

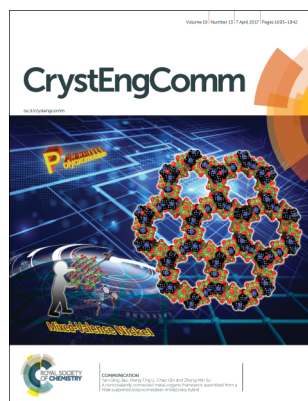
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A journal at the forefront of the design and understanding of solid-state and crystalline materials
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Cover

See Yan-Qing Jiao, Meng-Ting Li, Chao Qin and Zhong-Min Su, pp. 1721-1724.

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Inside cover

See Luciano Pandolfo and Claudio Pettinari, pp. 1701-1720.

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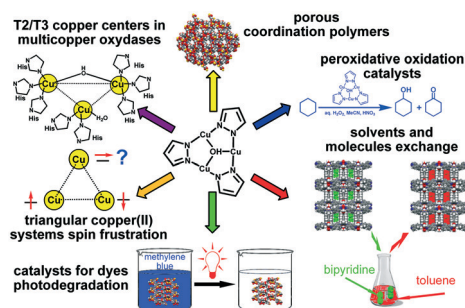
HIGHLIGHT

1701

Trinuclear copper(II) pyrazolate compounds: a long story of serendipitous discoveries and rational design

Luciano Pandolfo* and Claudio Pettinari*

The ease of obtaining the triangular $\text{Cu}_3(\mu_3\text{-OH})(\mu\text{-pz})_3$ moiety (pz = pyrazolate), and its supramolecular self-assemblies, uses and perspectives are reviewed.



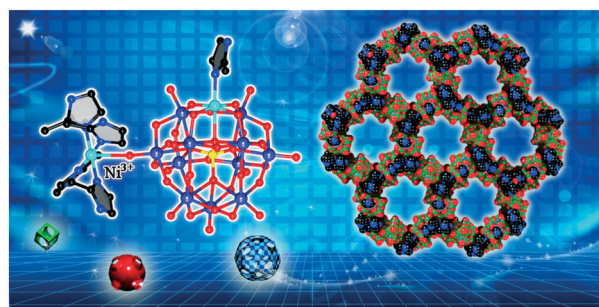
COMMUNICATIONS

1721

A noncovalently connected metal-organic framework assembled from a Ni(III)-supported polyoxometalate-imidazolate hybrid

Yan-Qing Jiao, Meng-Ting Li, Chao Qin* and Zhong-Min Su*

The first mixed-valence nickel-supported polyoxometalate-based metal-organic framework constructed via noncovalent interactions has been synthesized, exhibiting a hexagonal array of 1D large channels along the crystallographic *c* axis with a diameter of 18.83 Å.



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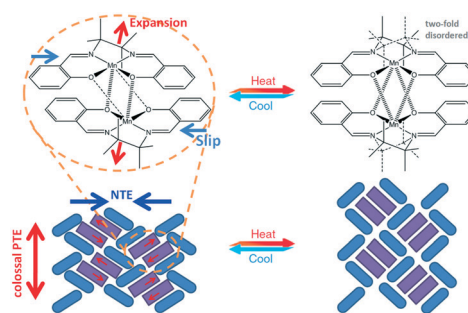
COMMUNICATIONS

1725

Deformable Mn(III)–Schiff-base dimer for anomalously large positive and negative anisotropic thermal expansions

Yu-Jun Su, Ke-Xin Wei, Bo Huang, Wei-Jian Xu, Wei-Xiong Zhang,* Ming-Hua Zeng and Xiao-Ming Chen

A new molecular crystal consisting of supramolecular layers assembled by a Mn(III)–Schiff-base dimer and fumaric acid reveals anomalously large positive and negative anisotropic thermal expansions in the layers.



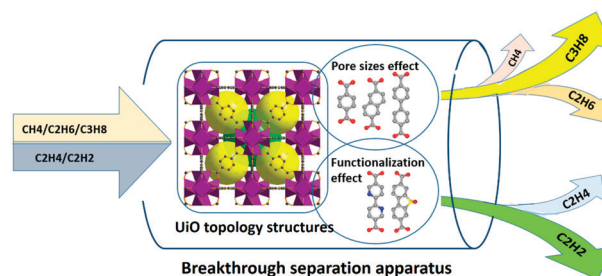
PAPERS

1729

Exploiting the pore size and functionalization effects in UiO topology structures for the separation of light hydrocarbons

Xiaoqing Wang, Libo Li, Yong Wang, Jian-Rong Li and Jinping Li*

A series of UiO topology structures were synthesized by choosing Zr-based clusters with variable length and functional group/site ligands, for exploring the pore size and functionalization effects on the adsorption and separation of light hydrocarbons.

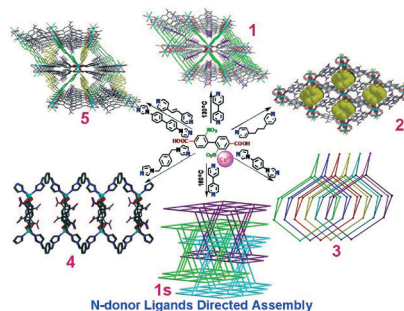


1738

N-donor auxiliary ligand-directed assembly of Co^{II} compounds with a 2,2'-dinitro-biphenyl-4,4'-dicarboxylate ligand: structures and magnetic properties

Jian-Yong Zhang,* Jun-Xia Shi, Liang-Yan Chen, Qin-Xiang Jia, Wei Deng* and En-Qing Gao

The self-assembly of Co^{II} ions and 2,2'-dinitrobiphenyl-4,4'-dicarboxylate ligands leads to the formation of six diverse coordination polymers templated by auxiliary N-donor bridging ligands.

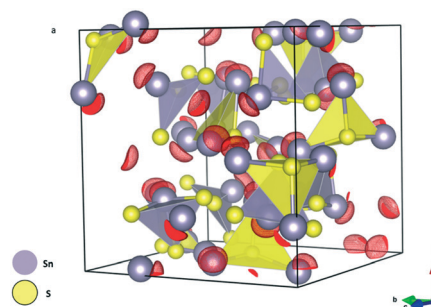


1751

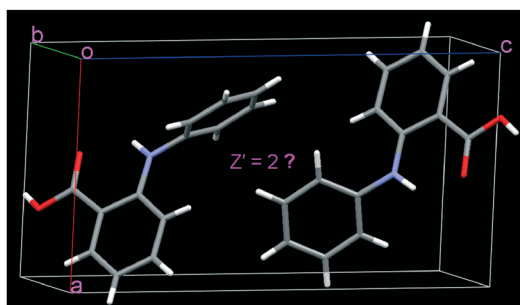
A new cubic prototype structure in the IV–VI monochalcogenide system: a DFT study

Elad Segev, Uri Argaman, Ran E. Abutbul, Yuval Golan and Guy Makov*

Stability, bonding and electronic properties of the novel π -phase in monochalcogenides are explored predicting new phases in GeS and GeSe.



1762

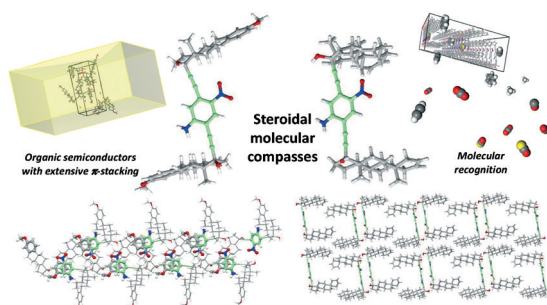


Fenamic acid crystal with two asymmetric units ($Z' = 2$): why $Z' = 2$ rather than $Z' = 1$

Fan Yang, Chao-Xian Yan, Xing Yang, Da-Gang Zhou and Pan-Pan Zhou*

Fenamic acid crystal with the asymmetric unit of $Z' = 2$ is associated with molecular electronic properties, cooperation between intermolecular hydrogen bonding and other interactions like $\pi \cdots \pi$.

1771

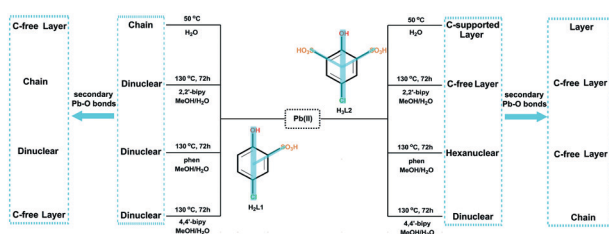


Synthesis of steroidal molecular compasses: exploration of the controlled assembly of solid organic materials

Nancy Aguilar-Valdez, Mauricio Maldonado-Domínguez, Rafael Arcos-Ramos,* Margarita Romero-Ávila, Rosa Santillan and Norberto Farfán*

Crystalline steroidal molecular compasses can be useful to develop self-assembled materials for molecular recognition and as organic semiconducting solids with extensive π -stacking.

1778

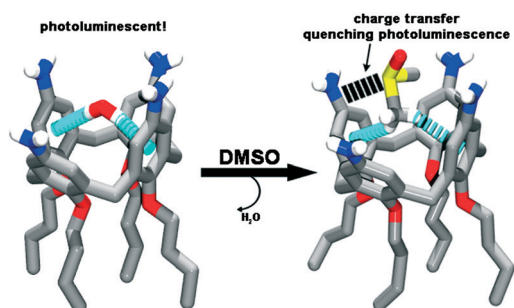


Effect of ligand configurations, secondary Pb–O interactions and auxiliary ligands on Pb(II)–mono/disulfonate complexes: syntheses, structures, and luminescence properties

Guo-Zhen Huang, Xin Zou, Zhi-Biao Zhu, Zhao-Peng Deng,* Li-Hua Huo and Shan Gao*

Eight Pb(II)–mono/disulfonates have been obtained which exhibit diverse structures with different ligand configurations, secondary Pb–O interactions and auxiliary ligands.

1792



Solvatomorphs of 25,26,27,28-tetrahydroxycalix[4]arene and 5,11,17,23-tetramino-25,26,27,28-tetrabutoxycalix[4]arene: quenching photoluminescence through switching the guest

Felipe Terra Martins,* Lauro June Queiroz Maia, Leonardo da Silva Neto, Cleiton Moreira da Silva, Ariel M. Sarotti and Ângelo de Fátima*

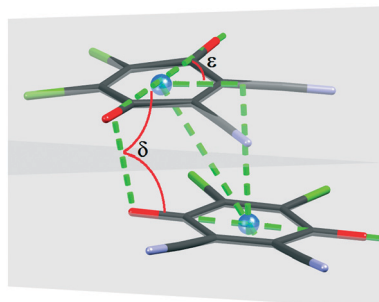
Controlling the solid state luminescence as the solvent molecule entrapped into the calix[4]arene cone.

1801

Spin pairing, electrostatic and dipolar interactions influence stacking of radical anions in alkali salts of 4,5-dichloro-3,6-dioxocyclohexa-1,4-diene-1,2-dicarbonitrile (DDQ)

Krešimir Molčanov* and Biserka Kojić-Prodić

π -stacking of DDQ radical anions is studied in a series of five novel alkali salts; the stacks are Peierls distorted or comprise equidistant radicals.

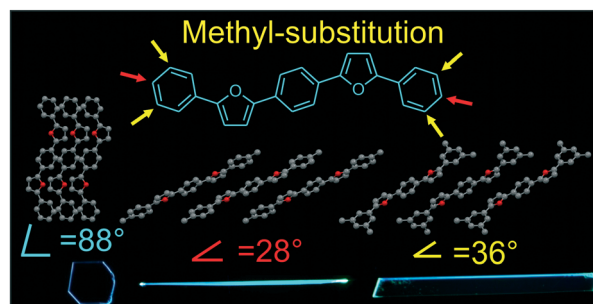


1809

Methyl substituent effect on structure, luminescence and semiconducting properties of furan/phenylene co-oligomer single crystals

Maxim S. Kazantsev,* Alina A. Beloborodova, Ekaterina S. Frantseva, Tatyana V. Rybalova, Vladislav G. Konstantinov, Inna K. Shundrina, Dmitry Yu. Paraschuk and Evgeny A. Mostovich

Methyl substitution tunes the molecular tilt angle, charge transport and luminescence of single crystals of the furan/phenylene co-oligomer BPFB.

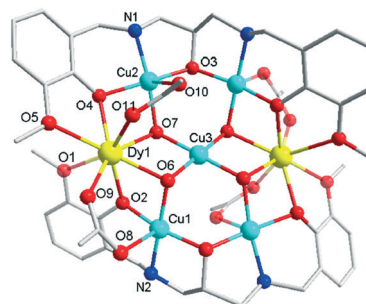


1816

Compartmental ligand approach for constructing 3d-4f heterometallic [Cu^I₅Ln^{III}₂] clusters: synthesis and magnetostructural properties

Lin Jiang, Bin Liu, Hao-Wen Zhao, Jin-Lei Tian,* Xin Liu* and Shi-Ping Yan

The employment of a reduced Schiff-base ligand, 1,3-bis(3-methoxy-salicylamino)-2-propanol (H₃L), with the assistance of acetate anions led to the isolation of eight heptanuclear heterometallic complexes containing [Cu₅Ln₂] cores.

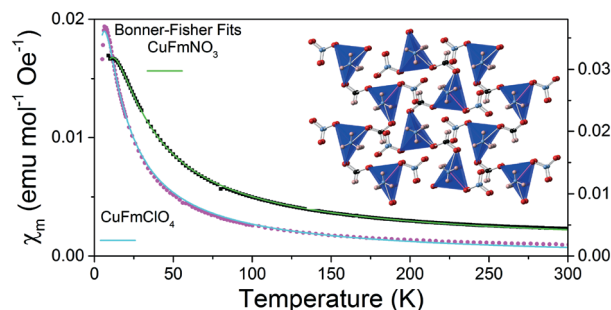


1831

Three coordination frameworks with copper formate based low dimensional motifs: synthesis, structure and magnetic properties

Sally M. Bovill, Richard J. C. Dixey and Paul J. Saines*

The magnetic properties of three new frameworks featuring copper formate chain and ladder motifs have been examined.



CORRECTION

1839

Correction: Synthesis, X-ray characterization, DFT calculations and Hirshfeld surface analysis of thiosemicarbazone complexes of M^{n+} ions ($n = 2, 3$; $M = Ni, Cd, Mn, Co$ and Cu)

Ghodrat Mahmoudi,* Alfonso Castiñeiras, Piotr Garczarek, Antonio Bauzá, Arnold L. Rheingold, Vasyl Kinzhybalov and Antonio Frontera*