC
Source: researchoutputwizard
Source ID: 3840
Research output: Contribution to journal › Article › Scientific › peer-review

Vectorial Photoinduced Charge Transfer in Langmuir-Blodgett Films of Porphyrin-Based Donor-Acceptor Systems

General information

Publication status: Published
MoE publication type: A3 Part of a book or another research book
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Tkachenko, N., Lemmetyinen, H.
Pages: 537-586
Publication date: 2012

Host publication information

Title of host publication: Multiporphyrin Arrays : Fundamentals and Applications
Place of publication: Singapore
Publisher: PAN STANFORD PUBLISHING
Editor: Dongho, K.
ISBN (Print): 978-981-4316-60-6
ISBN (Electronic): 978-981-4364-28-7
DOIs:
10.4032/9789814364287
URLs:
<http://www.panstanford.com/books/9789814316606.html>

Bibliographical note

ei ut-numeroa 30.8.2013
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source ID: 5431
Research output: Chapter in Book/Report/Conference proceeding > Chapter > Scientific > peer-review

Construction of bispirooxindoles containing three quaternary stereocentres in a cascade using a single multifunctional organocatalyst

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Urban circular bioeconomy (UrCirBio), Scripps Res Inst, Scripps Research Institute, Skaggs Inst Chem Biol, Scripps Res Inst, Scripps Research Institute, Dept Chem, Scripps Res Inst, Scripps Research Institute, Dept Mol Biol, Scripps Res Inst, Scripps Research Institute, Dept Chem & Mol Biol, Univ Lisbon, Universidade de Lisboa, Fac Farm, iMed UL
Contributors: Tan, B., Candeias, N. R., Barbas, C. F.
Number of pages: 5
Pages: 473-477
Publication date: Jun 2011
Peer-reviewed: Yes

Publication information

Journal: Nature Chemistry
Volume: 3
Issue number: 6
ISSN (Print): 1755-4330
Ratings:
Scopus rating (2011): CiteScore 9.74 SJR 7.548 SNIP 3.484
Original language: English
Keywords: ENANTIOSELECTIVE CONJUGATE ADDITION, C BOND FORMATION, NATURAL-PRODUCTS, STEREOCONTROLLED CREATION, CINCHONA ALKALOIDS, DOMINO REACTIONS, ALDER REACTIONS, OXINDOLES, THIOUREA, DERIVATIVES
DOIs:
10.1038/NCHEM.1039
Source: WOS
Source ID: 000290846300015
Research output: Contribution to journal > Article > Scientific > peer-review

Core-Structure-Motivated Design of a Phosphine-Catalyzed [3+2] Cycloaddition Reaction: Enantioselective Syntheses of Spirocyclopenteneoxindoles

A novel organocatalytic asymmetric [3 + 2] cycloaddition reaction between methyleneindolinones and allylic compounds yielding complex spirocyclopentaneoxindoles has been developed. It provides extraordinary levels of enantioselective control involving a chiral phosphine as a nucleophilic organocatalyst. Simple precursors were used under mild conditions to construct oxindole derivatives with high enantiopurity and structural diversity. This method should be useful in medicinal chemistry and diversity-oriented syntheses of these intriguing compounds.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Urban circular bioeconomy (UrCirBio), Scripps Res Inst, Scripps Research Institute, Skaggs Inst Chem Biol, Scripps Res Inst, Scripps Research Institute, Dept Chem & Mol Biol

Contributors: 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 (2011): CiteScore 9.94 SJR 5.478 SNIP 2.328

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

1,7- And 1,6-Regioisomers of Diphenoxy and Dipyrrolidinyl Substituted Perylene Diimides: Synthesis, Separation, Characterization, and Comparison of Electrochemical and Optical Properties

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Dubey, R. K., Efimov, A., Lemmetyinen, H.

Pages: 778-788

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Chemistry of Materials

Volume: 23

Issue number: 3

ISSN (Print): 0897-4756

Ratings:

Scopus rating (2011): CiteScore 7.38 SJR 3.488 SNIP 2.108

Original language: English

DOIs:

10.1021/cm1018647

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 5891

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

Anaerobic H₂ production at elevated temperature (60 °c) by enriched mixed consortia from mesophilic sources

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Karadag, D.

Pages: 458-465

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: International Journal of Hydrogen Energy

Volume: 36

Issue number: 1

ISSN (Print): 0360-3199

Ratings:

Scopus rating (2011): CiteScore 4.42 SJR 1.443 SNIP 1.828

Original language: English

DOIs:

10.1016/j.ijhydene.2010.10.003

Bibliographical note

Contribution: organisation=keb,FACT1=1

Source: researchoutputwizard

Source ID: 6299

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

A solid phase extraction technique for HPLC analysis of short chain fatty acid fluxes during microbial degradation of plant polymers

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Carver, S., Munster, U., Tuovinen, O. H.

Pages: 1546-1555

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Journal of Liquid Chromatography and Related Technologies

Volume: 34

Issue number: 15

ISSN (Print): 1082-6076

Ratings:

Scopus rating (2011): CiteScore 0.8 SJR 0.457 SNIP 0.46

Original language: English

DOIs:

10.1080/10826076.2011.575978

Bibliographical note

Contribution: organisation=keb bio,FACT1=1

Source: researchoutputwizard

Source ID: 5825

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

Bay Region Borylation of Perylene Bisimides

General information

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

Publication information

Journal: European Journal of Organic Chemistry
Volume: 2011
Issue number: 30
ISSN (Print): 1434-193X
Ratings:
Scopus rating (2011): CiteScore 3.2 SJR 1.576 SNIP 0.886
Original language: English
DOIs:
10.1002/ejoc.201101051

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source ID: 5882
Research output: Contribution to journal > Article > Scientific > peer-review

Biohydrogen production in alkalithermophilic conditions: Thermobrachium celere as a case study

General information

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

Publication information

Journal: Bioresource Technology
Volume: 102
Issue number: 18
ISSN (Print): 0960-8524
Ratings:
Scopus rating (2011): CiteScore 5.56 SJR 2.308 SNIP 2.516
Original language: English
DOIs:
10.1016/j.biortech.2011.01.028

Bibliographical note

Contribution: organisation=keb bio,FACT1=1
Source: researchoutputwizard
Source ID: 5851
Research output: Contribution to journal > Article > Scientific > peer-review

Carbon Nanotube Wiring of Donor-Acceptor Nanograins by Self-Assembly and Efficient Charge Transport

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Umeyama, T., Tezuka, N., Kawashima, F., Seki, S., Matano, Y., Yoshihide, N., Shishido, T., Nishi, M., Hirao, K., Lehtivuori, H., Tkachenko, N. V., Lemmetyinen, H., Imahori, H.
Pages: 4615-4619

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Angewandte Chemie (International Edition)

Volume: 50

Issue number: 20

ISSN (Print): 1433-7851

Ratings:

Scopus rating (2011): CiteScore 10.75 SJR 6.063 SNIP 2.353

Original language: English

DOIs:

10.1002/anie.201007065

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 7448

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

Comparison of sea surface microlayer and subsurface water bacterial communities in the Baltic sea

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Lindroos, A., Szabo, H. M., Nikinmaa, M., Leskinen, P.

Pages: 29-42

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Aquatic Microbial Ecology

Volume: 65

Issue number: 1

ISSN (Print): 0948-3055

Ratings:

Scopus rating (2011): CiteScore 2.45 SJR 1.434 SNIP 0.884

Original language: English

DOIs:

10.3354/ame01532

Bibliographical note

Contribution: organisation=keb bio,FACT1=1

Source: researchoutputwizard

Source ID: 6624

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

Covalent phthalocyanine-fullerene dyads: synthesis, electron transfer in solutions and molecular films

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Tkachenko, N. V., Efimov, A., Lemmetyinen, H.

Pages: 780-790

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Journal of Porphyrins and Phthalocyanines

Volume: 15

Issue number: 9-10

ISSN (Print): 1088-4246

Ratings:

Scopus rating (2011): CiteScore 1.4 SJR 0.545 SNIP 0.583

Original language: English

DOIs:

10.1142/S1088424611003732

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 7388

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

Dynamics of Photoinduced Charge Transfer of Fullerene Based Donor-Acceptor Systems: From Solution to Organized Molecular Films

General information

Publication status: Published

MoE publication type: A3 Part of a book or another research book

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Tkachenko, N. V., Lemmetyinen, H.

Pages: 405-440

Publication date: 2011

Host publication information

Title of host publication: Handbook of Carbon Nano Materials, Volume 2: Electron Transfer and Applications

Place of publication: Singapore

Publisher: World Scientific Publishing

Editors: D'Souza, F., Kadish, K. M.

ISBN (Print): 978-981-4327-81-7

ISBN (Electronic): 981-4350-21-4

Bibliographical note

myös isbn 978-981-4350-21-1.Poistettu tupla r=3293 tietokannassa portfolio12.
Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 7389

Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific › peer-review

Effect of Anion Ligation on Electron Transfer of Double-Linked Zinc Porphyrin - Fullerene Dyad

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Al-Subi, A. H., Niemi, M., Tkachenko, N. V., Lemmetyinen, H.

Pages: 3263-3271

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry A

Volume: 115

Issue number: 15

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131

Original language: English

DOIs:

10.1021/jp111234d

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 5676

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

Effects of fullerene encapsulation on structure and photophysical properties of porphyrin-linked single-walled carbon nanotubes

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Umeyama, T., Mihara, J., Hayashi, H., Kadota, N., Chukharev, V., Tkachenko, N., Lemmetyinen, H., Yoshida, K., Isoda, S., Imahori, H.

Pages: 11781-11783

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Chemical Communications

Volume: 47

Issue number: 42

ISSN (Print): 1359-7345

Ratings:

Scopus rating (2011): CiteScore 5.96 SJR 2.889 SNIP 1.326

Original language: English

DOIs:

10.1039/c1cc15011a

Bibliographical note

Contribution: organisation=keb,FACT1=1

Source: researchoutputwizard

Source ID: 7446

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

Electronic Structure Manipulation of (Benzothiazole)zinc Complexes: Synthesis, Optical and Electrochemical Studies of 5-Substituted Derivatives

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Dey, S., Efimov, A., Giri, C., Rissanen, K., Lemmetyinen, H.

Pages: 6226-6232

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: European Journal of Organic Chemistry

Volume: 2011

Issue number: 31

ISSN (Print): 1434-193X

Ratings:

Scopus rating (2011): CiteScore 3.2 SJR 1.576 SNIP 0.886

Original language: English

DOIs:

10.1002/ejoc.201100186

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 5881

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

Enhanced performance and stability of inverted organic solar cells by using novel zinc-benzothiazole complexes as anode buffer layer

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Dey, S., Vivo, P., Efimov, A., Lemmetyinen, H.

Pages: 15587-15592

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry

Volume: 21

ISSN (Print): 0959-9428

Ratings:

Scopus rating (2011): SJR 2.614 SNIP 1.539

Original language: English

DOIs:

10.1039/c1jm13256c

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 5883

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

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

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Martiskainen, J., Kananavicius, R., Linnanto, J., Lehtivuori, H., Keraenen, M., Aumanen, V., Tkachenko, N., Korppi-Tommola, J.

Pages: 195-207

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Photosynthesis Research

Volume: 107

Issue number: 2

ISSN (Print): 0166-8595

Ratings:

Scopus rating (2011): CiteScore 2.86 SJR 1.32 SNIP 1.09

Original language: English

DOIs:

10.1007/s11120-011-9626-4

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 6759

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

Fused Alq3 derivatives: syntheses and photophysical characteristics

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Contributors: Heiskanen, J. P., Tolkki, A. E., Lemmetyinen, H. J., Hormi, O. E. O.
Pages: 14766-14775
Publication date: 2011
Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry
Volume: 21
ISSN (Print): 0959-9428
Ratings:
Scopus rating (2011): SJR 2.614 SNIP 1.539
Original language: English
DOIs:
10.1039/C1JM12424B

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source ID: 6068
Research output: Contribution to journal > Article > Scientific > peer-review

Indole-olefin-oxazoline (IndOlefOx)-ligands: synthesis and utilization in asymmetric Rh-catalyzed conjugate addition

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering
Contributors: Kuuloja, N., Tois, J., Franzen, R.
Pages: 468-475
Publication date: 2011
Peer-reviewed: Yes

Publication information

Journal: Tetrahedron : Asymmetry
Volume: 22
Issue number: 4
ISSN (Print): 0957-4166
Ratings:
Scopus rating (2011): CiteScore 2.69 SJR 1.301 SNIP 0.812
Original language: English
DOIs:
10.1016/j.tetasy.2011.02.020

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source ID: 6472
Research output: Contribution to journal > Article > Scientific > peer-review

Optical, Electrochemical, and Photovoltaic Effects of an Electron-Withdrawing Tetrafluorophenylene Bridge in a Push -Pull Porphyrin Sensitizer Used for Dye-Sensitized Solar Cells

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Mathew, S., Iijima, H., Toude, Y., Umeyama, T., Matano, Y., Ito, S., Tkachenko, N. V., Lemmetyinen, H., Imahori, H.
Pages: 14415-14424
Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 115

Issue number: 29

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2011): CiteScore 4.92 SJR 2.339 SNIP 1.465

Original language: English

DOIs:

10.1021/jp2030208

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 6767

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

Photochemical processes for dithiocarbamate metal complexes. Photochemistry of Ni(II)(n-Bu₂NCS₂)₂ complex in CCl₄

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Kolomeets, A. V., Plyusnin, V. F., Grivin, V. P., Larionov, S. V., Lemmetyinen, H.

Pages: 164-172

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Journal of Photochemistry and Photobiology, A: Chemistry

Volume: 220

Issue number: 2-3

ISSN (Print): 1010-6030

Ratings:

Scopus rating (2011): CiteScore 2.84 SJR 0.978 SNIP 1.355

Original language: English

DOIs:

10.1016/j.jphotochem.2011.04.007

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 6407

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

Photochemistry of Dithiocarbamate Cu(II) Complex in CCl₄

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Plyusnin, V. F., Kolomeets, A. V., Grivin, V. P., Larionov, S. V., Lemmetyinen, H.

Pages: 1763-1773

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry A

Volume: 115

Issue number: 10

ISSN (Print): 1089-5639

Ratings:

Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131

Original language: English

DOIs:

10.1021/jp105755f

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 7028

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

Photochromic processes in di(mercaptoquinolino)Ni(II) complex and perfluordiphenyl disulfide solutions

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Vorobyev, D., Kolomeets, A., Ivanov, Y., Bogdanchikov, G., Grivin, V., Plyusnin, V., Larionov, S., Lemmetyinen, H.

Pages: 1196-1202

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Photochemical & Photobiological Sciences

Volume: 10

Issue number: 7

ISSN (Print): 1474-905X

Ratings:

Scopus rating (2011): CiteScore 2.63 SJR 1.028 SNIP 0.947

Original language: English

DOIs:

10.1039/c1pp05061c

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 7536

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

Photocurrent generation in fullerene-phthalocyanine composite by in situ cationic polymerization

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Lintinen, K., Storbacka, L., Efimov, A., Tolkki, A., Tkachenko, N., Lemmetyinen, H.

Pages: 909-916

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Solar Energy Materials and Solar Cells

Volume: 95

Issue number: 3

ISSN (Print): 0927-0248

Ratings:

Scopus rating (2011): CiteScore 5.16 SJR 2.182 SNIP 2.548

Original language: English

DOIs:

10.1016/j.solmat.2010.11.018

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source ID: 6635
Research output: Contribution to journal > Article > Scientific > peer-review

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Wijesinghe, C. A., Niemi, M., Tkachenko, N. V., Subbaiyan, N. K., Zandler, M. E., Lemmetyinen, H., DSouza, F.
Pages: 391-400
Publication date: 2011
Peer-reviewed: Yes

Publication information

Journal: Journal of Porphyrins and Phthalocyanines
Volume: 15
Issue number: 5-6
ISSN (Print): 1088-4246
Ratings:
Scopus rating (2011): CiteScore 1.4 SJR 0.545 SNIP 0.583
Original language: English
DOIs:
10.1142/S108842461100329X

Bibliographical note

poistettu tupla r=3530
Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source ID: 7565
Research output: Contribution to journal > Article > Scientific > peer-review

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

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Lemmetyinen, H., Tkachenko, N. V., Efimov, A., Niemi, M.
Pages: 397-412
Publication date: 2011
Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics
Volume: 13
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.184
Original language: English
DOIs:
10.1039/C0CP01106A

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source ID: 6590
Research output: Contribution to journal > Article > Scientific > peer-review

Photoinduced processes in chromophore-gold nanoparticle assemblies

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Kotiaho, A., Lahtinen, R., Lemmetyinen, H.

Pages: 813-821

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Pure and Applied Chemistry

Volume: 83

Issue number: 4

ISSN (Print): 0033-4545

Ratings:

Scopus rating (2011): CiteScore 2.56 SJR 1.21 SNIP 1.054

Original language: English

DOIs:

10.1351/PAC-CON-10-08-19

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 6436

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

Photophysics and photoelectrochemical properties of nanohybrids consisting of fullerene-encapsulated single-walled carbon nanotubes and poly(3-hexylthiophene)

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Tezuka, N., Umeyama, T., Matano, Y., Shishido, T., Yoshida, K., Ogawa, T., Isoda, S., Stranius, K., Chukharev, V., Tkachenko, N. V., Lemmetyinen, H., Imahori, H.

Pages: 741-750

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Energy & Environmental Science

Volume: 4

Issue number: 3

ISSN (Print): 1754-5692

Ratings:

Scopus rating (2011): CiteScore 9.96 SJR 3.737 SNIP 2.497

Original language: English

DOIs:

10.1039/C0EE00482K

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 7373

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

Poly(b-amino ester)-DNA complexes: Time-resolved fluorescence and cellular transfection studies

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: Vuorimaa, E., Ketola, T., Green, J. J., Hanzlikova, M., Lemmetyinen, H., Langer, R., Anderson, D. G., Urtti, A., Yliperttula, M.
Pages: 171-176
Publication date: 2011
Peer-reviewed: Yes

Publication information

Journal: Journal of Controlled Release
Volume: 154
Issue number: 2
ISSN (Print): 0168-3659
Ratings:

Scopus rating (2011): CiteScore 6.33 SJR 2.763 SNIP 2.089

Original language: English

DOIs:

10.1016/j.jconrel.2011.06.016

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 7546

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

Preparation of triethylammonium tetra-arylborates (TETABs): coupling partners for the Suzuki reaction

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Kuuloja, N., Kylmälä, T. M., Tois, J. E., Sjöholm, R. E., Franzen, R. G.

Pages: 1052-1063

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Synthetic Communications

Volume: 41

Issue number: 7

ISSN (Print): 0039-7911

Ratings:

Scopus rating (2011): CiteScore 1.13 SJR 0.432 SNIP 0.53

Original language: English

DOIs:

10.1080/00397911003718086

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 6471

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

Role of Polyplex Intermediate Species on Gene Transfer Efficiency: Polyethylenimine-DNA Complexes and Time-Resolved Fluorescence Spectroscopy

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Ketola, T., Hanzlikova, M., Urtti, A., Lemmetyinen, H., Yliperttula, M., Vuorimaa, E.

Pages: 1895-1902

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry Part B

Volume: 115

Issue number: 8

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2011): CiteScore 3.62 SJR 1.801 SNIP 1.223

Original language: English

DOIs:

10.1021/jp109984c

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 6357

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

Self-assembled monolayers (SAMs) of porphyrin deposited inside photonic crystal fibre (PCF)

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Optoelectronics Research Centre, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Veselov, A. A., Thur, C., Efimov, A., Guina, M., Lemmetyinen, H., Tkachenko, N. V.

Pages: 1858-1861

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Physica Status Solidi A: Applications And Materials Science

Volume: 208

Issue number: 8

ISSN (Print): 1862-6300

Ratings:

Scopus rating (2011): CiteScore 1.66 SJR 0.971 SNIP 0.98

Original language: English

DOIs:

10.1002/pssa.201084135

Bibliographical note

SA Project ActiveFiber
Contribution: organisation=keb kem,FACT1=0.5
Contribution: organisation=orc,FACT2=0.5

Source: researchoutputwizard

Source ID: 7506

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

Structure of porphyrin-fullerene dyad monolayer on the water surface and solid substrate

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Dyakova, Y. A., Suvorova, E. I., Orekhov, A. S., Alekseev, A. S., Klechkovskaya, V. V., Tereshchenko, E. Y., Tkachenko, N. V., Lemmetyinen, H., Feigin, L. A., Kovalchuka, M. V.

Number of pages: 7

Pages: 157-163

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Crystallography Reports

Volume: 56

Issue number: 1

ISSN (Print): 1063-7745

Ratings:

Scopus rating (2011): CiteScore 0.29 SJR 0.241 SNIP 0.31

Original language: English

DOIs:

10.1134/S1063774511010093

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 2063

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

Study of PEGylated Lipid Layers as a Model for PEGylated Liposome Surfaces: Molecular Dynamics Simulation and Langmuir Monolayer Studies

General information

Publication status: Published

MoE 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

Contributors: Stepniewski, M., Pasenkiewicz-Gierula, M., Rog, T., Danne, R., Orłowski, A., Karttunen, M., Urtti, A., Yliperttula, M., Vuorimaa, E., Bunker, A.

Pages: 7788-7798

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Langmuir

Volume: 27

Issue number: 12

ISSN (Print): 0743-7463

Ratings:

Scopus rating (2011): CiteScore 4.42 SJR 2.051 SNIP 1.341

Original language: English

DOIs:

10.1021/la200003n

Bibliographical note

poistettu tupla r=2135
Contribution: organisation=fys,FACT1=0.5
Contribution: organisation=keb kem,FACT2=0.5

Source: researchoutputwizard

Source ID: 7309

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

Synthesis and photovoltaic properties of thiopheneimide-fused thiophene alternating copolymers with different alkyl side chains

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry

Contributors: Umeyama, T., Oodoi, M., Yoshikawa, O., Sagawa, T., Yoshikawa, S., Evgenia, D., Tezuka, N., Matano, Y., Stranius, K., Tkachenko, N., Lemmetyinen, H., Imahori, H.

Pages: 12454-12461

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry

Volume: 21
Issue number: 33
ISSN (Print): 0959-9428
Ratings:
Scopus rating (2011): SJR 2.614 SNIP 1.539
Original language: English
DOIs:
10.1039/C1JM11531F

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Source: researchoutputwizard
Source ID: 7447
Research output: Contribution to journal > Article > Scientific > peer-review

The excited states of a porphine-quinone complex under an external electrostatic field calculated by TDDFT

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Computational Science X (CompX), Frontier Photonics
Contributors: Aittala, P. J., Cramariuc, O., Hukka, T. I.
Pages: 226-231
Publication date: 2011
Peer-reviewed: Yes

Publication information

Journal: Chemical Physics Letters
Volume: 501
Issue number: 4-6
ISSN (Print): 0009-2614
Ratings:
Scopus rating (2011): CiteScore 2.38 SJR 1.159 SNIP 1.004
Original language: English
DOIs:
10.1016/j.cplett.2010.11.042

Bibliographical note

Contribution: organisation=keb kem,FACT1=1
Publisher name: Elsevier
Source: researchoutputwizard
Source ID: 5671
Research output: Contribution to journal > Article > Scientific > peer-review

Ultrafast excitation transfer and charge stabilization in a newly assembled photosynthetic antenna-reaction center mimic composed of boron dipyrin, zinc porphyrin and fullerene

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics
Contributors: D'Souza, F., Wijesinghe, C. A., El-Khouly, M. E., Hudson, J., Niemi, M., Lemmetyinen, H., Tkachenko, N. V., Zandler, M. E., Fukuzumi, S.
Pages: 18168-18178
Publication date: 2011
Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics
Volume: 13
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.184

Original language: English

DOIs:

10.1039/c1cp90147h

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 5861

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

Ultrafast pump-probe spectroscopy of IrCl₆²⁻ complex in alcohol solutions

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics

Contributors: Glebov, E., Kolomeets, A., Pozdnyakov, I., Plyusnin, V., Tkachenko, N. V., Lemmetyinen, H.

Pages: 1709-1714

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Photochemical & Photobiological Sciences

Volume: 10

Issue number: 10

ISSN (Print): 1474-905X

Ratings:

Scopus rating (2011): CiteScore 2.63 SJR 1.028 SNIP 0.947

Original language: English

DOIs:

10.1039/c1pp05138e

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Source ID: 5976

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

Utilization of IndPHOX-ligands in palladium-catalysed asymmetric allylic aminations

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering

Contributors: Wang, Y., Vaismaa, M., Hämäläinen, A., Tois, J., Franzen, R.

Pages: 524-529

Publication date: 2011

Peer-reviewed: Yes

Publication information

Journal: Tetrahedron : Asymmetry

Volume: 22

Issue number: 5

ISSN (Print): 0957-4166

Ratings:

Scopus rating (2011): CiteScore 2.69 SJR 1.301 SNIP 0.812

Original language: English

DOIs:

10.1016/j.tetasy.2011.03.004

Bibliographical note

Contribution: organisation=keb kem,FACT1=1

Source: researchoutputwizard

Photopolymerizable liquid fullerene, phthalocyanine and porphyrin derivatives: synthesis, analysis and photocurrent generation

Photopolymerizable liquid monomers of fullerene, phthalocyanine and porphyrin were synthesized, polymerized and used as photoactive materials in organic solar cell structures. The design of the molecules requires the combination of three major parts: the functional core of the original molecules, alkylic side chains for liquid state and polymerizable end groups. The harsh conditions of the chromophore synthesis require a modular design, where the chromophore core and polymerizable tails are synthesized separately, and combined later by mild acylation. A means of ultra-thin-film polymerization, both photo and thermal, were devised. All of the chromophores could be polymerized as ultrathin films. Because of their high absorbances, it was possible to use UV-Vis spectroscopy to monitor polymerization indirectly; as the films were of only a few monomer units thick, it was possible to dissolve the unreacted monomer residues afterwards and thus determine polymerization degrees as a function of the absorbance of the polymerized film. The molecules were studied extensively to yield the parameters for thin film preparation, photopolymerization, and photocurrent generation. While the monomers were liquid at room temperature, the hardness of the polymers was that of crosslinked epoxy plastics. The porphyrin monomer was used to study photopolymerization kinetics due to its unique self-photoinitiating properties. Polarization modulation IR spectroscopy was used to study real-time photopolymerization of the porphyrin monomer at varying temperatures, yielding rate constants and the activation energy of the reaction. It was the first published study of ultra-thin-film polymerization kinetics. The monomers were polymerized in situ to form bilayers, bulk heterojunctions or hybrids of both, to create a photoactive structure for photocurrent generation. An extensive set of samples was prepared and studied. The monomers employed in this work were optimized for easy photopolymerizability and as such produced unoptimal power conversion efficiency. Nevertheless the basic structure of the polymer lends itself well to modification for improved organic photovoltaic performance.

General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Department of Chemistry and Bioengineering

Contributors: Lintinen, K.

Number of pages: 96

Publication date: 3 Dec 2010

Publication information

Place of publication: Tampere

Publisher: Tampere University of Technology

ISBN (Print): 978-952-15-2492-9

ISBN (Electronic): 978-952-15-2494-3

Original language: English

Publication series

Name: Tampere University of Technology. Publication

Publisher: Tampere University of Technology

Volume: 942

ISSN (Print): 1459-2045

Electronic versions:

lintinen.pdf

URLs:

<http://urn.fi/URN:NBN:fi:tty-201011111359>**Bibliographical note**

Awarding institution: Tampere University of Technology

Source: researchoutputwizard

Source ID: 8651

Research output: Book/Report > Doctoral thesis > Collection of Articles

Computational study of charge transfer in a porphine: quinone complex and novel alkoxypridylindolizine derivatives

Finding ways to control electron transfer (ET) between molecules or molecular systems and to investigate efficient theoretical methods capable of describing ET is important for being able to design better molecular electronic devices. In this Thesis the capability of computational methods based on density functional theory (DFT) to describe charge transfer is studied in two molecular systems. In addition, the possibility to control ET by strong electric fields is investigated. The molecular structure and excited states of three alkoxypridylindolizine derivatives are studied by using DFT and time-dependent DFT (TDDFT). In addition, the influence of an external electrostatic field of the order of magnitude of 10⁹ V/m and of an electric field induced by ambient helical peptides on ET in a porphine-2,5-dimethyl-1,4-benzoquinone (PQ) complex is studied with TDDFT and the approximate coupled cluster singles and doubles (CC2) method. The calculations

show that the absorption spectra of the studied indolizine derivatives are characterized by a band arising from the intramolecular CT between the indolizine ring and the pyridyl substituent attached to it and the hybrid functionals reproduce the experimental absorption spectra of the derivatives well within TDDFT. However, the same functionals are not as good in describing the fluorescence properties of the indolizine derivatives, namely the CT excited state of a derivative is obtained with too low an energy, which prevents the relaxation of the correct state. This problem can be circumvented by applying an exchange-correlation (XC) functional with a high fraction of Hartree-Fock (HF) exchange but this is done in the expense of the quantitative accuracy. According to the calculations, perturbation generated either by an external electrostatic field or by ambient Aib peptides affects the energies of the locally excited Q and B states of porphine in the PQ complex clearly less than the energy of the lowest CT state. Hence, it is possible to select a locally excited state (Q or B) of the PQ complex whose photoexcitation leads to ET from porphine to quinone. The results presented show that TDDFT applied with the current XC functionals provides an efficient way to study the qualitative picture of the excited states under the influence of an external electric field.

General information

Publication status: Published
MoE publication type: G4 Doctoral dissertation (monograph)
Organisations: Department of Chemistry and Bioengineering
Contributors: Aittala, P.
Number of pages: 87
Publication date: 26 Nov 2010

Publication information

Place of publication: Tampere
Publisher: Tampere University of Technology
ISBN (Print): 978-952-15-2479-0
ISBN (Electronic): 978-952-15-2488-2
Original language: English

Publication series

Name: Tampere University of Technology. Publication
Publisher: Tampere University of Technology
Volume: 936
ISSN (Print): 1459-2045
Electronic versions:
aittala.pdf
URLs:
<http://urn.fi/URN:NBN:fi:tty-201011051351>

Bibliographical note

Awarding institution: Tampere University of Technology
Source: researchoutputwizard
Source ID: 7642
Research output: Book/Report > Doctoral thesis > Monograph

Multilayered thin films for organic photovoltaics

This work investigates the photoinduced interactions between different organic chromophores, thus identifying possible materials for organic photovoltaic applications. The intermolecular electron transfer (ET) in layered structures centered on a covalently bridged porphyrin-fullerene dyad (P-F) was studied by means of electrical and spectroscopic methods. When excited, the dyad initiates the vectorial ET in the films, and secondary processes take place after the charge separation between the porphyrin and fullerene moieties of P-F. This study showed that violanthrone-79 (V-79) and two different perylene derivatives (PDI and PTCDI) were capable to accept electrons from the photoinduced fullerene anion of P-F. Longer-lived electrical and spectroscopic signals were achieved when the film structures were expanded to multilayered configurations containing an electron-donor, the P-F dyad, and an electron-acceptor. The electron-donor material used was poly(3-hexylthiophene) (PHT). The film deposition technique was switched from the Langmuir-Blodgett (LB) to Langmuir-Schäfer (LS) or thermal evaporation methods in order to achieve stronger photoelectrical signal amplitudes. As a result of the information gained in the ET studies, photovoltaic devices were prepared based on the studied compounds. The photocurrent generated from the ultrathin film systems studied in this Thesis can be easily measured with a three-electrode photoelectrochemical cell. In fact, the deposition of a metal top-electrode on the solar cell would damage the underlying organics, thus leading to short-circuiting problems. However, since the liquid cells suffer of poor performances and low stability, it was aimed to build layered cells with a metal top-electrode. The first step in this direction was the optimization of the organics|top-electrode junction, in order to protect the thin organic films. This was achieved with the introduction of a thin tris-8-hydroxy-quinolato aluminum (Alq3) layer in the cell, which successfully enhanced both the efficiency and the lifetime of the devices. Finally, multilayered cells based on a donor-acceptor pair sandwiched between an electron-donor and an electron-acceptor were developed, demonstrating that it is possible to design photovoltaic devices starting from the valuable information offered by the ET studies. The molecule chosen to this aim was the phthalocyanine-fullerene dyad, H2Pc-C60ee, which could be easily deposited as spin-coated layer.

General information

Publication status: Published
MoE publication type: G4 Doctoral dissertation (monograph)
Organisations: Department of Chemistry and Bioengineering
Contributors: Vivo, P.
Number of pages: 86
Publication date: 29 Oct 2010

Publication information

Place of publication: Tampere
Publisher: Tampere University of Technology
ISBN (Print): 978-952-15-2450-9
ISBN (Electronic): 978-952-15-2461-5
Original language: English

Publication series

Name: Tampere University of Technology. Publication
Publisher: Tampere University of Technology
Volume: 918
ISSN (Print): 1459-2045
Electronic versions:
vivo.pdf
URLs:
<http://urn.fi/URN:NBN:fi:ty-201010071329>

Bibliographical note

Awarding institution: Tampere University of Technology
Source: researchoutputwizard
Source ID: 9598
Research output: Book/Report > Doctoral thesis > Monograph

Boronic Acids and Esters in the Petasis-Borono Mannich Multicomponent Reaction

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Scripps Res Inst, Scripps Research Institute, Skaggs Inst Chem Biol, Scripps Res Inst, Scripps Research Institute, Dept Chem & Mol Biol, Scripps Res Inst, Scripps Research Institute, Dept Mol Biol, Univ Lisbon, Universidade de Lisboa, Fac Farm, iMed UL
Contributors: 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 (2010): SJR 18.613 SNIP 10.967
Original language: English
Keywords: ALPHA-AMINO-ACIDS, BETA-TURN MIMETICS, N-ACYLIMINIUM IONS, STEREOSELECTIVE-SYNTHESIS , ORGANOBORONIC ACIDS, SOLID-PHASE, 3-COMPONENT REACTION, PRACTICAL SYNTHESIS, HYDROXY ALDEHYDES, FORMAL SYNTHESIS
DOIs:
10.1021/cr100108k
Source: WOS
Source ID: 000283395800014
Research output: Contribution to journal > Literature review > Scientific > peer-review

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

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Univ Lisbon, Universidade de Lisboa, Fac Farm, iMed UL

Contributors: 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 (2010): SJR 3.014 SNIP 1.308

Original language: English

Keywords: N-HETEROCYCLIC CARBENES, BAEYER-VILLIGER OXIDATION, CROSS-COUPPLING REACTIONS, MOLECULAR-OXYGEN, ZINC-OXIDE, COMPLEXES, EFFICIENT, KETONES, ESTERS, POLYMERIZATION

DOIs:

10.1021/ol100302e

Source: WOS

Source ID: 000278616800003

Research output: Contribution to journal › Article › Scientific › peer-review