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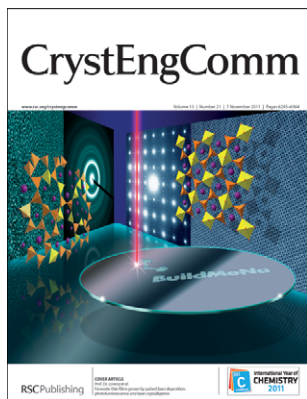
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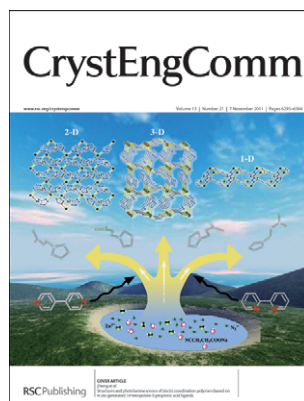
## IN THIS ISSUE

ISSN 1499-8033 CODEN CRECF4 13(21) 6295–6564 (2011)



### Cover

See Prof. Dr. Lorenz *et al.*, pp. 6377–6385.  
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### Inside cover

See Zheng *et al.*, pp. 6386–6392.  
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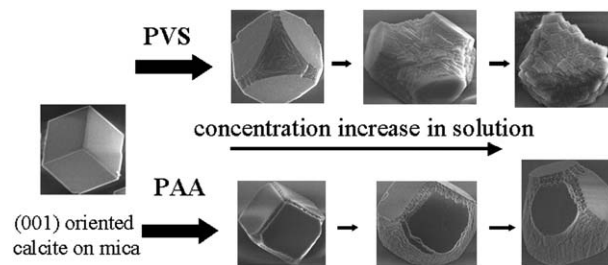
## COMMUNICATIONS

6311

### Additive-dependent morphogenesis of oriented calcite crystals on mica

Xu-Rong Xu,\* Han-Hua Pan, Rui-Kang Tang and Kilwon Cho\*

We have demonstrated the highly controlled preparation of (001) oriented calcite crystals on (001) mica surface and show two kinds of morphogenesis of (001) oriented calcite on mica in the presence of poly(vinyl sulfonate) and poly(acrylic acid). The present experiment is a good model system for studying the effect of additives in biomineralization.

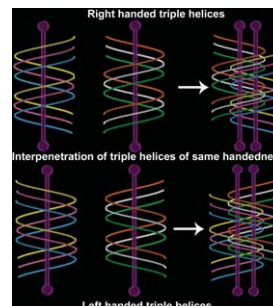


6315

### A hydrogen bonded cocrystal with an unusual interweaving between the adjacent triple-helices

Amit Delori and William Jones\*

Triple-helices of same handedness interpenetrated with each other.



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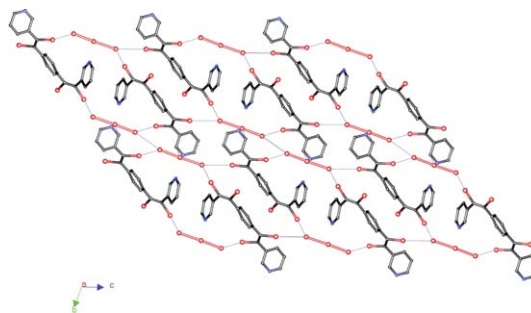
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6319

**CT-adduct vs. pyridinium polyhalide salt formation in the reactions between polypyridyl donors and dihalogens: reactivity of 1,4-di-(3'-pyridylethynyl)benzene towards Br<sub>2</sub> and I<sub>2</sub>**

M. C. Aragoni, M. Arca,\* S. J. Coles, F. A. Devillanova, M. B. Hursthouse, S. L. Coles (née Huth), F. Isaia, V. Lippolis and A. Mancini

The joint X-ray diffraction and FT-Raman investigations of the products obtained by reacting the title dipyrindyl donor with I<sub>2</sub>/Br<sub>2</sub> illustrate how the competition between the Lewis and Brønsted–Lowry basicity can be exploited for the design of supramolecular architectures.

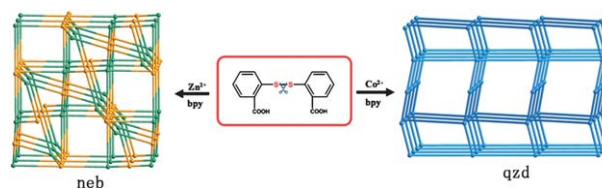


6323

**Topological variability of Zn(II) and Co(II) 3D coordination polymers obtained through solvothermal *in situ* disulfide cleavage**

Yang Bu, Feilong Jiang, Shuquan Zhang, Jie Ma, Xingjun Li and Maochun Hong\*

Two 3D coordination polymers with neb and qzd topology have been solvothermally prepared by *in situ* generation of a 2-sulfobenzoic acid ligand from a 2,2'-dithiobisbenzoic acid precursor through oxidative cleavage of its disulfide bond.

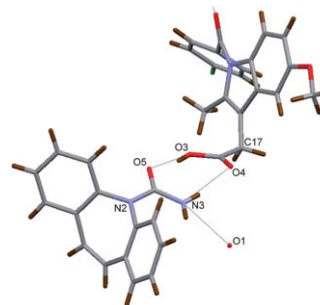


6327

**A carbamazepine-indomethacin (1 : 1) cocrystal produced by milling**

Mridul Majumder, Graham Buckton, Clare Rawlinson-Malone, Adrian C. Williams, Mark J. Spillman, Norman Shankland and Kenneth Shankland\*

An X-ray amorphous mixture of carbamazepine and indomethacin transforms upon annealing to produce a novel 1 : 1 cocrystal.

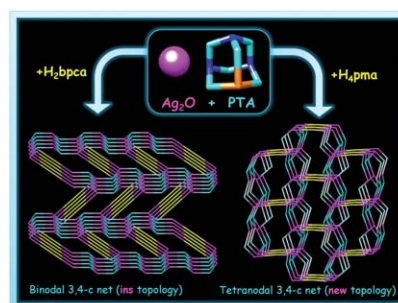


6329

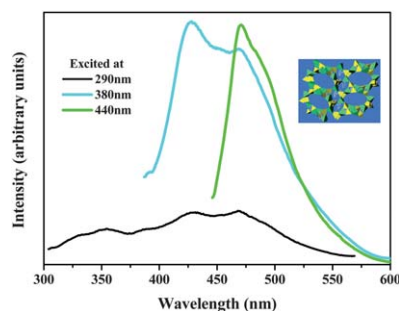
**Crystal engineering with 1,3,5-triaza-7-phosphaadamantane (PTA): first PTA-driven 3D metal–organic frameworks**

Alexander M. Kirillov,\* Sabina W. Wiczorek, M. Fátima C. Guedes da Silva, Jerzy Sokolnicki, Piotr Smoleński\* and Armando J. L. Pombeiro\*

Two new topologically distinct silver–organic frameworks have been prepared, thus opening up the use of PTA as a versatile *N,P*-building block in crystal engineering of 3D networks.



6334

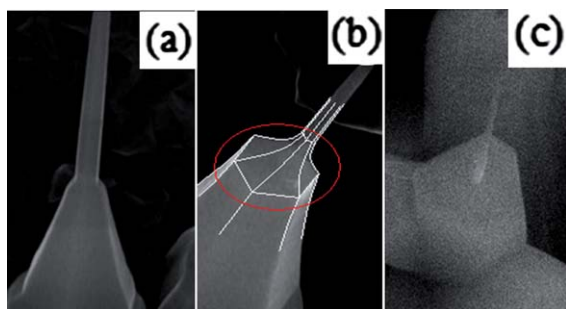


### New zinc diphosphonates with bright tunable luminescence and 12-member ring channels

Ruibiao Fu,\* Shengmin Hu and Xintao Wu\*

Ten new isomorphous 3D zinc diphosphonates with a 12MR ellipsoid-like channel and high thermal stability, display bright tunable luminescence.

6337

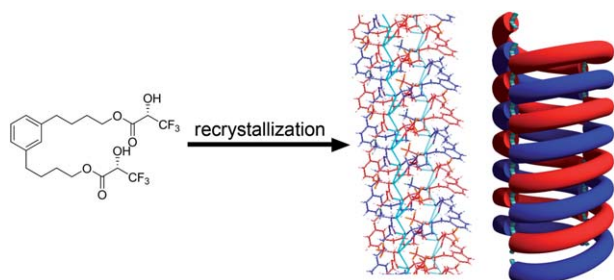


### Controllable growth of hierarchical AlN nanostructures based on dynamic equilibrium

Min Sun, Xinglong Wu,\* Chengyu He and Paul K. Chu

One-dimensional hierarchical AlN nanostructures comprising a thin nanowire on top of a nanocolumn were synthesized *via* a vapor–liquid–solid growth mechanism.

6342

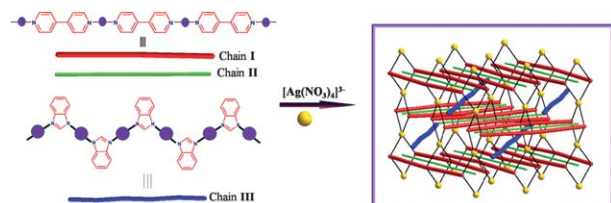


### A crystal engineering weaving of half-spiral molecules by hydrogen bonding chains into tube structures

Keisuke Kataoka, Masato Yanagi and Toshimasa Katagiri\*

We have woven molecules into a tube structure by hydrogen bonding chains of trifluorolactate, *via* a crystal engineering procedure.

6345



### An unprecedented supramolecular network with channels filled by 1D coordination polymer chains: Cocrystallization of Ag(I)-4,4'-bipyridine and Ag(I)-benzimidazole complexes

Song-Liang Cai, Sheng-Run Zheng,\* Jing-Bo Tan, Mei Pan, Jun Fan and Wei-Guang Zhang\*

A coordination polymer containing both  $[\text{Ag}(4,4'\text{-bipyridine})]_n$  and  $[\text{Ag}(\text{benzimidazole})]_n$  chains, which represents the first example of cocrystallization of two 1D chains was synthesized.



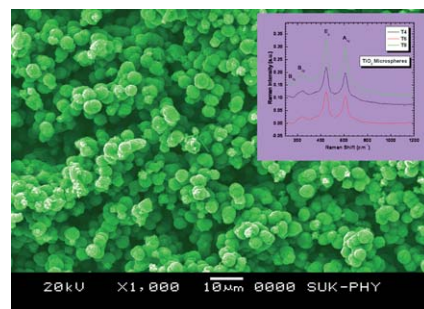
## COMMUNICATIONS

6349

**Hydrothermal synthesis of rutile TiO<sub>2</sub> with hierarchical microspheres and their characterization**

Sawanta S. Mali, Chirayath A. Betty, Popatrao N. Bhosale and Pramod S. Patil\*

In the present study, novel rutile TiO<sub>2</sub> films with primary microspheres and secondary nanospheres have been deposited on glass substrates *via* a simple hydrothermal process.

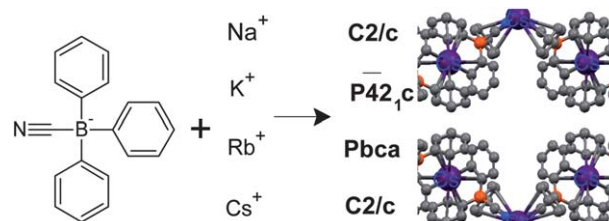


6352

**Crystal data behind efficient cesium recognition: triphenylcyanoborates of potassium, rubidium, and cesium**

Alexander Y. Nazarenko\* and Victor N. Nemykin

Alkali metal triphenylcyanoborates form different coordination polymer networks in solid state enabling selective separation of cesium ions.

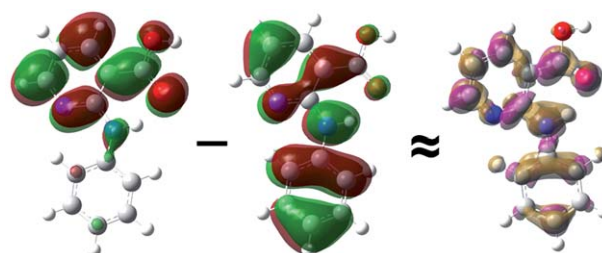


6356

**Electronic origin of pyridinyl N as a better hydrogen-bonding acceptor than carbonyl O**

Tonglei Li,\* Panpan Zhou and Alessandra Mattei

The local distribution of LUMO dominates the HOMO around carbonyl O, making it less willing to share its electrons to electron-deprived atoms. Pyridinyl N is however different.

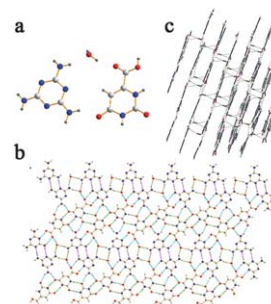


6361

**The influence of water on dielectric property in cocrystal compound of [orotic acid][melamine]·H<sub>2</sub>O**

Hao-Ran Xu, Qian-Chong Zhang, Yan-Ping Ren,\* Hai-Xia Zhao,\* La-Sheng Long, Rong-Bin Huang and Lan-Sun Zheng

An organic cocrystal compound consisting of melamine, orotic acid and water molecules was synthesized under hydrothermal conditions.



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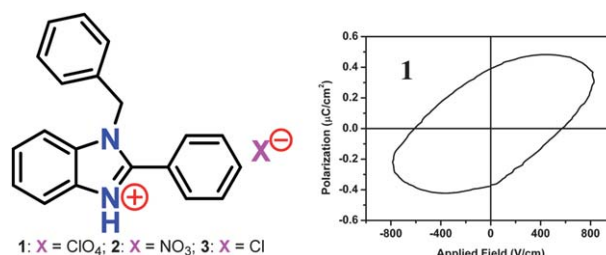
## COMMUNICATIONS

6365

**Nonlinear optical and ferroelectric materials based on 1-benzyl-2-phenyl-1*H*-benzimidazole salts**

Yong-Tao Wang,\* Gui-Mei Tang, Chao He, Shi-Chen Yan, Qi-Chao Hao, Long Chen, Xi-Fa Long,\* Tian-Duo Li and Seik Weng Ng\*

Three benzimidazole-based salts crystallize in the chiral *P*1 space group, which display second harmonic generation (SHG) responses and ferroelectric behaviors.

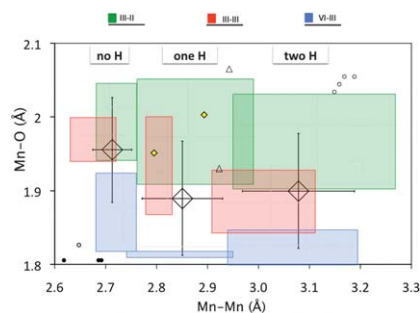


6369

**Can oxidation states and the protonation pattern of oxomanganese complexes be recognized from their structures?**

Arturo Robertazzi, Artur Galstyan and Ernst Walter Knapp\*

In this work, the authors propose a quantum-chemically based tool that can “recognize” the oxidation state and/or the protonation pattern of oxomanganese complexes from simple structural information.

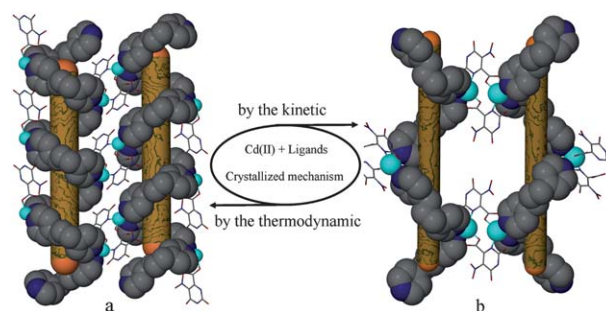


6373

**Self-assembly of metal–organic frameworks: From packing helical channels to 2-fold interpenetration helical layers**

Xing Li,\* Yue Bing, Mei-Qin Zha, Yun-Xiao Liang, Jian-Guo Pan and Dong-Jie Wang

Two kinds of metal–organic frameworks with different helical structures were successfully assembled by stratified solution diffusion or hydrothermal methods, in which TGA, XRD, crystallization mechanisms and quantitative calculations are discussed.



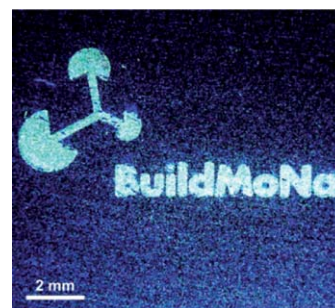
## PAPERS

6377

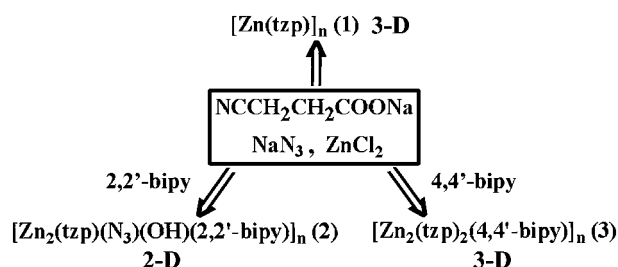
**Fresnoite thin films grown by pulsed laser deposition: photoluminescence and laser crystallization**

Alexander Müller, Michael Lorenz,\* Kerstin Brachwitz, Jörg Lenzner, Kai Mittwoch, Wolfgang Skorupa, Marius Grundmann and Thomas Höche

Luminescent logo of the Leipzig Graduate School of Natural Sciences BuildMoNa written by pulsed CO<sub>2</sub> laser in a 500 nm thin fresnoite Ba<sub>2</sub>TiSi<sub>2</sub>O<sub>8</sub> film.



6386

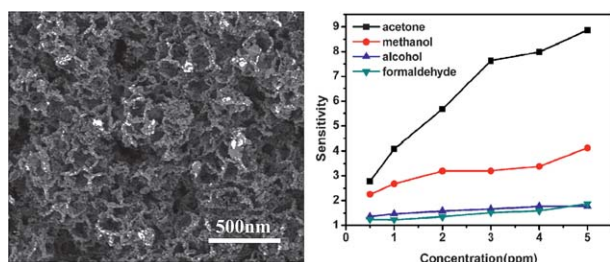


### Structures and photoluminescence of zinc(II) coordination polymers based on *in situ* generated 1*H*-tetrazolate-5-propionic acid ligands

Mei-Feng Wu, Zhi-Fa Liu, Shuai-Hua Wang, Jun Chen, Gang Xu, Fa-Kun Zheng,\* Guo-Cong Guo\* and Jin-Shun Huang

Three novel Zn(II) coordination polymers based on *in situ* generated 1*H*-tetrazolate-5-propionic acid were obtained in the absence/presence of co-ligands.

6393



### Porous WO<sub>3</sub> with enhanced photocatalytic and selective gas sensing properties

Zhong Xie, Yuguang Zhu, Jing Xu, Hongtao Huang, Di Chen\* and Guozhen Shen\*

Nanoparticle-assembled porous WO<sub>3</sub> products were synthesized at room temperature, showing excellent photocatalytic properties and high sensitivity to organic gases.

6399

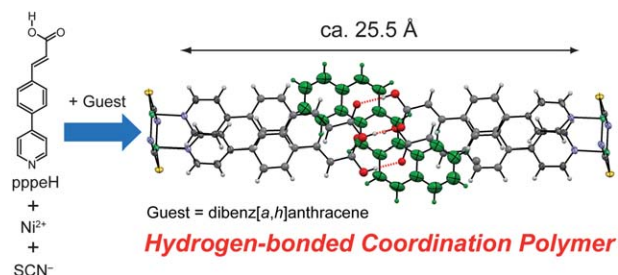


### Multiple phase-transitions upon selective CO<sub>2</sub> adsorption in an alkyl ether functionalized metal-organic framework—an *in situ* X-ray diffraction study

Sebastian Henke, D. C. Florian Wieland, Mikhail Meilikhov, Michael Paulus, Christian Sternemann, Kirill Yusenkov and Roland A. Fischer\*

An *in situ* X-ray diffraction study of an alkyl ether functionalized metal-organic framework reveals multiple phase transitions in this material upon carbon dioxide adsorption.

6405



### Synthesis, X-ray crystal structures and inclusion properties of a hydrogen-bonded coordination polymer [Ni(SCN)<sub>2</sub>(pppeH)<sub>2</sub>](guest)<sub>x</sub>

Ryo Sekiya\* and Shin-ichi Nishikiori\*

Self-assembly of Ni<sup>2+</sup>, SCN<sup>-</sup>, pppeH and a guest afforded new inclusion compounds in which pppeH dimers work as 25.5 Å long bridges.

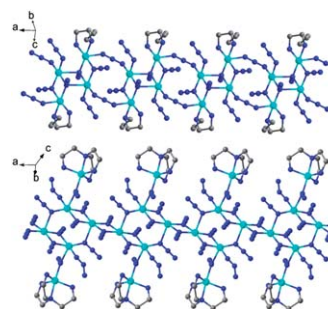


6415

### Novel copper-azido magnetic molecular tapes: syntheses, structures, and magnetic properties

Zhi-Guo Gu,\* Jing-Jing Na, Bao-Xiang Wang, Hong-Ping Xiao and Zaijun Li

Three one dimensional copper-azido molecular tapes with different chelating amine ligands have been synthesized and structurally characterized. In addition, magnetic properties of complexes **1–3** were investigated.

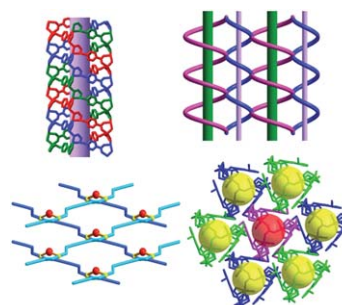


6422

### Syntheses, crystal structures and optical properties of six homochiral coordination networks based on phenyl acid-amino acids

Xiu-Li Yang, Ming-Hua Xie, Chao Zou and Chuan-De Wu\*

Six homochiral coordination networks based on two new phenyl acid-amino acids present interesting structural patterns, and metal coordination environments dependent second-order nonlinear optics (NLO) properties.



6431

### Syntheses, structures and photoluminescent properties of a series of Ag(I) coordination architectures based on 2,4-diamino-6-methyl-1,3,5-triazine and dicarboxylates: from a 0D discrete molecule to a 3D infinite network

Di Sun, Yun-Hua Li, Hong-Jun Hao, Fu-Jing Liu, Yang Zhao, Rong-Bin Huang\* and Lan-Sun Zheng

Five novel Ag(I) mixed ligand coordination complexes were synthesized and characterized. The diverse structures were found to be remarkably influenced by different dicarboxylates as well as the solvent systems.

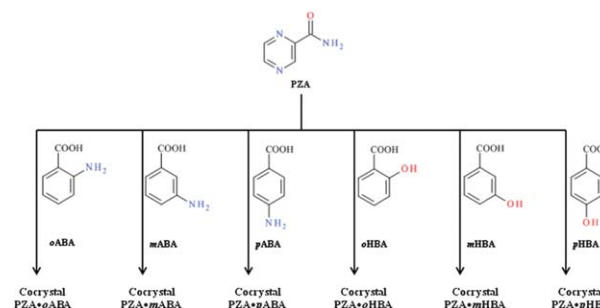


6442

### Pyrazinamide cocrystals and the search for polymorphs

Heba Abourahma,\* Devon S. Cocuzza, Jesus Melendez and Jennifer M. Urban

The synthesis and characterization of six related cocrystals of pyrazinamide that do not appear to exhibit polymorphism is reported.



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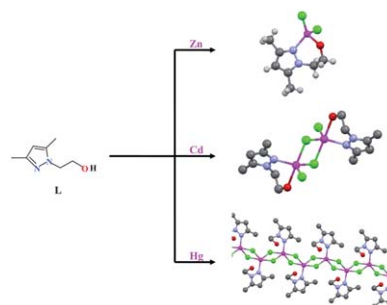
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## PAPERS

6451

**Molten salt growth and magnetic properties of octahedral  $\text{CoFe}_2\text{O}_4$  crystals: effects of synthesis conditions**Guangbin Ji,\* Xiaohui Lin, Yanyan Sun,  
Syed Ahmed Ali Trimizi, Hailin Su and Youwei DuWell defined octahedral  $\text{CoFe}_2\text{O}_4$  crystals were obtained in a series of molten salt systems.

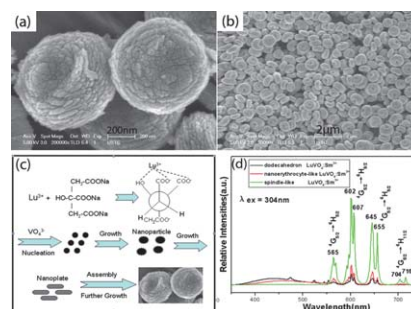
6457

**Variable behaviour of flexible *N,O*-mixed pyrazole ligand towards  $\text{Zn(II)}$ ,  $\text{Cd(II)}$  and  $\text{Hg(II)}$  ions. Synthesis, crystal structure and fluorescent properties**Miguel Guerrero, Josefina Pons,\* Josep Ros,  
Mercè Font-Bardia, Oriol Vallcorba, Jordi Rius,  
Vicenç Branchadell and Arben MerkoçiThree metal–organic frameworks based on a *N,O*-mixed pyrazole ligand have been synthesized and their photoluminescent properties are investigated.

6471

 **$\text{LuVO}_4\text{:Ln}^{3+}$  ( $\text{Ln} = \text{Sm, Eu, Dy, Er}$  and  $\text{Tm}$ ) with high uniform size and morphology: Controlled synthesis, growth mechanism and optical properties**

Youjin Zhang,\* Hongmei He, Wei Zhu and Ao Zheng

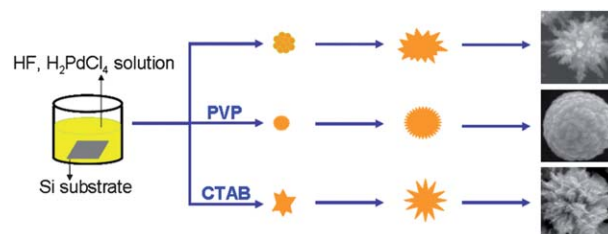
Nanoerythrocyte-like  $\text{LuVO}_4$  have been synthesized by an  $\text{Na}_3\text{Cit}$ -assisted hydrothermal method and the morphology-dependent optical properties of  $\text{LuVO}_4\text{:Ln}^{3+}$  were investigated.

6481

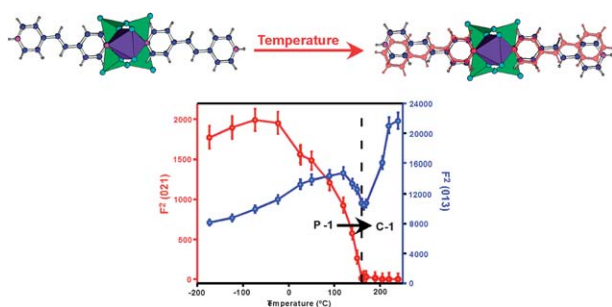
**Palladium crystals of various morphologies for SERS enhancement**

Li-Miao Chen\* and You-Nian Liu

Palladium nanostructures with urchin-like, hemispherical, flower-like, and plate-like morphologies were controllably deposited on silicon substrates at room temperature.



6488

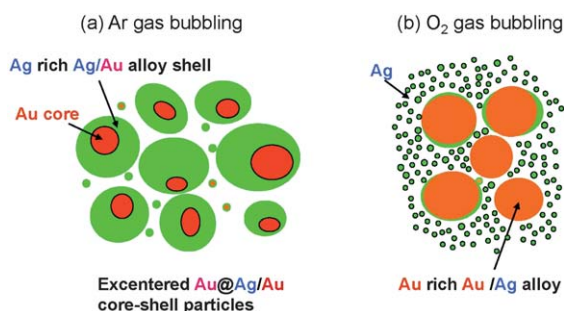


**{Co(HBpe)<sub>2</sub>}(V<sub>4</sub>O<sub>12</sub>): pedal motion induced order–disorder *P1* → *C1* transition and disrupted *C1* → *C2/m* displacive transition due to thermal instability**

Roberto Fernández de Luis, M. Karnele Urtiaga, José L. Mesa, Joseba Orive Gómez de Segura, Teófilo Rojo and María I. Arriortua\*

Order–disorder induced structural transition due to the pedal motion of the HBpe ligand in a one dimensional polymeric compound, {Co(HBpe)<sub>2</sub>}(V<sub>4</sub>O<sub>12</sub>).

6499

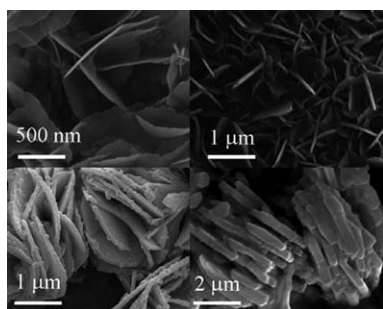


**Effects of gas bubbling for shape, size, and composition changes in Au–Ag bimetallic nanoparticles including polygonal Au seeds under oil-bath heating at 150 °C**

Md. Jahangir Alam and Masaharu Tsuji\*

Excentered Au core Ag-rich Ag/Au alloy shell or Au-rich Au/Ag alloy particles were prepared after heating AgNO<sub>3</sub>/PVP/ethylene glycol solution involving polygonal Au nanocrystals, under oil-bath heating under Ar or O<sub>2</sub> gas bubbling.

6507

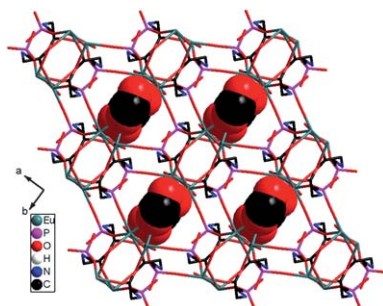


**Thickness tunable Cu<sub>2</sub>ZnSnSe<sub>4</sub> nanosheets**

Liang Shi\* and Quan Li

Quaternary Cu<sub>2</sub>ZnSnSe<sub>4</sub> single crystalline nanosheets have been synthesized in a controlled manner with a solvothermal approach by simply modifying the reaction conditions.

6511



**Two isomorphous 3-D lanthanide oxalatophosphonate frameworks based on glyphosate: syntheses, crystal structures, and luminescence properties**

Lijuan Zhang, Sheng Xu, Yunshan Zhou,\* Xiaorui Zheng, Chao Yu, Zonghai Shi, Sadaf ul Hassan and Chao Chen

3-D luminescent lanthanide oxalatophosphonate frameworks possessing 1-D channels accommodating oxalates and lattice water molecules as troglodytes were synthesized.



## PAPERS

6520

**Networking of macrocycles: 1D and 2D coordination polymers of dithia-18-crown-6 with copper(II) and copper(I)**

In-Hyeok Park and Shim Sung Lee\*

Cu<sup>I</sup> and Cu<sup>II</sup> coordination polymers of 1,10-dithia-18-crown-6 (L) with unusual networking modes involving an exocyclic coordination are presented.

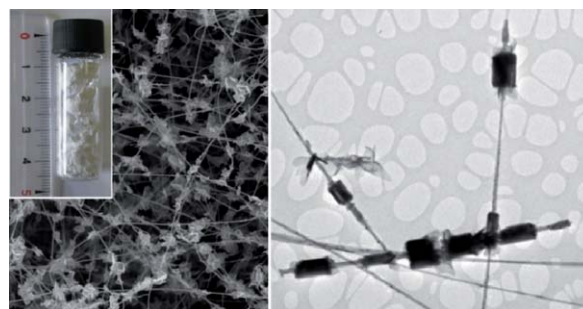


6526

**Boron nitride multiwall nanotubes decorated with BN nanosheets**

Mikhael Bechelany,\* Arnaud Brioude, Samuel Bernard, Pierre Stadelmann, David Cornu and Philippe Miele

We report a simple chemical-route for large scale synthesis of long multiwall boron nitride nanotubes decorated with BN nanosheets.

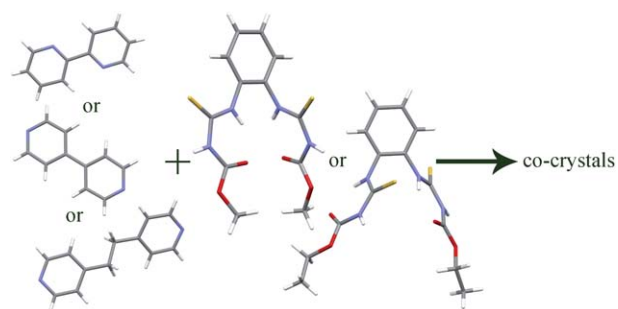


6531

**Packing incentives and a reliable N–H⋯N–pyridine synthon in co-crystallization of bipyridines with two agrochemical actives**

Elisa Nauha, Erkki Kolehmainen and Maija Nissinen\*

A reliable NH⋯N synthon is observed in co-crystals of two agrochemical actives with bipyridine derivatives.

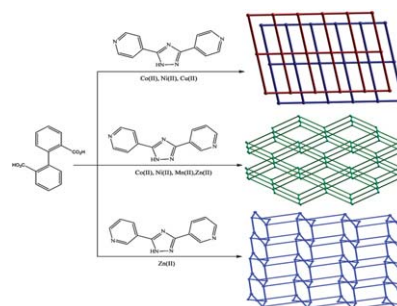


6538

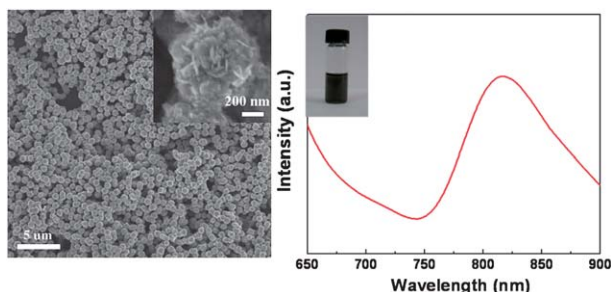
**Coordination assemblies of Co<sup>II</sup>/Ni<sup>II</sup>/Mn<sup>II</sup>/Zn<sup>II</sup> with 1,1'-biphenyl-2,2'-dicarboxylic acid and three positional isomeric ligands: structural diversity and properties**

Fu-Ping Huang, He-Dong Bian,\* Qing Yu, Jin-Lei Tian, Hong Liang, Shi-Ping Yan,\* Dai-Zheng Liao and Peng Cheng

We present here 8 coordination polymers generated from bpdcc and positional isomeric bpt ligands. This work indicates that the isomeric effects of the bpt connectors. Moreover, the magnetic and luminescent properties of these corresponding complexes have been investigated.



6549

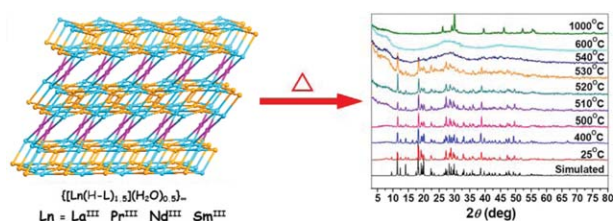


### One-pot self-assembly of flower-like Cu<sub>2</sub>S structures with near-infrared photoluminescent properties

Na Li, Xiaoling Zhang,\* Shutang Chen, Wen Yang,\* Huaizhi Kang and Weihong Tan\*

In the present study, a simple one-pot route by using a green, phosphine-free oleic acid as the single capping solvent has been employed to obtain flower-like Cu<sub>2</sub>S nanoparticles with near-infrared (NIR) photoluminescence (PL) emission.

6555



### Highly-thermostable lanthanide–organic coordination frameworks with *N*-protonated 2,6-dihydroxypyridine-4-carboxylate exhibiting unusual 3-D mixed-connected network topology

Shao-Ming Fang, Min Hu, Li-Ran Jia, Cong Wang, Qiang Zhang, Song-Tao Ma, Miao Du\* and Chun-Sen Liu\*

Four isostructural 3-D lanthanide–organic frameworks with *N*-protonated 2,6-dihydroxypyridine-4-carboxylate have been presented, which show the exceptionally high thermal stability (up to 530°C) and unusual (4,5,7)-connected network topology.

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