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A journal at the forefront of the design and understanding of solid-state and crystalline materials
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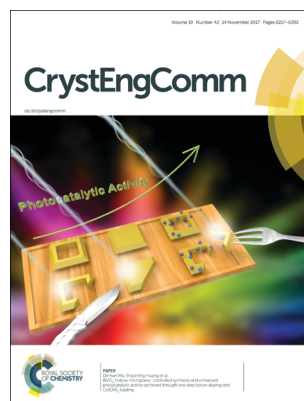
IN THIS ISSUE

ISSN 1466-8033 CODEN CRECF4 19(42) 6217-6392 (2017)



Cover

See Lauren E. Hatcher and Paul R. Raithby, pp. 6297-6304. Image reproduced by permission of Lauren E. Hatcher from *CrystEngComm*, 2017, 19, 6297.



Inside cover

See De-Kun Ma, Shaoming Huang *et al.*, pp. 6305-6313. Image reproduced by permission of De-Kun Ma from *CrystEngComm*, 2017, 19, 6305.

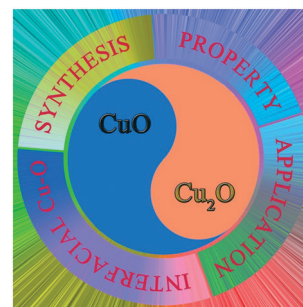
HIGHLIGHT

6225

Hollow Cu_xO ($x = 2, 1$) micro/nanostructures: synthesis, fundamental properties and applications

Shaodong Sun,* Qing Yang, Shuhua Liang* and Zhimao Yang*

In this review, we comprehensively summarize the important advances in hollow Cu_xO micro/nanostructures, including the universal synthesis strategies, the interfacial Cu-O atomic structures as well as the intrinsic properties, and potential applications. Remarks on emerging issues and promising research directions are also discussed.



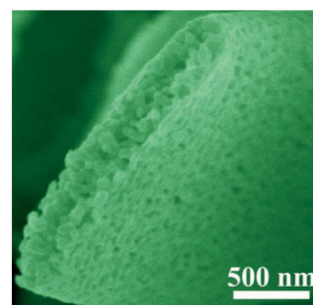
COMMUNICATIONS

6252

Electrospun BiVO_4 nanobelts with tailored structures and their enhanced photocatalytic/ photoelectrocatalytic activities

Huabing Liu, Weiyu Yang, Lin Wang, Huilin Hou* and Fengmei Gao*

We reported the fabrication of BiVO_4 nanobelts with tailored structures by a versatile electrospinning method.



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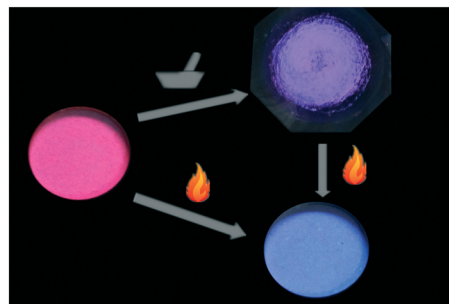
COMMUNICATIONS

6259

Reversible mechanochromic and thermochromic luminescence switching via hydrogen-bond-directed assemblies in a zinc coordination complex

Rui Zou, Jie Zhang,* Shuzhi Hu, Fei Hu, Haoyu Zhang and Zhiyong Fu*

A zinc coordination complex with terpyridyl derivative as ligand exhibits mechanochromic and thermochromic luminescence behaviors with reversible color changes visible to the naked eye from pink to blue-purple upon mechanical grinding and from blue-purple to pink upon heating.

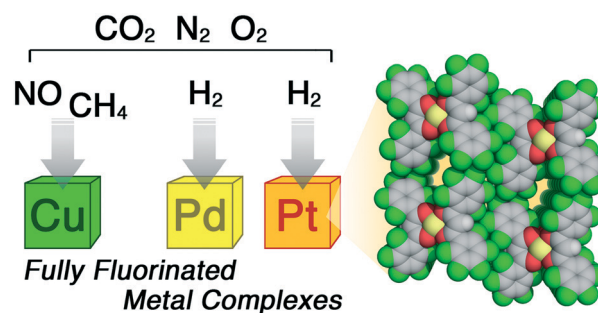


6263

Enhanced adsorption of small gas molecules in metal (Cu^{2+} , Pd^{2+} , Pt^{2+}) complexes induced by ligand fluorination

Akiko Hori,* Ryu Gonda and Izabela I. Rzeznicka

Fully fluorinated coordination complexes show two types of guest recognition events: 1:1 selective recognition of CO_2 and metal ion-selective adsorption of N_2 , O_2 , H_2 , NO , and CH_4 .



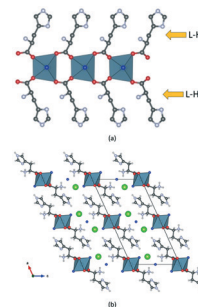
PAPERS

6267

Ionic co-crystals of enantiopure and racemic histidine with calcium halides

O. Shemchuk, L. Degli Esposti, F. Grepioni and D. Braga*

Ionic co-crystals (ICCs) of L- and DL-histidine with CaCl_2 , CaBr_2 and CaI_2 were prepared by mechanochemical and solution methods and were structurally characterized by either single crystal or powder X-ray diffraction methods.

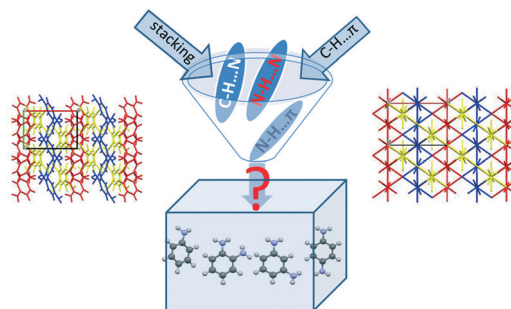


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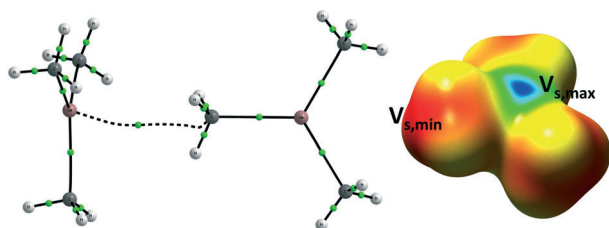
Acceptor properties of amino groups in aminobenzene crystals: study from the energetic viewpoint

Svitlana V. Shishkina,* Irina S. Konovalova, Oleg V. Shishkin and Alexander N. Boyko

The role of the $\text{N-H}\cdots\text{N}$ hydrogen bonds in the organization of the crystals of the aniline and diaminobenzenes has been studied.



6289

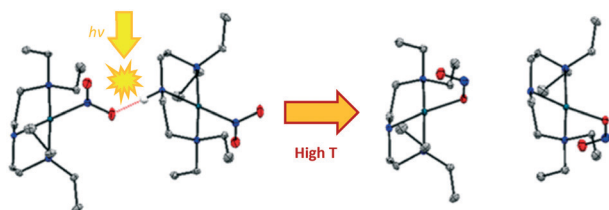
 π -hole bonding (5 kcal/mol)

Alkyl groups as electron density donors in π -hole bonding

Jorge Echeverría

A combined structural and computational analysis has demonstrated that alkyl groups can act as Lewis bases in π -hole bonding.

6297

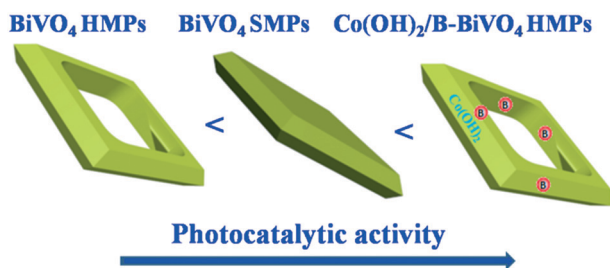


The impact of hydrogen bonding on 100% photo-switching in solid-state nitro-nitrito linkage isomers

Lauren E. Hatcher* and Paul R. Raithby

Temperature-regulated control of photo-induced linkage isomer switching engineered through intermolecular hydrogen bonding to the nitro-(η^1 -NO₂) group.

6305

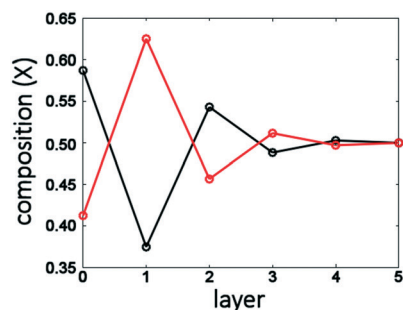


BiVO₄ hollow microplates: controlled synthesis and enhanced photocatalytic activity achieved through one-step boron doping and Co(OH)₂ loading

Abraham Adenle, De-Kun Ma,* De-Peng Qu, Wei Chen and Shaoming Huang*

BiVO₄ hollow microplates co-modified by boron doping and Co(OH)₂ nanoparticle loading achieved enhanced photocatalytic activity.

6314



A revised thermodynamic model for crystal surfaces. I. Theoretical aspects

Marco Bruno*

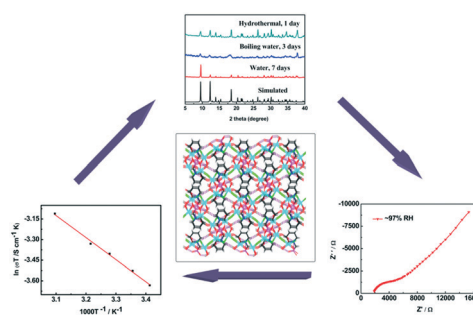
A revised thermodynamic model to study surface segregation.

6325

One, two, and three-dimensional metal–organic coordination polymers derived from enantiopure organic phosphorate: homochirality, water stability and proton conduction

Xiaoqiang Liang, Kun Cai, Feng Zhang, Jia Liu* and Guangshan Zhu

A multifunctional ligand reacts with metal ions to generate three new coordination polymers, where **3** has a high water stability, a moderate proton conductivity and a lower activation energy.

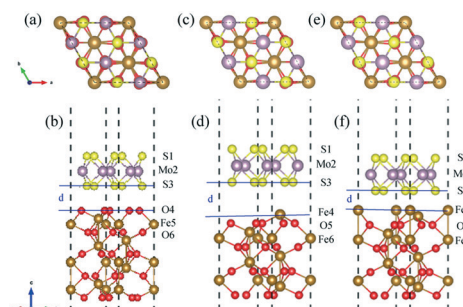


6333

Electronic and optical properties of MoS₂/α-Fe₂O₃(0001) heterostructures: a first-principles investigation

Haijun Pan,* Xiangying Meng, Xiwei Qi and Gaowu Qin

This study investigates the effect of interfacial structure of MoS₂/α-Fe₂O₃(0001) heterostructure on its photocatalytic activity.

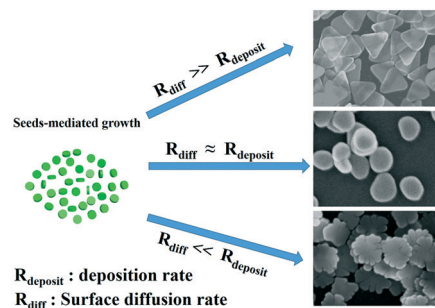


6339

Branched Ag nanoplates: synthesis dictated by suppressing surface diffusion and catalytic activity for nitrophenol reduction

Taixing Tan, Shun Zhang and Cheng Wang*

Highly branched Ag nanoplates were achieved at extremely low Ag atoms surface diffusion rate, fulfilled *via* the Cu under potential deposition.

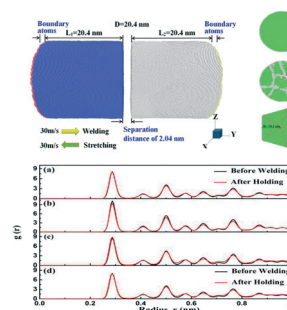


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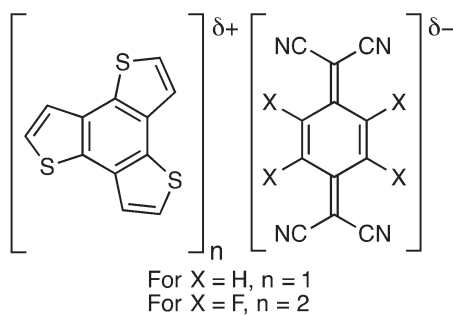
Formation of gold composite nanowires using cold welding: a structure-based molecular dynamics simulation

Hongjian Zhou, Yuehui Xian, Runni Wu, Guoming Hu and Re Xia*

Cold welding between nanowires with various grain structures is researched using molecular dynamics simulation.



6355



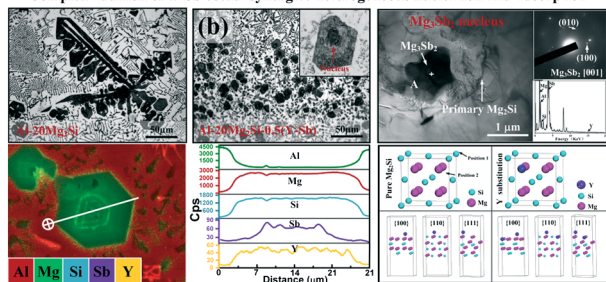
Structure and characterization of charge transfer complexes of benzo[1,2-*b*:3,4-*b'*:5,6-*b''*]trithiophene [C_{3h} -BTT]

Qian Qin,* Joel T. Mague, Khadija Z. Moses, Elizabeth M. Carnicom and Robert J. Cava

Four charge-transfer complexes of C_{3h} -BTT (**2**) with the organic acceptors TCNQ, F_4 TCNQ, chloranil, and fluoranil were prepared and crystallographically characterized.

6365

Complex addition of Y-Sb could synergize heterogeneous nucleation and adsorption

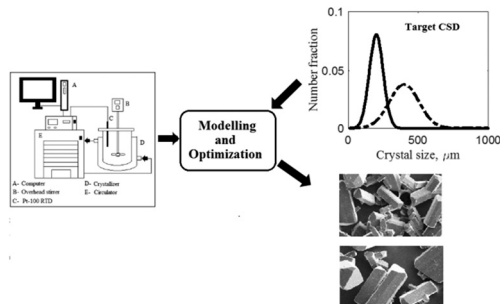


Refinement and modification of primary Mg_2Si in an Al-20 Mg_2Si alloy by a combined addition of yttrium and antimony

Hui-Yuan Wang, Jia-Ning Zhu, Jie-Hua Li, Chao Li, Min Zha,* Cheng Wang, Zhi-Zheng Yang and Qi-Chuan Jiang

The complex modification of primary Mg_2Si in an Al-20 Mg_2Si alloy by simultaneous addition of yttrium (Y) and antimony (Sb) was investigated in the present work.

6373

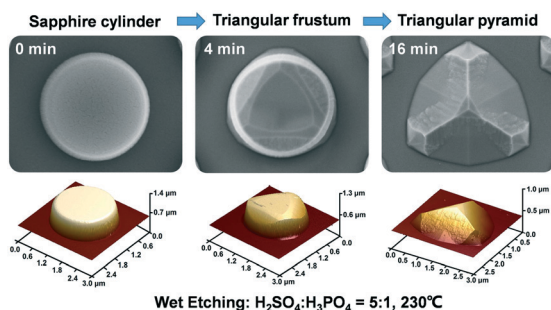


Particle engineering by optimization for the unseeded batch cooling crystallization of L-asparagine monohydrate

Stutee Bhoi, Maheswata Lenka and Debasis Sarkar*

A model-based optimization approach is proposed to obtain temperature profiles to achieve the target CSD in a batch cooling crystallization process.

6383



Crystallographic and topographical evolutions of a cylinder patterned sapphire substrate etched with a sulfuric acid and phosphoric acid mixture: an SEM and AFM study

Jian Shen, Dan Zhang, You Wang and Yang Gan*

Using cylinders as a model system, the full spectrum of crystallographic and topographical evolutions of patterned sapphire substrates is exhibited.