

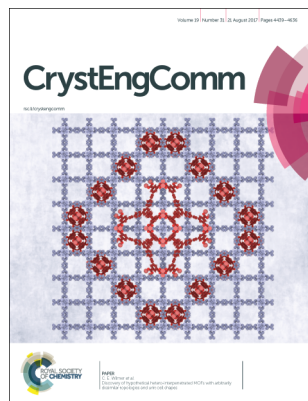
# CrystEngComm

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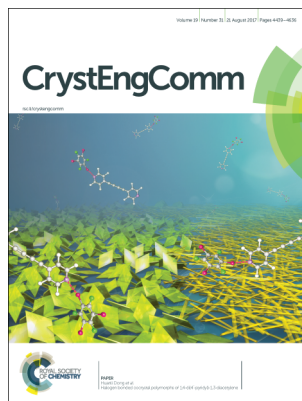
## IN THIS ISSUE

ISSN 1466-8033 CODEN CRECF4 19(31) 4439-4636 (2017)



### Cover

See C. E. Wilmer *et al.*, pp. 4497-4504.  
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### Inside cover

See Huanli Dong *et al.*, pp. 4505-4509.  
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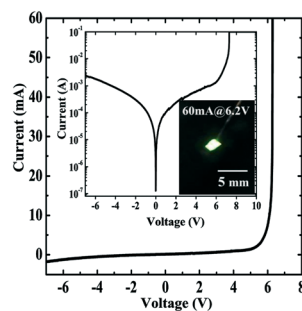
## HIGHLIGHTS

4448

### Efficient pure green emission from Er-doped Ga<sub>2</sub>O<sub>3</sub> films

Zhengwei Chen, Katsuhiko Saito, Tooru Tanaka and Qixin Guo\*

This review describes recent advances in the properties of Er-doped Ga<sub>2</sub>O<sub>3</sub> films and light-emitting devices based on these films.

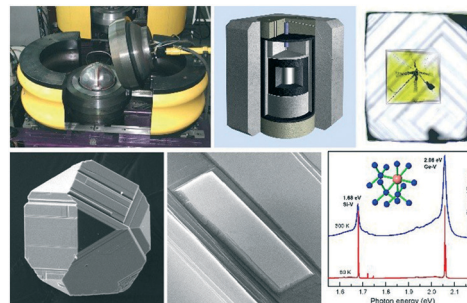


4459

### High-pressure crystallization and properties of diamond from magnesium-based catalysts

Yuri N. Palyanov,\* Igor N. Kupriyanov, Alexander F. Khokhryakov and Yuri M. Borzdov

HPHT diamond synthesis using catalysts based on magnesium demonstrates a number of intriguing characteristics. In this highlight, we review the major characteristics of the growth, morphology, internal structure, and defect and impurity content of diamonds crystallized using Mg-based catalysts.



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# CrystEngComm

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

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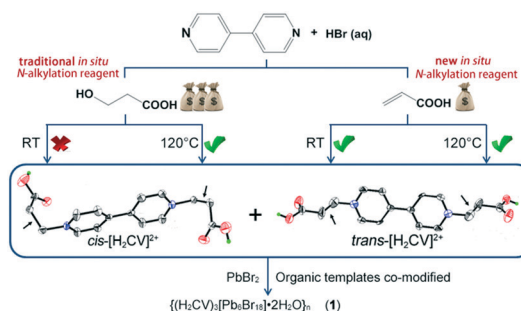


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### Viologen-templated bromoplumbate: a new *in situ* synthetic method and energy gap engineering

Cai Sun, Ming-Sheng Wang,\* Xian Zhang, Ning-Ning Zhang, Lin-Rong Cai and Guo-Cong Guo\*

A new *in situ* synthesis strategy for viologen-based compounds was developed, which is much milder than the traditional solvothermal method.

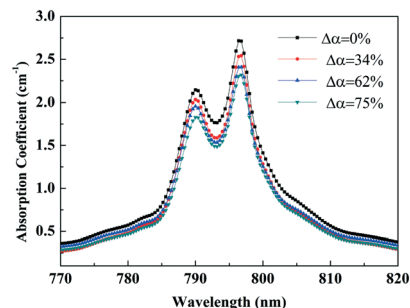


4480

### Re-clustering of neodymium ions in neodymium, buffer ion-codoped alkaline-earth fluoride transparent ceramics

Yiguang Jiang, Benxue Jiang,\* Nan Jiang, Pande Zhang, Shuilin Chen, Jintai Fan, Liangbi Su, Jiang Li and Long Zhang\*

We systematically present the relationship between the optical properties and deformation of Nd,B-codoped MF<sub>2</sub> (B = buffer ions; M = alkaline earth metal ions) transparent ceramics.

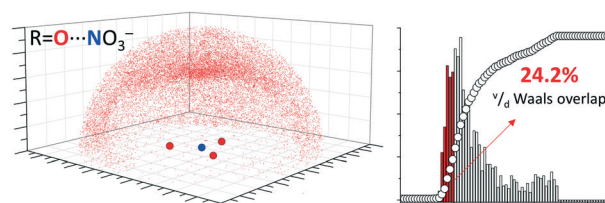


4485

### Coordinated nitrate anions can be directional $\pi$ -hole donors in the solid state: a CSD study

Tiddo J. Mooibroek\*

Within the CSD  $sp^2$  O-atoms cluster closer to the  $\pi$ -hole of  $NO_3^-$  when nitrate is coordinated to a metal.

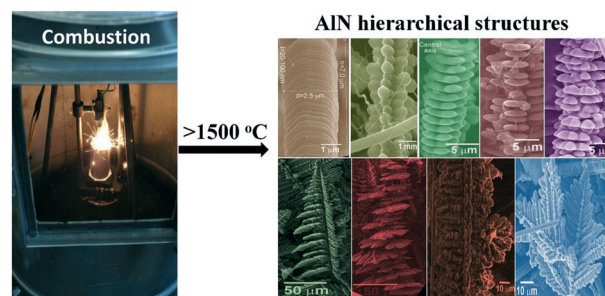


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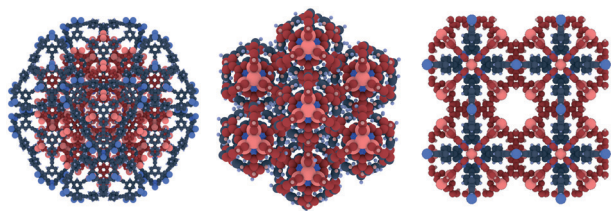
### Tailoring the morphology of AlN: from 6-fold patterned crystals to multilayer hierarchical structures

H. H. Nersisyan, S. H. Lee, J. H. Choi, B. U. Yoo, T.-H. Lee, H. Suh, J.-G. Kim and J. H. Lee\*

Combustion of inorganic powder mixtures is not only one of the chemical routes of fabrication of advanced inorganic materials but is also drawing attention as a high-temperature process to grow inorganic nanocrystals of various shapes and morphology.



4497

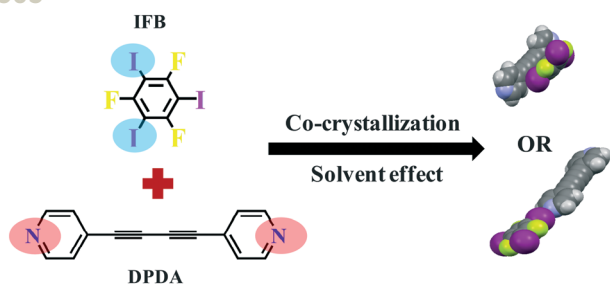


### Discovery of hypothetical hetero-interpenetrated MOFs with arbitrarily dissimilar topologies and unit cell shapes

K. B. Sezginel, T. Feng and C. E. Wilmer\*

Interpenetration is a commonly observed phenomenon in metal organic frameworks (MOFs) where multiple frameworks are entangled with each other. Using a novel algorithm described here, 18 hypothetical hetero-interpenetrated MOFs were discovered.

4505

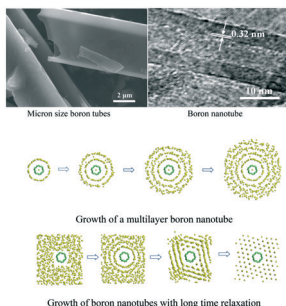


### Halogen bonded cocrystal polymorphs of 1,4-di(4'-pyridyl)-1,3-diacetylene

Pan Zhang, Geetha Bolla, Gege Qiu, Zhibin Shu, Qingqing Yan, Qingyuan Li, Shang Ding, Zhenjie Ni, Weigang Zhu, Huanli Dong,\* Yonggang Zhen and Wenping Hu

Two cocrystals based on IFB and DPDA are controllably prepared under solvent effects demonstrating different photo-physical properties.

4510

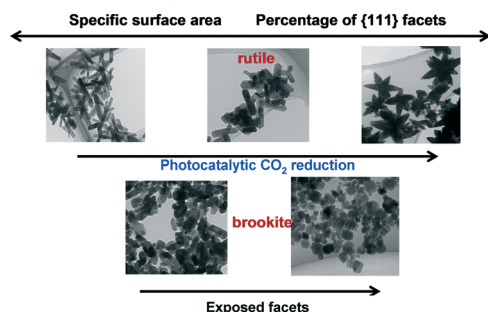


### Growth of single crystalline boron nanotubes in a Cu alloy

Yuying Wu, Yifan Li, Houwen Chen, Zuxin Sun, Na Wang, Jingyu Qin, Hui Li, Xiufang Bian and Xiangfa Liu\*

Herein, we report the successful synthesis of single crystalline boron nanotubes in a Cu alloy via a novel and simple direct melt reaction process.

4519



### Amino acid-assisted controlling the shapes of rutile, brookite for enhanced photocatalytic CO<sub>2</sub> reduction

Quang Duc Truong,\* Thi Hang Le and Huu Thu Hoa

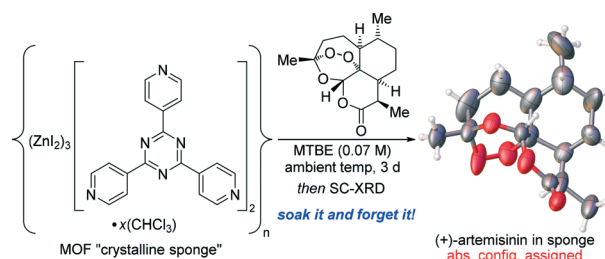
Rutile and brookite titania with tunable shape have been synthesized. The investigation results show that the photocatalytic CO<sub>2</sub> reduction activity of rutile increases with increasing percentage of {111} surface and brookite with exposed {210} facets exhibit a notable photocatalytic reduction of CO<sub>2</sub> to methanol.

4528

### The crystalline sponge method: a solvent-based strategy to facilitate noncovalent ordered trapping of solid and liquid organic compounds

Timothy R. Ramadhar,\* Shao-Liang Zheng, Yu-Sheng Chen and Jon Clardy\*

A new simple procedure for inclusion of solid and unstable liquid compounds into a crystalline sponge for rapid elucidation is described.

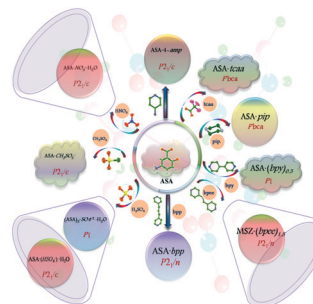


4535

### Structural landscape of multicomponent solids of 5-aminosalicylic acid

Pramod Kumar Goswami, Vineet Kumar, Ram Thaimattam\* and Arunachalam Ramanan\*

Crystallization of ten new multicomponent solids of 5-aminosalicylic acid with various inorganic and organic cofomers has been achieved by mechanochemical and solvent evaporation techniques.

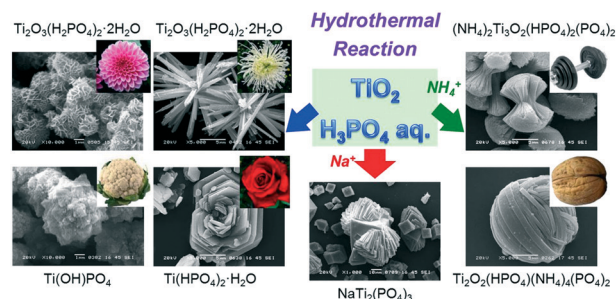


4551

### Nanostructured titanium phosphates prepared via hydrothermal reaction and their electrochemical Li- and Na-ion intercalation properties

Y. Zhu, G. Hasegawa,\* K. Kanamori, T. Kiyomura, H. Kurata, K. Hayashi and K. Nakanishi

A series of titanium phosphates with various morphologies are fabricated via a simple hydrothermal reaction of  $\text{TiO}_2$  in  $\text{H}_3\text{PO}_4$  aq.

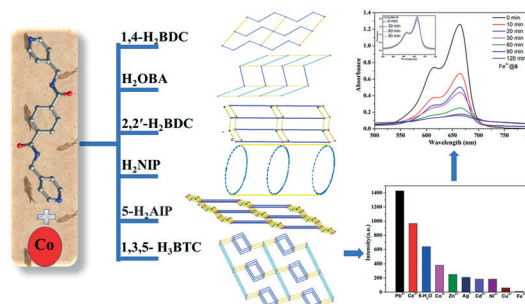


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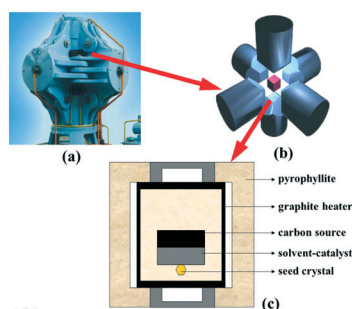
### Fluorescent recognition of $\text{Fe}^{3+}$ and $\text{Fe}^{3+}$ -functionalized composite materials for enhancing photocatalytic activities of $\text{Co}^{\text{II}}$ complexes

Ying Xiong, Guocheng Liu,\* Xiuli Wang,\* Juwen Zhang, Hongyan Lin and Xiaoting Sha

Six new  $\text{Co}^{\text{II}}$  complexes (1–6) based on a bi-methylene-bridged bis-pyridyl-bis-amide have been synthesized. 5 and 6 exhibit photoluminescent sensing selectivity for  $\text{Fe}^{3+}$  ions, and  $\text{Fe}^{3+}$ -functionalized composites  $\text{Fe}^{3+}@5$  and  $\text{Fe}^{3+}@6$  show photocatalytic properties for the degradation of organic dyes.



4571

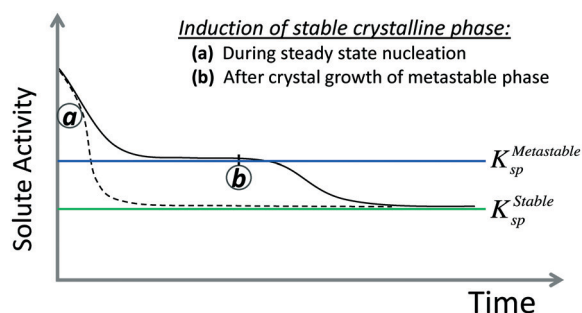


### Synthesis and characterization of boron and nitrogen co-doped diamond crystals under high pressure and high temperature conditions

Meihua Hu,\* Ning Bi, Shangsheng Li, Taichao Su, Qiang Hu, Hongan Ma and Xiaopeng Jia

In this study, diamond crystals co-doped with boron and nitrogen were synthesized via a temperature gradient method at 5.3–5.8 GPa and 1300–1550 °C by adding B and N dopants to a system of carbon and an Fe-based solvent catalyst.

4576

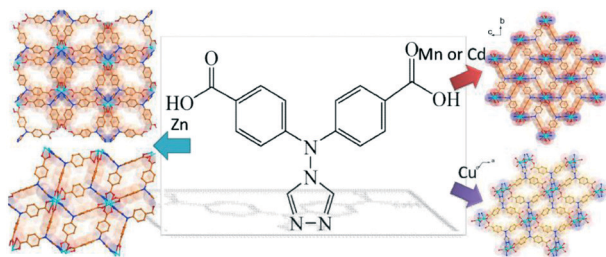


### Induction time of a polymorphic transformation

Wenhao Sun\* and Gerbrand Ceder

We analyze the processes governing the lifetimes of transient metastable polymorphs, within the context of classical nucleation theory.

4586

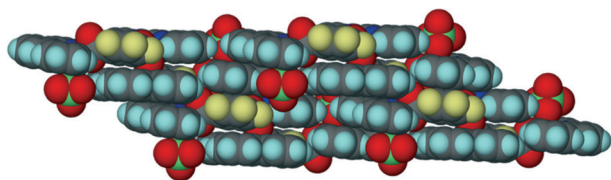


### A series of transition metal coordination polymers based on a rigid bi-functional carboxylate-triazolate tecton

Nan-nan Mao, Peng Hu, Fan Yu, Xi Chen, Gui-lin Zhuang,\* Tian-le Zhang and Bao Li\*

By utilizing a pre-designed bi-functional ligand, five new transition-metal-based coordination polymers have been constructed and structurally characterized, along with their luminescence or magnetic properties.

4595



### Interaction between aromatic rings as organizing tools and semi-coordination in Cu(II) compounds

Sergio Martínez-Vargas, Alejandro Dorazco-González, Simón Hernández-Ortega, Rubén A. Toscano, José Enrique Barquera-Lozada and Jesús Valdés-Martínez\*

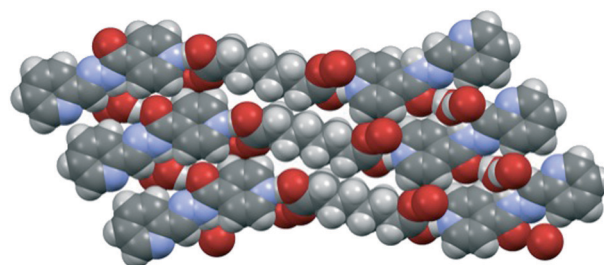
We present the use of the interaction between aromatic rings as the main tool in the organization of coordination compounds in a crystal.

4605

### Exploring binding preferences in co-crystals of conformationally flexible multitopic ligands

Erika L. Krueger, Abhijeet S. Sinha, John Desper and Christer B. Aakeröy\*

A series of conformationally flexible, bipyridine-based ligands were co-crystallized with nine aliphatic dicarboxylic acids of varying carbon chain lengths.

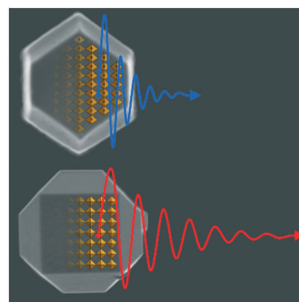


4615

### Facet-controlled preparation of hybrid perovskite microcrystals in the gas phase and the remarkable effect on optoelectronic properties

T. Kollek and S. Polarz\*

Particle shape of hybrid perovskite microcrystals influences PL properties *via* differences in the abundant facets and associated surface trap states.

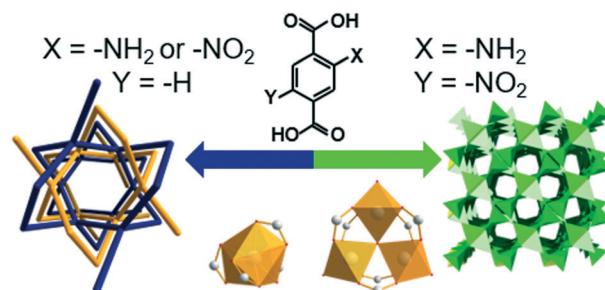


4622

### Investigation of the effect of polar functional groups on the crystal structures of indium MOFs

Martin Krüger, Martin Albat, A. Ken Inge and Norbert Stock\*

$-NH_2/-NO_2$  functionalized linker resulted in In-MOF structures with *qtz* or *ncb* topology, containing  $[In(-CO_2)_4]^-$  polyhedra and ultra-tetrahedra, respectively.



4629

### Switchable dielectric phase transition originating from disorder–order transformation and distortion in $\{[(C_4H_4N_2)Co(H_2O)_4]SO_4 \cdot 2H_2O\}_n$

Rong Mu, Guan-Cheng Xu,\* Ying-Ying Zhang, Li Zhang and Dian-Zeng Jia\*

Disorder–order transition of the  $SO_4^{2-}$  and distortion of the  $[(C_4H_4N_2)Co(H_2O)_4]^{2+}$  chain induce the phase transition of  $\{[(C_4H_4N_2)Co(H_2O)_4]SO_4 \cdot 2H_2O\}_n$ .

