

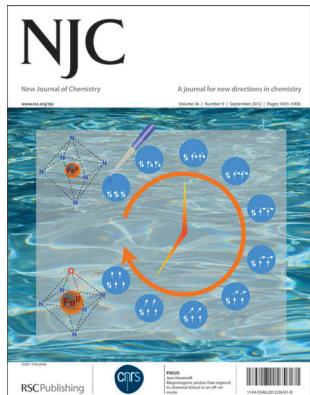


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IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 36(9) 1693–1908 (2012)



Cover

See Jens Hasserodt,
 pp. 1707–1712.
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Inside cover

See Shu-Peng Zhang and
 Hai-Ou Song, pp. 1733–1738.
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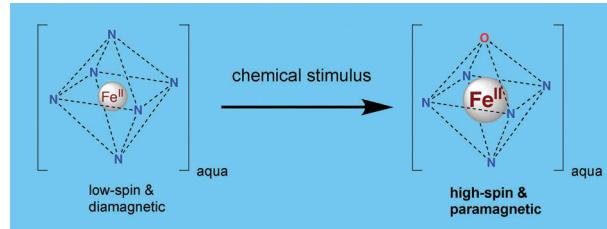
FOCUS

1707

Magnetogenic probes that respond to chemical stimuli in an off-on mode

Jens Hasserodt*

Robust ferrous chelates of cage-like, poly-aza ligands can be made to respond to chemical conversion by a target reactant in aqueous solution by changing the magnetic properties of the sample in a binary off-on fashion.



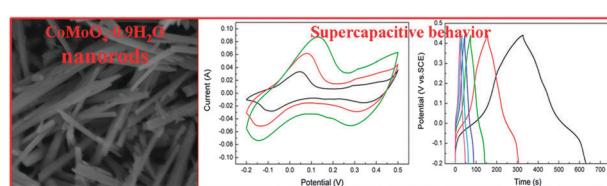
LETTERS

1713

Hydrothermal process for the fabrication of CoMoO₄·0.9H₂O nanorods with excellent electrochemical behavior

Mao-Cheng Liu, Ling-Bin Kong,* Xue-Jing Ma, Chao Lu, Xiao-Ming Li, Yong-Chun Luo and Long Kang

A hydrothermal process is developed to fabricate one-dimensional CoMoO₄·0.9H₂O nanorods with excellent electrochemical behavior. It provides a new research strategy for the application of binary oxides in supercapacitors.



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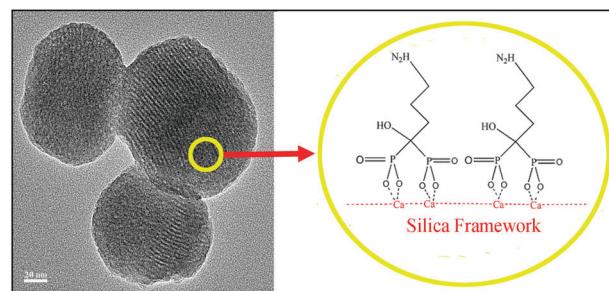
LETTERS

1717

Calcium doped mesoporous silica nanoparticles as efficient alendronate delivery vehicles

Jinlou Gu,* Meng Huang, Jiapeng Liu, Yongsheng Li, Wenru Zhao and Jianlin Shi*

Calcium doped mesoporous silica nanoparticles were successfully prepared and employed as efficient drug carriers for alendronate delivery. The incorporation of calcium ions dramatically enhanced the drug loading capacity and sustained release rate. The loaded alendronate more efficiently inhibited the growth of HeLa cancer cells than free drug.

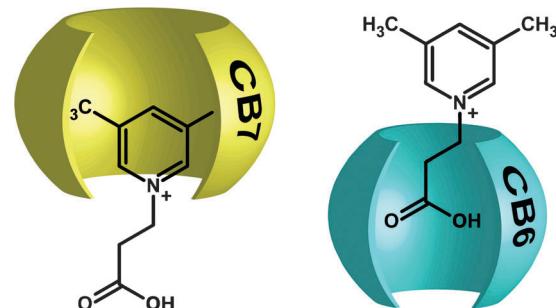


1721

Effects of cucurbituril size on the binding of a lutidine guest

Jan Svec, Vladimir Sindelar* and Angel E. Kaifer*

The size of cucurbituril hosts dramatically influences their binding features with a lutidine guest.

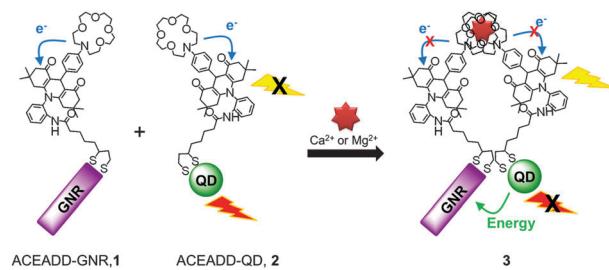


1725

Metal ion-induced dual fluorescent change for aza-crown ether acridinedione-functionalized gold nanorods and quantum dots

Ranganathan Velu, Nayoun Won, Jungheon Kwag, Sungwook Jung, Jaehyun Hur, Sungjee Kim* and Nokyung Park*

A pair of aza-crown ether acridinedione-functionalized quantum dots and gold nanorods has been developed for a selective metal ion sensor *via* ratiometric fluorescence modulations.

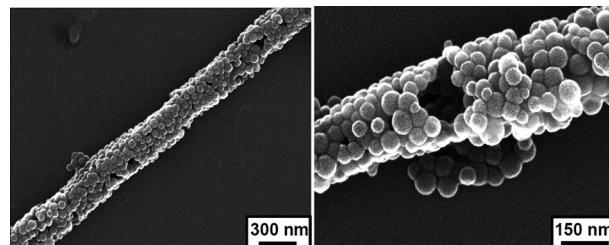


1729

Facile fabrication of free-standing microtubes composed of colloidal spheres

Xiaoyan Liu and Jianguo Huang*

Free-standing microtubes composed of polystyrene microspheres were fabricated by a facile electrostatic self-assembly approach templated with porous alumina membranes.



New process for crystal data files

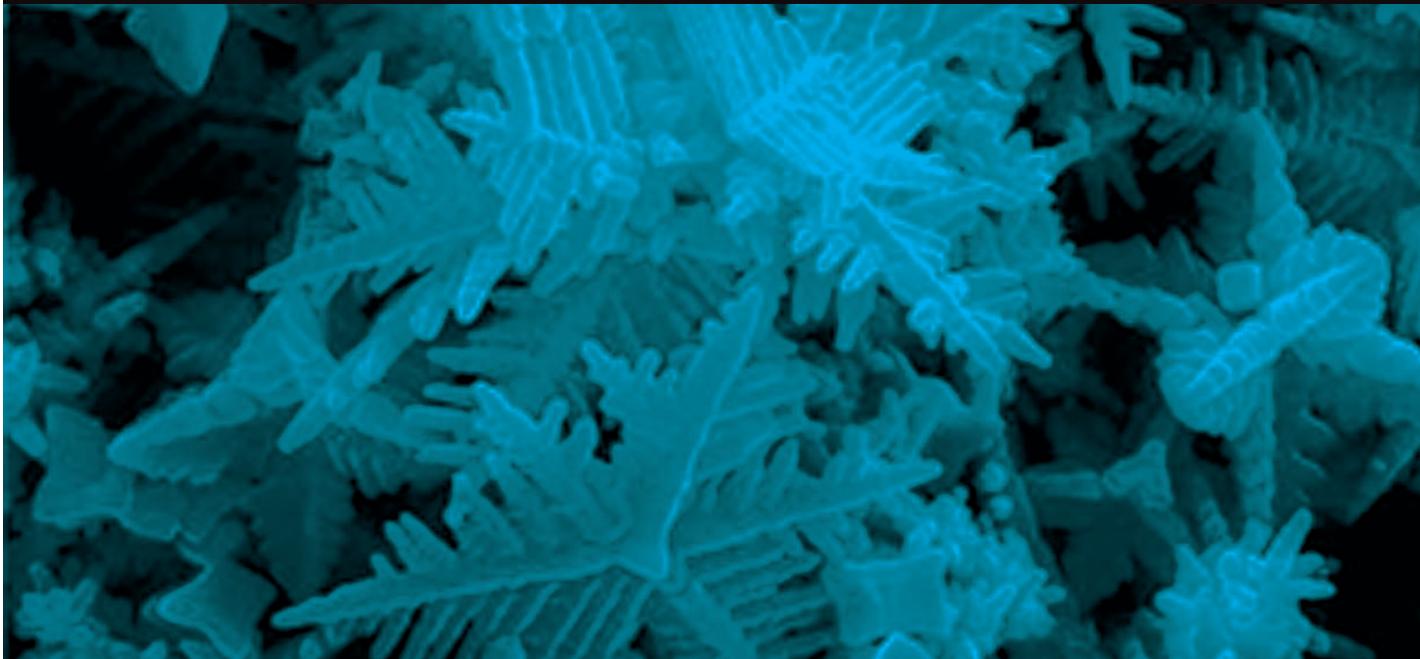


Image courtesy of Professor Gang Chen and Dr Rencheng Jin DOI: 10.1039/C2CE06417K

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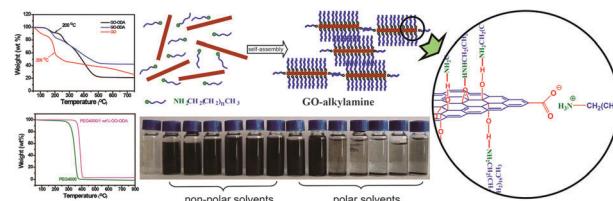
PAPERS

1733

Supramolecular graphene oxide-alkylamine hybrid materials: variation of dispersibility and improvement of thermal stability

Shu-Peng Zhang* and Hai-Ou Song

A simple and effective self-assembly method improving thermal stability and dispersibility of graphene oxide-based hybrid materials.

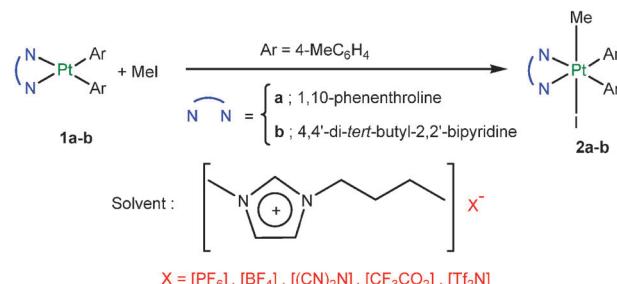


1739

Influence of anionic components of ionic liquid solvents on oxidative addition reactions of organoplatinum(II) complexes with MeI

S. Masoud Nabavizadeh,* Hajar Sepehrpour, Hamid R. Shahsavari and Mehdi Rashidi*

The effects of several imidazolium-based ionic liquids on the rate of the oxidative addition reactions of organoplatinum(II) complexes with MeI were investigated and showed a dependence on the nature of the anionic component of the ionic liquids.

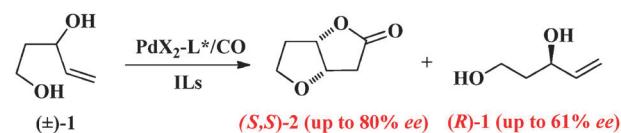


1744

Kinetic resolution of pent-4-ene-1,3-diol by Pd(II)-catalysed oxycarbonylation in ionic liquids

Jana Doháňová, Angelika Lásiková, Martial Toffano, Tibor Gracza* and Giang Vo-Thanh*

The kinetic resolution of (\pm) -1 by Pd(II)-catalysed oxycarbonylation in ionic liquid under carbon monoxide atmosphere in the presence of chiral catalyst, *p*-benzoquinone and acetic acid was investigated, giving enantioenriched (S,S) -2 (80% ee) and (R,R) -2 (57% ee).

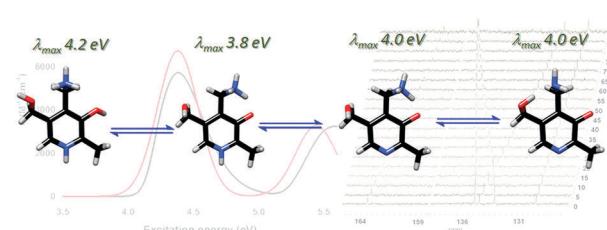


1751

Towards a detailed description of pyridoxamine tautomeric species

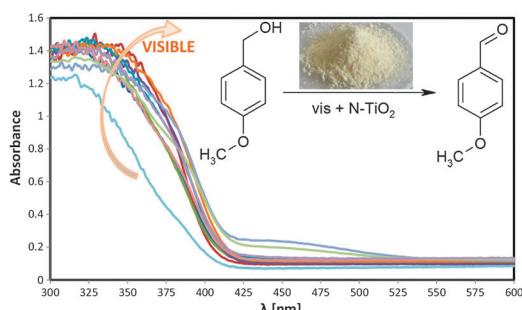
Miquel Adrover, Catalina Caldés, Bartolomé Vilanova, Juan Frau, Josefa Donoso and Francisco Muñoz*

Physico-chemical properties of minor tautomers in complex ionic and tautomer mixtures can be derived from a combined use of theoretical and experimental methodologies: the case of pyridoxamine.



PAPERS

1762

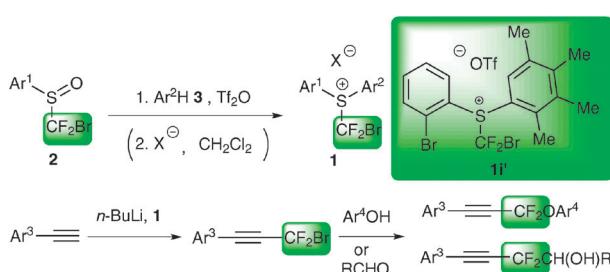


Enhancing selectivity in photocatalytic formation of *p*-anisaldehyde in aqueous suspension under solar light irradiation *via* TiO₂ N-doping

Sedat Yurdakal,* Vincenzo Augugliaro, Vittorio Loddo, Giovanni Palmisano and Leonardo Palmisano*

The enhancement of selectivity in photocatalytic formation of *p*-anisaldehyde in aqueous suspension under solar light irradiation *via* TiO₂ N-doping is presented by analysing a number of doped and undoped home-prepared catalysts and the influence of light irradiation energy.

1769

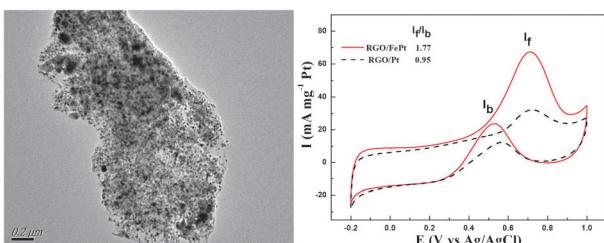


Efficient synthesis of unsymmetrical *S*-(bromodifluoromethyl) diarylsulfonium salts for electrophilic bromodifluoromethylating reagents

Guokai Liu, Satoru Mori, Xin Wang, Shun Noritake, Etsuko Tokunaga and Norio Shibata*

A series of unsymmetrical *S*-(bromodifluoromethyl)- diarylsulfonium salts were readily synthesized for bromodifluoromethylation of alkynes.

1774

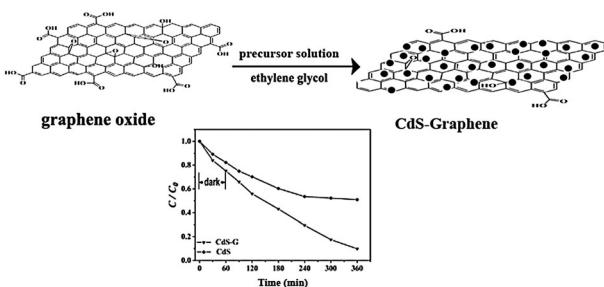


Reduced graphene oxide supported FePt alloy nanoparticles with high electrocatalytic performance for methanol oxidation

Zhenyuan Ji, Guoxing Zhu, Xiaoping Shen,* Hu Zhou, Chaomin Wu and Min Wang

A reduced graphene oxide supported FePt alloy electrocatalyst was prepared by a facile *in situ* co-reduction route, which exhibit enhanced catalytic performance for methanol oxidation.

1781



CdS-Graphene nanocomposite: synthesis, adsorption kinetics and high photocatalytic performance under visible light irradiation

Shugang Pan and Xiaoheng Liu*

CdS-Graphene nanocomposite was prepared using graphene oxide as the raw material and showed high catalytic effects under visible light irradiation.

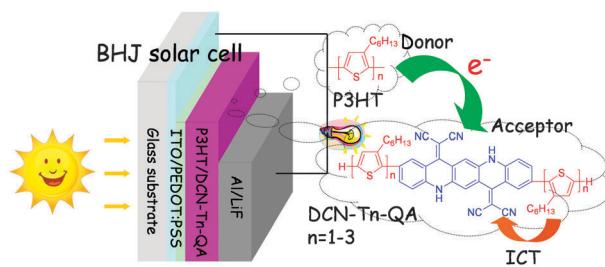
PAPERS

1788

Oligo(3-hexylthiophene)-functionalized dicyano-ethylene substituted quinacridone derivatives: synthesis, characterizations and applications as acceptors in photovoltaic devices

Chenguang Wang, Weiping Chen, Shanyong Chen, Shanshan Zhao, Jingying Zhang,* Dengli Qiu and Yue Wang*

A series of new organic acceptors were synthesized and employed as acceptors to fabricate organic solar cells (OSCs).

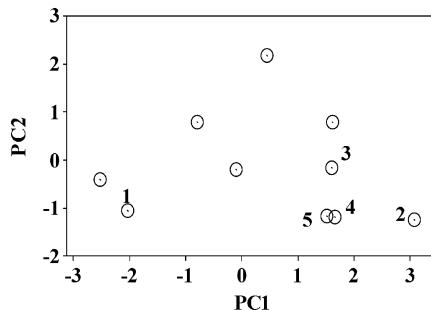


1798

Linear free-energy relationships for water/hexadec-1-ene and water/deca-1,9-diene partitions, and for permeation through lipid bilayers; comparison of permeation systems

Michael H. Abraham*

Analysis of equation coefficients shows that membranes have very different permeation properties (key to graphic: 1 egg lecithin, 2 intestinal absorption, 3 skin, 4 brain perfusion, 5 cerasome).

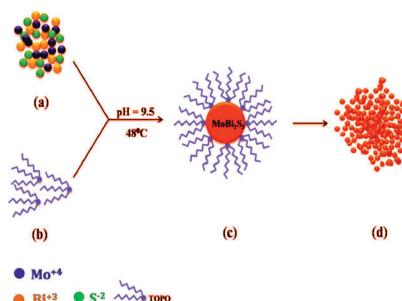


1807

Effect of surfactant on optical and structural properties of chemically deposited MoBi_2S_5 thin films

Nita B. Pawar, Sawanta S. Mali, Manauti M. Salunkhe, Rahul M. Mane, Pramod S. Patil and Popatrao N. Bhosale*

TOPO mediated nanocrystalline MoBi_2S_5 mixed metal chalcogenide thin films for solar cell applications.

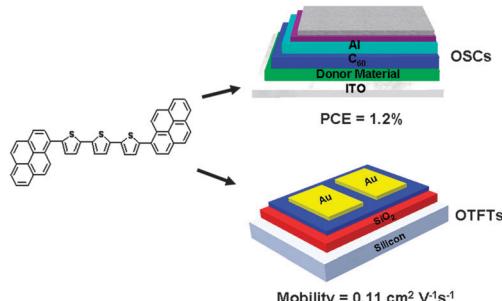


1813

Pyrene end-capped oligothiophene derivatives for organic thin-film transistors and organic solar cells

Jongchul Kwon, Jung-Pyo Hong, Seunguk Noh, Tae-Min Kim, Jang-Joo Kim,* Changhee Lee,* Seonghoon Lee* and Jong-In Hong*

The 5,5''-di(pyren-1-yl)-2,2':5',2''-terthiophene-based OTFT and OSC devices exhibited a field effect mobility of $0.11 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and a power conversion efficiency of 1.2%, respectively.



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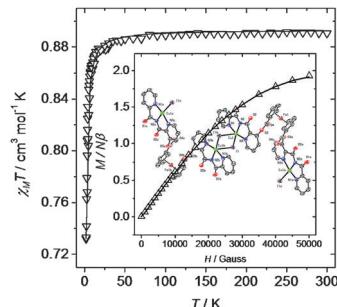
PAPERS

1819

Electrochemical, spectroscopic, magnetic and structural studies of complexes bearing ferrocenyl ligands of *N*-(3-hydroxypicolinoyl)picolinamide

Gilles Gasser,* Cristina Mari, Michelle Burkart, Stephen J. Green,* Joan Ribas, Helen Stoeckli-Evans* and James H. R. Tucker*

The synthesis and in-depth characterisation including X-ray crystallography and electrochemistry of two new ligands, derivatives of ferrocene, and their metal complexes is described.

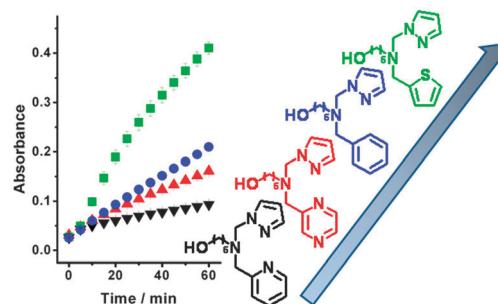


1828

Rate enhancement of the catechol oxidase activity of a series of biomimetic monocopper(II) complexes by introduction of non-coordinating groups in *N*-tripodal ligands

Ronan Marion, Nidal M. Saleh, Nicolas Le Poul, Didier Floner, Olivier Lavastre and Florence Geneste*

Catecholase activity of copper complexes with asymmetrical tripodal *N*-ligands is enhanced by decreasing the basicity and the steric hindrance of the heterocyclic donor. Bidentate derivatives exhibit even higher performances.

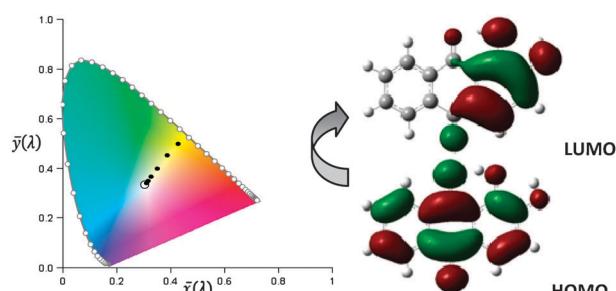


1836

Color prediction from first principle quantum chemistry computations: a case of alizarin dissolved in methanol

Piotr Cysewski,* Tomasz Jeliński, Maciej Przybyłek and Aleksander Shyichuk

Accurate color prediction of alizarin from first principle TD-DFT computations.

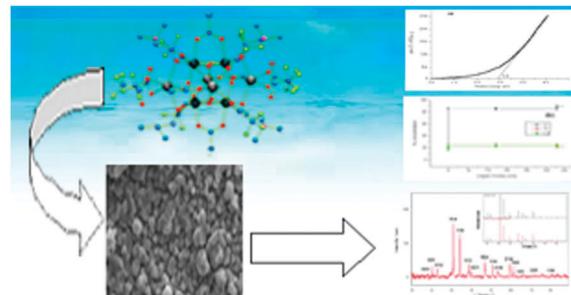


1844

CdTiO₃ thin films from an octa-nuclear bimetallic single source precursor by aerosol assisted chemical vapor deposition (AACVD)

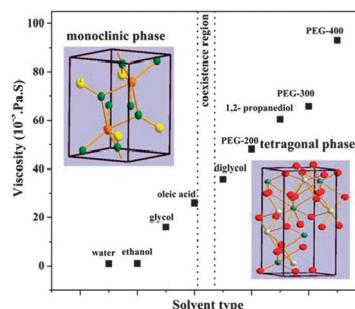
Shahzad Abu Bakar, Syed Tajammul Hussain and Muhammad Mazhar*

Mesoporous, crack free and crystalline CdTiO₃ thin films have been deposited from bimetallic molecular complex [Cd₄Ti₄(dmae)₄(TFA)₈(OAc)₄O₆] **1** by using AACVD.



PAPERS

1852

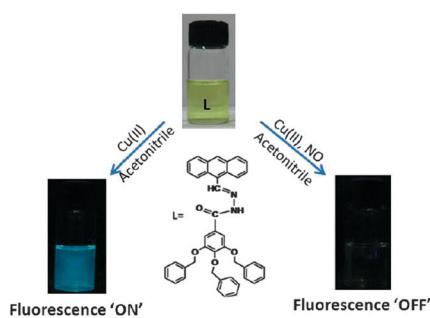


Solvent-driven polymorphic control of CdWO₄ nanocrystals for photocatalytic performances

**Yunjian Wang, Xiangfeng Guan,* Liping Li, Huan Lin,
Xuxu Wang and Guangshe Li***

The polymorph control of CdWO₄ nanocrystals was achieved by a solvent-driven approach and these nanocrystals showed improved photo-catalytic performances.

1859

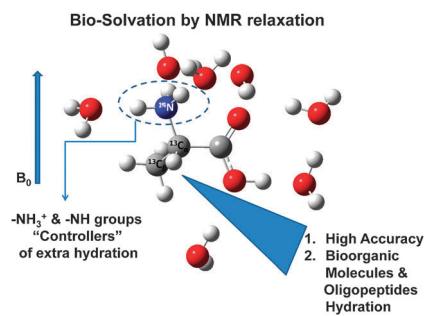


Detection of Cu(II) and NO by ‘on–off’ aggregation in poly(aryl ether) dendron derivatives

Chanchal Agarwal and Edamana Prasad*

Poly(aryl ether) dendrons with anthracene units attached through an acylhydrazone moiety were synthesized and fluorescence response from the system was recorded in presence of Cu(II) and NO at ambient conditions. The results suggest that specific binding with copper(II) at micromolar concentration leads to a ‘fluorescent on’ signal, followed by a ‘fluorescent off’ signal in the presence of nanomolar concentration of NO.

1866

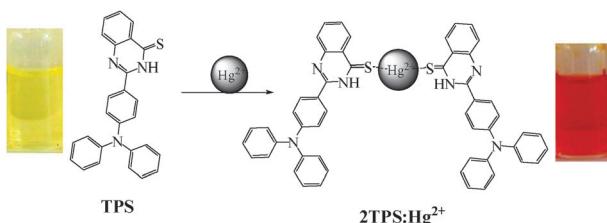


A “hidden” role of amino and imino groups is unveiled during the micro-solvation study of three biomolecule groups in water

Panteleimon G. Takis, Vasilios S. Melissas* and
Anastassios N. Troganis*

A novel NMR spectroscopic approach with DFT calculations unravels the hydration grade of amino acids, acetyl-amino acids and betaines in protonated and neutral pH forms, while revealing the “controlling” role of the N-terminus and the – NH group near the C-terminus in peptide solvation.

1879



A highly selective and naked-eye sensor for Hg^{2+} based on quinazoline-4(3H)-thione

Qunbo Mei,* Lingxia Wang, Bo Tian, Fang Yan,
Bin Zhang, Wei Huang and Bihai Tong*

A highly selective colorimetric and fluorescent sensor TPS was designed and showed a satisfactory selectivity, sensitivity and reversibility for Hg^{2+} . It can be used for “naked-eye” detection of Hg^{2+} .

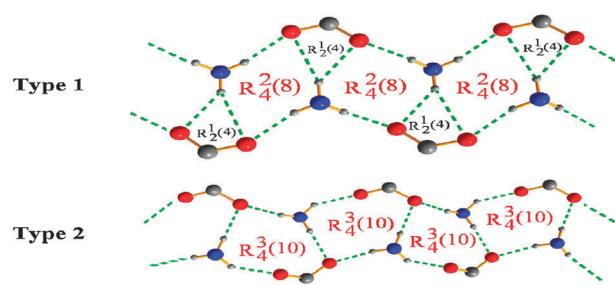
PAPERS

1884

Proton-transfer supramolecular salts resulting from 3,5-dinitrobenzoic acid and aminomethyl pyridine

Xue-Hua Ding, Lin-Fang Cui, Yong-Hua Li,* Shi Wang and Wei Huang*

Different hydrogen-bonding patterns of two heterosynthons are observed in ammonium carboxylate salts.

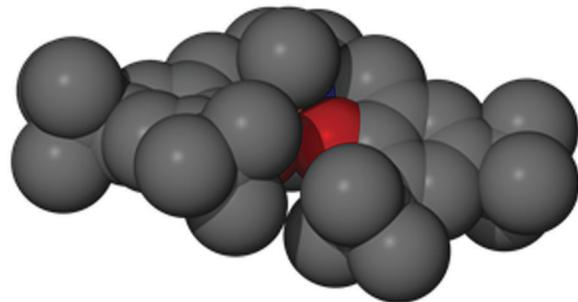


1891

Al(III)-homopiperazine complexes and their exploitation for the production of polyesters

Stuart L. Hancock, Matthew D. Jones,* Conrad J. Langridge and Mary F. Mahon

A series of Al(III)-homopiperazine complexes have been prepared for the production of polyesters.

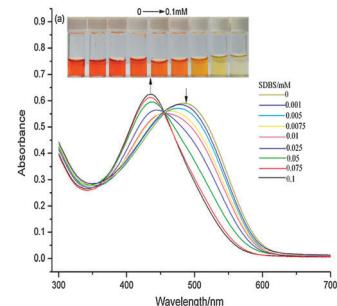


1897

A novel polythiophene derivative as a sensitive colorimetric and fluorescent sensor for anionic surfactants in water

Lin Wang, Qilong Feng, Xiangyong Wang, Meishan Pei and Guangyou Zhang*

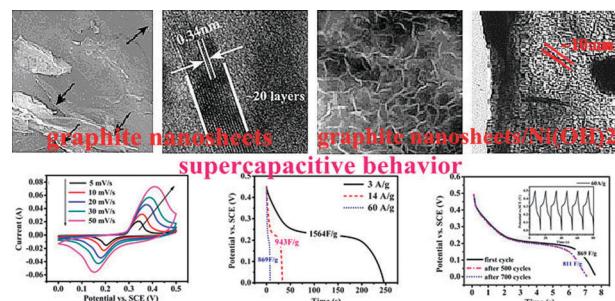
We have developed a sensitive colorimetric and fluorescent sensor for anionic surfactants in water based on a novel cationic polythiophene derivative, which has not been reported so far, especially, a new method for the polymerization of cationic polythiophene derivatives is found.



1902

Electrodeposited Ni(OH)₂ nanoflakes on graphite nanosheets prepared by plasma-enhanced chemical vapor deposition for supercapacitor electrode

Xin Wang, Yayu Wang, Cuimei Zhao, Yunxiao Zhao, Baoyu Yan and Weitao Zheng*

The Ni foam/graphite nanosheets/Ni(OH)₂ composite electrode prepared by plasma-enhanced chemical vapor deposition and electrochemical deposition with no binders and additives presents a high specific capacitance, high rate capability and excellent cycling stability.

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