

RSC Advances

An international journal to further the chemical sciences

www.rsc.org/advances

RSC Publishing is a not-for-profit publisher and a division of the Royal Society of Chemistry. Any surplus made is used to support charitable activities aimed at advancing the chemical sciences. Full details are available from www.rsc.org

IN THIS ISSUE

ISSN 2046-2069 CODEN RSCACL 2(19) 7307–7600 (2012)



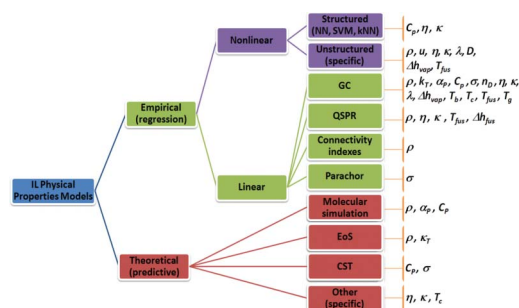
REVIEWS

7322

Predictive methods for the estimation of thermophysical properties of ionic liquids

João A. P. Coutinho,* Pedro J. Carvalho and Nuno M. C. Oliveira

Review on predictive models for the estimation of thermophysical properties of ionic liquids with a critical assessment of the quality of the models and their areas of applicability.



7347

Reflections on the chemistry of the Fischer–Tropsch synthesis

Olusola O. James,* Biswajit Chowdhury, M. Adediran Mesubi and Sudip Maity*

Reflections on the chemistry of FTS yields clearer pictures about the mechanism of the reaction and tools for its molecular engineering.

Chemistry of Fischer-Tropsch Synthesis



**Rational catalyst design for FTS
Molecular engineering**

EDITORIAL STAFF

Editor

Sarah Ruthven

Deputy editor

Kathleen Too

Senior publishing editor

Sophia Anderton

Publishing editorsCatherine Bacon, Amaya Camara-Campos,
Ian Coates, Lucy Gilbert, Charles Quigg**Publishing assistants**

Rachel Blakeburn, Natalie Ford, Paul Gibb, Peter Moorby

Publisher

Emma Wilson

For queries about submitted papers, please contact Sophia Anderton, Senior publishing editor, in the first instance. E-mail: advances@rsc.org

For pre-submission queries please contact Sarah Ruthven, Editor. E-mail: advances-rsc@rsc.org

RSC Advances (ISSN 2046-2069) is published by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

The Royal Society of Chemistry takes reasonable care in the preparation of this publication but does not accept liability for the consequences of any errors or omissions. Inclusion of an item in this publication does not imply endorsement by The Royal Society of Chemistry of the content of the original documents to which that item refers.

Advertisement sales: Tel +44 (0) 1223 432246;
Fax +44 (0) 1223 426017; E-mail advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

RSC Advances

An international journal to further the chemical sciences

www.rsc.org/advances

EDITORIAL BOARD

ChairMike D. Ward, University of Sheffield,
UK**Associate editors**

James D. Batteas, Texas A&M
University, USA
Russell J. Cox, University of Bristol, UK
Marcos N. Eberlin, University of
Campinas, Brazil
Matthias Epple, Universität Duisburg-
Essen, Germany

Changming Li, Nanyang
Technological University, Singapore
T. N. Guru Row, Indian Institute of
Science, Bangalore, India
Suning Wang, Queen's University,
Canada
Urs Welz-Biermann, Evonik Degussa
Taiwan Ltd., China

INFORMATION FOR AUTHORS

Full details on how to submit material for publication in RSC Advances are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: <http://www.rsc.org/advances>.

Submissions: The journal welcomes submissions of manuscripts for publication as Communications, Full papers and Reviews. Communications must report preliminary research findings that are original and of immediate interest. Full papers must describe science that will be of benefit to the community and are judged according to originality, quality of scientific content and contribution to existing knowledge. For Reviews, potential writers should contact the Editorial Office before embarking on their work (advances-rsc@rsc.org).

Authors may reproduce/republish portions of their published contribution without seeking permission from the RSC, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of The Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2012. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

Royal Society of Chemistry: Registered Charity No. 207890.

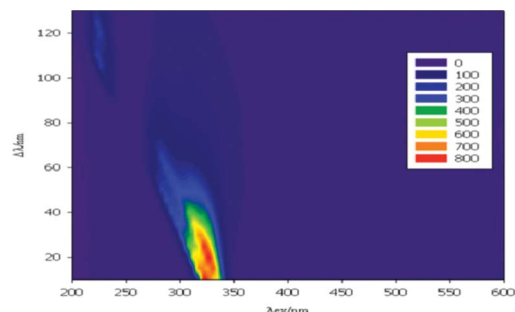
COMMUNICATIONS

7367

Facile approach to the synthesis of carbon nanodots and their peroxidase mimetic function in azo dyes degradation

Afsaneh Safavi,* Fatemeh Sedaghati, Hamidreza Shahbaazi and Elaheh Farjami

Carbon nanodots are prepared *via* a one-pot synthesis using a microwave-assisted ionic liquid (MAIL) method. Moreover, a novel application of CDs as peroxidase mimetic compounds for azo dyes degradation is explained.

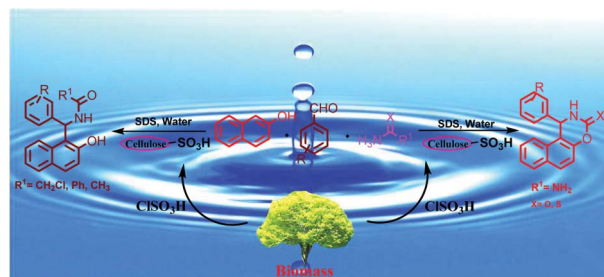


7371

Micelle promoted supramolecular carbohydrate scaffold-catalyzed multicomponent synthesis of 1,2-dihydro-1-aryl-3H-naphth[1,2-e][1,3]oxazin-3-one and amidoalkyl naphthols derivatives in aqueous medium

Atul Kumar,* Maneesh Kumar Gupta and Mukesh Kumar

Micelle promoted natural carbohydrate scaffold catalyzed synthesis of 1,2-dihydro-1-aryl-3H-naphth[1,2-e][1,3]oxazin-3-one and amidoalkyl naphthol derivatives have been developed *via* multicomponent one pot reaction.

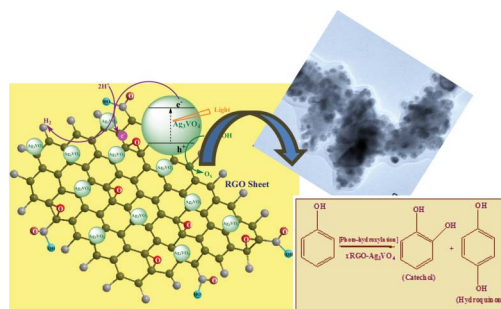


7377

Visible light induced photo-hydroxylation of phenol to catechol over RGO-Ag₃VO₄ nanocomposites without the use of H₂O₂

D. P. Das,* R. K. Barik, J. Das, P. Mohapatra and K. M. Parida*

RGO-Ag₃VO₄ nanocomposites prepared by a novel one-pot photochemical synthesis route show unusual selectivity towards catechol in the photo-hydroxylation of phenol with complete conversion.

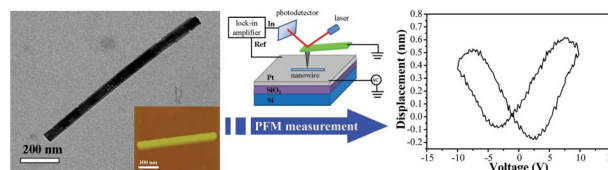


7380

Piezoelectric properties of rhombic LiNbO₃ nanowires

Zhong Chen, Jingyun Huang,* Yefeng Yang, Ye Wang, Yongjun Wu, Haiping He, Xiaoyan Wei, Zhizhen Ye, Huarong Zeng, Honglin Cong and Zhongyong Jiang

Low magnification TEM image, topographic image, and the typical *D-V* “butterfly” curve of a single LiNbO₃ nanowire.



High Impact Materials Science

Covering all aspects of materials science from the synthesis of materials through to a diversity of applications



Scan the QR code, search and view the latest articles online



Materials Physical Organic Inorganic Nanoscience
Food Biological Environmental Analytical Energy
Catalysis Chemical Biology & Medicinal General Chemistry

RSC Publishing

www.rsc.org/MaterialsPort

Registered Charity Number 207890

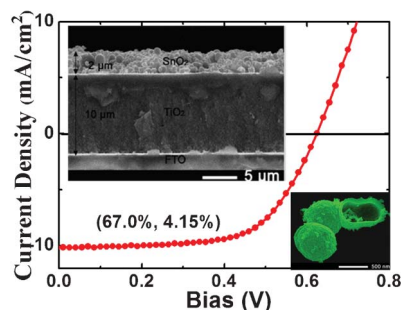
COMMUNICATIONS

7384

Hollow SnO₂ microspheres for high-efficiency bilayered dye sensitized solar cell

Jing Chen,* Chen Li, Feng Xu, Yidan Zhou, Wei Lei, Litao Sun and Yan Zhang

We report a bilayered DSSC using the hollow SnO₂ microspheres as the top layer and TiO₂ as the bottom layer. The power conversion efficiency (PCE) of the bilayered DSSC was 4.15%.

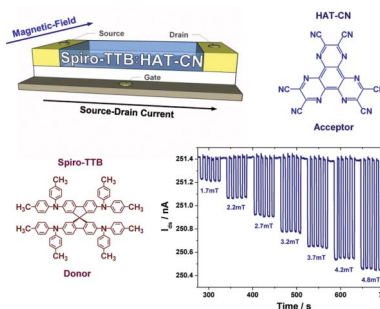


7388

Magnetoresistive field-effect transistors based on organic donor-acceptor blends

Thomas Reichert, Tobat P. I. Saragi* and Josef Salbeck

We present magnetoresistive transistors based on donor-acceptor blends, which are sensitive to magnetic fields as low as 1.7 mT.

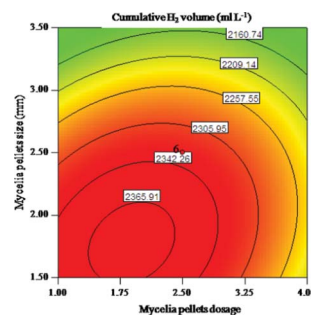


7391

Optimization of immobilization parameters of *Thermoanaerobacterium thermosaccharolyticum* W16 on a new carrier for enhanced hydrogen production

Lei Zhao, Guang-Li Cao, Jing Yao, Hong-Yu Ren, Fang Ma, Nan-Qi Ren and Ai-Jie Wang*

A new biological carrier mycelia pellet was adopted for enhanced hydrogen production by *Thermoanaerobacterium thermosaccharolyticum* W16.

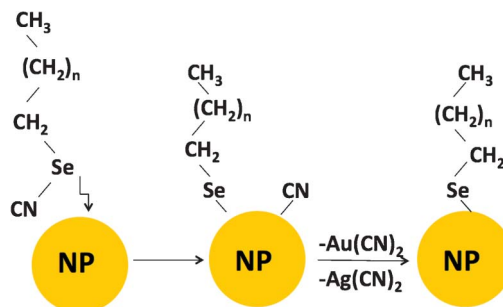


7396

Synthesis of Au and Ag nanoparticles with alkylselenocyanates

Oksana Zaluzhna, Chris Zangmeister and YuYe J. Tong*

We report the first successful synthesis of Au and Ag nanoparticles (NPs) with alkylselenocyanates as the source of protecting ligands.



RSC e-membership

Chemical science at your fingertips

£20

for 12 months



RSC e-membership enables you to...

- **ACCESS** expert knowledge and keep current with 12 digital editions of the award-winning *Chemistry World* magazine
- **INTERACT** with specialists in your field and discuss the science that matters to you by joining an RSC Interest Group
- **ENGAGE** with tens of thousands of users worldwide on MyRSC, the online professional community for chemical scientists

Join today and connect with the global scientific community through the RSC, the central hub for chemical science www.rsc.org/emembership

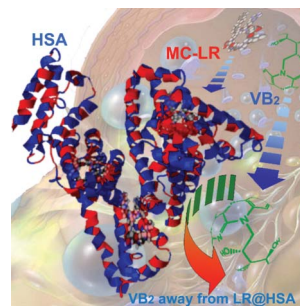
COMMUNICATIONS

7400

MC-LR@HSA: non-covalent interaction and effect

Chao Song, Yan-Qin Zi and Hong-Wen Gao*

Microcystin-LR binding to subdomains IA, IIA, IIIA and IIB of HSA induced the HSA conformation to transfer from α -helix to β -pleated sheet and random coils so that HSA transport of vitamin B₂ (VB₂) was inhibited.

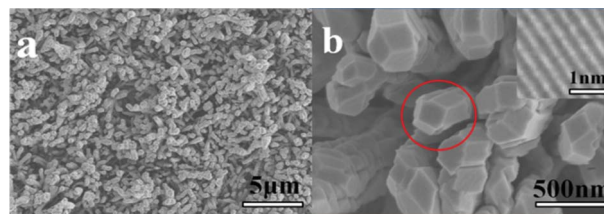


7403

Single-phase tungsten carbide nanopillar arrays prepared by chemical vapor deposition

Feng Teng, Jiangtao Wang, Xiuyun An, Bingan Lu, Yurong Su, Chengshi Gong, Peng Zhang, Zhenxing Zhang and Erqing Xie*

Single-phase tungsten carbide nanopillar arrays have been prepared by hot filament chemical vapor deposition with carbonized tungsten filaments as precursors.



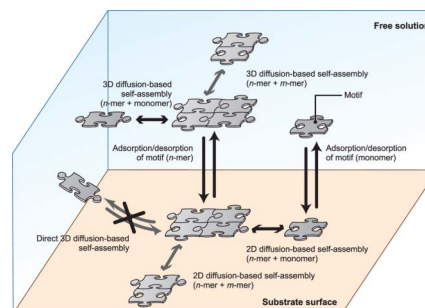
PAPERS

7406

Theoretical model of substrate-assisted self-assembly of DNA nanostructures

Shogo Hamada* and Satoshi Murata*

The theoretical model of a novel DNA self-assembly methodology called “substrate-assisted self-assembly” is proposed and compared with experiments.

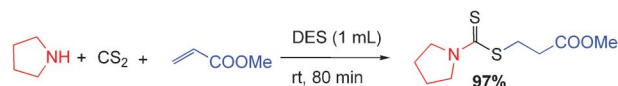


7413

A highly efficient synthesis of dithiocarbamates in green reaction media

Najmadin Azizi* and Elham Gholibeglo

A deep eutectic solvent (DES) and polyethylene glycol (PEG) promoted the environmentally friendly and fast synthesis of dithiocarbamate derivatives *via* a one-pot, three-component condensation of an amine, carbon disulfide, and a variety of electrophilic reagents in high yields and short reaction times without organic solvents and tedious work-up.



7417

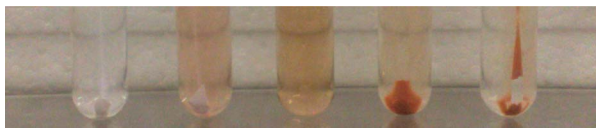
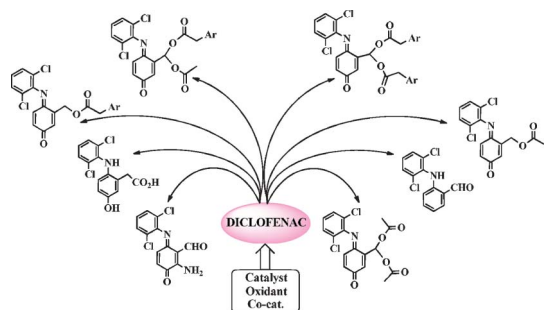


Photo-induced electron transfer in supramolecular materials of titania nanostructures and cytochrome *c*

Clemerson F. B. Dias, Juliana C. Araújo-Chaves, Katia C. U. Mugnol, Fabiane J. Trindade, Oswaldo L. Alves, Antonio C. F. Caires, Sergio Brochsztain, Frank N. Crespilho, Jivaldo R. Matos, Otaciro R. Nascimento and Iseli L. Nantes*

The interaction of TiO₂ nanoparticles and titanate nanotubes with cytochrome *c* is studied for understanding the effects of titania nanostructures on the photoreduction of heme iron.

7427

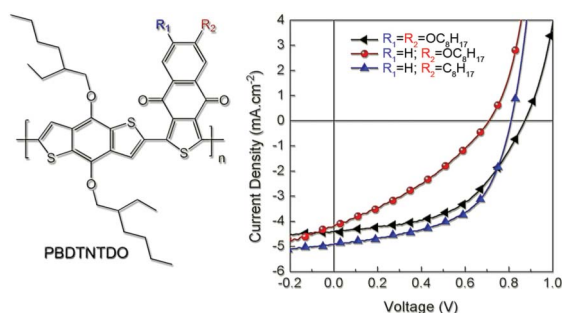


Oxidation of diclofenac catalyzed by manganese porphyrins: synthesis of novel diclofenac derivatives

Cláudia M. B. Neves, Mário M. Q. Simões,* M. Rosário M. Domingues, Isabel C. M. S. Santos, M. Graça P. M. S. Neves,* Filipe A. Almeida Paz, Artur M. S. Silva and José A. S. Cavaleiro

The *in vitro* formation of new diclofenac derivatives, initially resulting from oxidative decarboxylation, similar to what happens *in vivo*, is revealed. Manganese(III) porphyrins are the catalysts whereas hydrogen peroxide is the oxidant.

7439

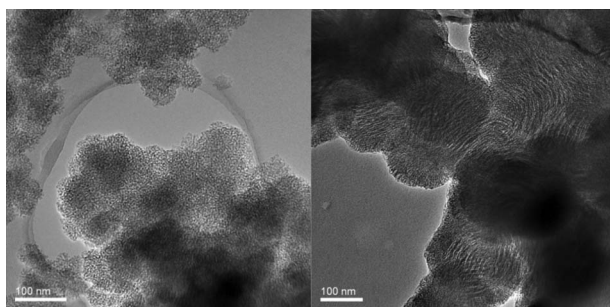


Copolymers from naphtho[2,3-*c*]thiophene-4,9-dione derivatives and benzodithiophene: synthesis and photovoltaic applications

Xuwen Chen, Bo Liu, Yingping Zou,* Wanjun Tang, Yongfang Li and Dequan Xiao

Three donor–acceptor (D–A) copolymers from a benzodithiophene (BDT) donor unit and a naphtho[2,3-*c*]thiophene-4,9-dione (NTDO) acceptor unit with different side chains were synthesized. Preliminary investigations showed power conversion efficiencies (PCEs) of 1.96% for PBDTNTDO-C1 and 2.21% for PBDTNTDO-C3.

7449



Bio-derived oleyl surfactants as porogens for the sustainable synthesis of micelle-templated mesoporous silica

Christian P. Canlas and Thomas J. Pinnavaia*

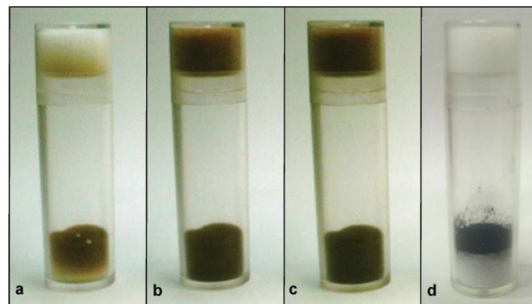
Bio-derived oleyl-NH₂ and -NH-(CH₂)₃NH₂ surfactants are effective templating agents for the hydrogen bonded assembly of mesoporous silica with well expressed wormhole (left) and lamellar (right) framework structures.

7456

Nontoxic, nonvolatile, and highly efficient osmium catalysts for asymmetric dihydroxylation of alkenes and application to one mol-scale synthesis of an anticancer drug, camptothecin intermediate

Ryo Akiyama, Norio Matsuki, Hiroshi Nomura, Hisao Yoshida, Tomoko Yoshida and Shū Kobayashi*

Nontoxic, nonvolatile, and highly efficient osmium catalysts have been developed and one mol-scale preparation of a key intermediate for camptothecin, an anticancer drug, has been demonstrated.

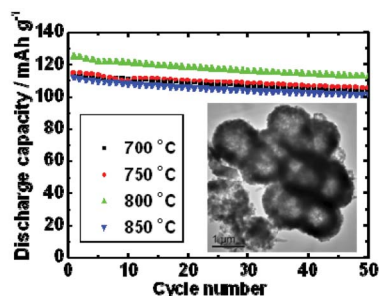


7462

Nano LiMn_2O_4 with spherical morphology synthesized by a molten salt method as cathodes for lithium ion batteries

Xuan Zhao, M. V. Reddy, Hanxing Liu,* S. Ramakrishna, G. V. Subba Rao and B. V. R. Chowdari*

LiMn_2O_4 synthesized by a molten salt method at various temperatures, hollow spherical morphology particles delivered high and stable electrochemical performance.

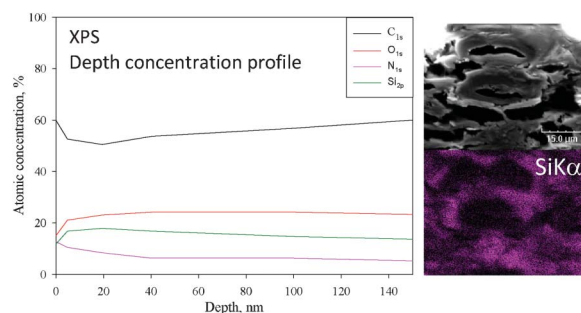


7470

Strengthening of degraded cellulosic material using a diamine alkylalkoxysilane

Zied Souguir, Anne-Laurence Dupont,* Kateryna Fatyeyeva, Gérard Mortha, Hervé Cheradame, Stéphane Ipert and Bertrand Lavédrine

The physicochemical modifications in papers upon introducing AEAPMDMS as a dry strength and deacidification agent were explored. Depth penetration inside the fibers was evidenced with XPS.

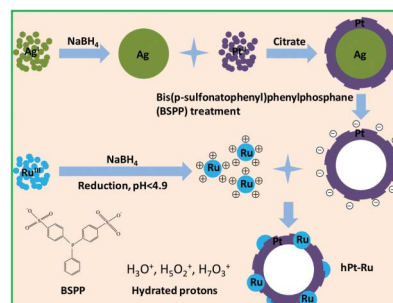


7479

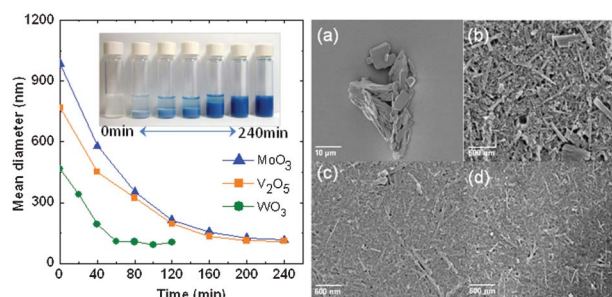
Electrostatic interaction based hollow Pt and Ru assemblies toward methanol oxidation

Feng Ye, Jinhua Yang, Weiwei Hu, Hui Liu, Shijun Liao, Jianhuang Zeng* and Jun Yang*

A solution route for the assembly of hollow Pt nanospheres and ultrafine Ru nanoparticles based on electrostatic interaction was demonstrated.



7487

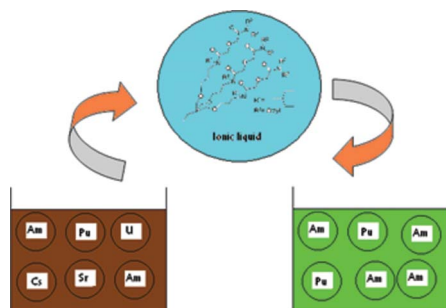


Wet-milled transition metal oxide nanoparticles as buffer layers for bulk heterojunction solar cells

Jen-Hsien Huang, Tzu-Yen Huang, Hung-Yu Wei, Kuo-Chuan Ho and Chih-Wei Chu*

In this study, we used high-energy grinding to prepare solutions of well-dispersed transition metal oxides for application in photovoltaic devices.

7492

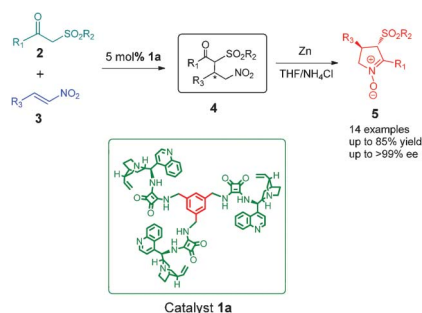


Extraction of Am(III) using novel solvent systems containing a tripodal diglycolamide ligand in room temperature ionic liquids: a 'green' approach for radioactive waste processing

A. Sengupta, P. K. Mohapatra,* M. Iqbal, W. Verboom, J. Huskens and S. V. Godbole

Extraction of actinide ions from acidic feed solutions was investigated using novel solvent systems containing a tripodal diglycolamide (T-DGA) in three room temperature ionic liquids (RTIL), viz. [C₄mim][NTf₂], [C₆mim][NTf₂] and [C₈mim][NTf₂].

7501

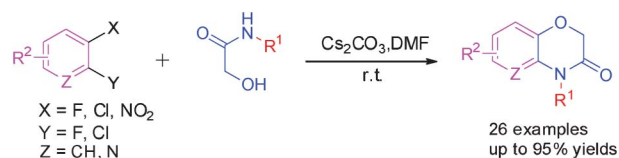


An expedient approach to highly enantioenriched cyclic nitrones mediated by robust and recoverable C₃-symmetric cinchonine-squaramide catalysts

Xin Han, Xiangfei Wu, Chang Min, Hai-Bing Zhou and Chune Dong*

The C₃-symmetric cinchonine-squaramide catalyzed asymmetric Michael addition of β -ketosulfones to nitroalkenes is presented. Subsequent transformation leads to chiral cyclic nitrones with excellent results (up to 85% yield and >99% ee). The catalyst can be recovered and reused for six cycles without losing activity and selectivity.

7506



A tandem coupling/smiles rearrangement/cyclization approach to 1,4-benzooxazinones or 1,4-pyridooxazinones under mild conditions

Chunjing Zhan, Jiong Jia,* Bingchuan Yang, Aiping Huang, Yanli Liu and Chen Ma*

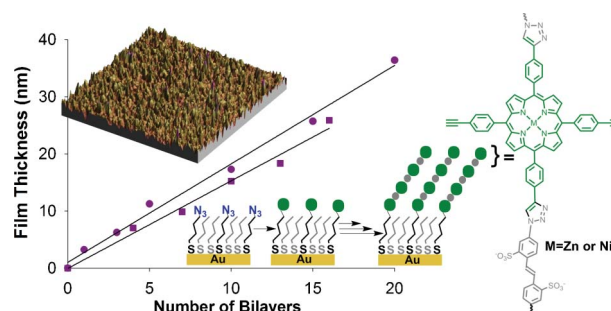
1,4-Benzooxazinones or 1,4-pyridooxazinones were easily obtained by a one-pot coupling/Smiles rearrangement/cyclization process.

7513

Layer-by-layer assembly of Zn(II) and Ni(II) 5,10,15,20-tetra(4-ethynylphenyl)porphyrin multilayers on Au using copper catalyzed azide-alkyne cycloaddition

Alexandra Krawicz, Joseph Palazzo, Gwo-Ching Wang and Peter H. Dinolfo*

We have developed a versatile layer-by-layer (LbL) fabrication method to assemble porphyrin based multilayers on Au surfaces utilizing copper(I) catalyzed azide-alkyne cycloaddition (CuAAC) as both a means of anchoring the films to the surface and coupling the individual molecular layers together.

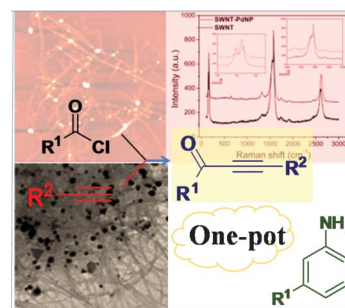


7523

Anchored palladium nanoparticles onto single walled carbon nanotubes: Efficient recyclable catalyst for N-containing heterocycles

Subhankar Santra, Priyadarshi Ranjan, Parthasarathi Bera, Prasenjit Ghosh and Swadhin K. Mandal*

Anchored palladium nanoparticles on chemically functionalized single walled carbon nanotubes (SWNTs-PdNPs) are used for a recyclable acyl Sonogashira reaction.

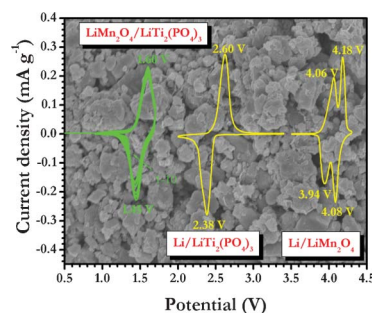


7534

Electrochemical performance of NASICON type carbon coated $\text{LiTi}_2(\text{PO}_4)_3$ with a spinel LiMn_2O_4 cathode

V. Aravindan, W. Chuiling and S. Madhavi*

Eco-friendly, thermally safe Li-ion batteries are demonstrated using NASICON type $\text{LiTi}_2(\text{PO}_4)_3$ as the anode with a commercially available LiMn_2O_4 cathode, the cell delivered appreciable performance during electrochemical cycling.

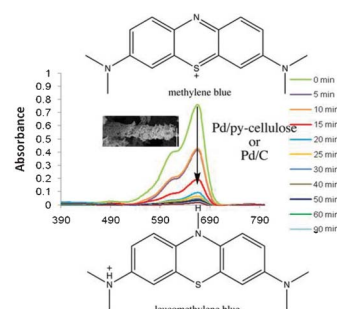


7540

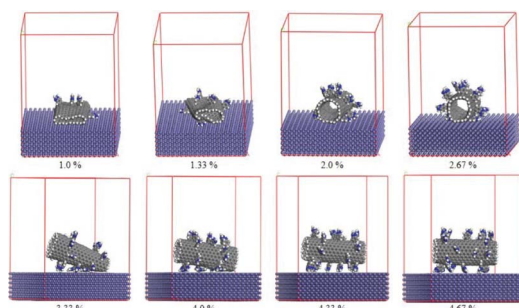
Novel Pd based catalyst for the removal of organic and emerging contaminants

Mallikarjuna N. Nadagouda,* Ishan Desai, Carlo Cruz and Duck J. Yang

Autocatalytic reduction of Au, Pd, and Pt crystals on polypyrrole-coated biodegradable cellulose fibers for waste water treatment.



7549



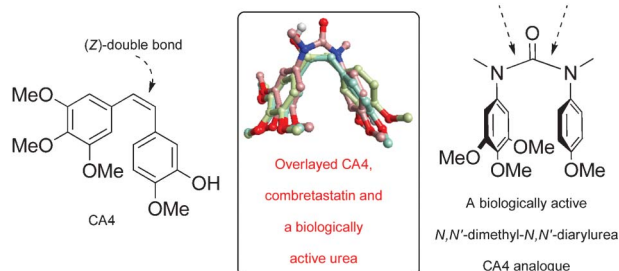
Collapse and Stability of functionalized Carbon Nanotubes on Fe (1 0 0) Surface

Cui-Cui Ling, Qing-Zhong Xue,* Nuan-Nuan Jing and Dan Xia

Carbon nanotubes modified by appropriate inhibitor groups can maintain their cylindrical structure on Fe surface and give them the potential to be used as nanocontainers for maintaining or transporting molecules.

7557

Conformationally 'fixed' urea mimics (Z)-double bond

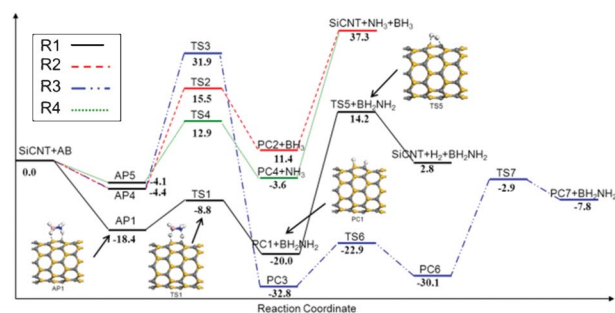


Exploiting conformationally restricted *N,N'*-dimethyl-*N,N'*-diarylureas as biologically active C=C double bond analogues: synthesis and biological evaluation of combretastatin A-4 analogues

Timothy J. Snape,* Katherine Karakoula, Farzana Rowther and Tracy Warr

Biologically active diarylureas, which occupy similar space to combretastatin A-4 (CA4), have been prepared. The results show that the ureas most like CA4, regarding benzene ring oxygenation and overall shape, are the most active.

7561

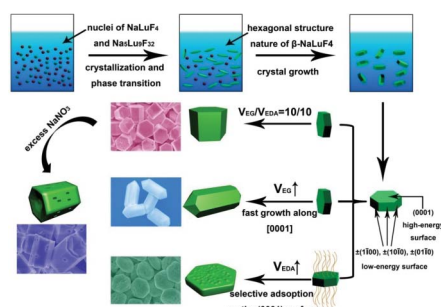


Theoretical study on the possibility of using silicon carbide nanotubes as dehydrogenation catalysts for ammonia-borane

Fenglei Cao and Huai Sun*

A new catalyst for the dehydrogenation of ammonia-borane is reported.

7569



Morphology-controllable synthesis and enhanced luminescence properties of β -NaLuF₄:Ln (Ln = Eu, Tb and Ce/Tb) microcrystals by solvothermal process

Fei He, Na Niu, Zhenguang Zhang, Xiao Zhang, Dong Wang, Ling Bai, Shili Gai, Xingbo Li and Piaoping Yang*

Schematic illustration for the formation process of β -NaLuF₄ MCs prepared at different conditions.

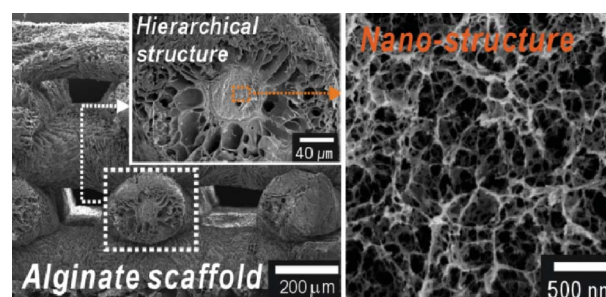
PAPERS

7578

Cryogenically direct-plotted alginate scaffolds consisting of micro/nano-architecture for bone tissue regeneration

Hyeong Jin Lee and Geun Hyung Kim*

Three dimensional multi-layered alginate scaffolds showed hierarchical core(nano)-shell(micro)-structured struts by using a combination of cryogenic and cross-linking processes.

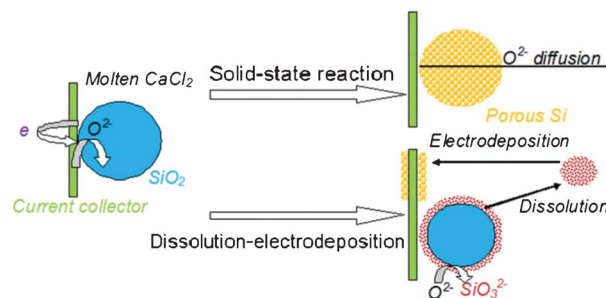


7588

Verification and implications of the dissolution–electrodeposition process during the electro-reduction of solid silica in molten CaCl_2

Wei Xiao, Xin Wang, Huayi Yin, Hua Zhu, Xuhui Mao and Dihua Wang*

The verified dissolution–electrodeposition of solid silica in molten CaCl_2 addresses the continuous silicon extraction and controllable electrolytic extraction of nanostructured silicon.



7594

A route to hydroxylfluorenes: TsOH-mediated condensation reactions of 1,3-diketones with propargylic alcohols

Liang-Feng Yao, Davin Tan, Xiaohe Miao and Kuo-Wei Huang*

An efficient method to prepare hydroxylfluorenes by TsOH-mediated tandem alkylation/rearrangements of propargylic alcohols with 1,3-diketones is described.

