

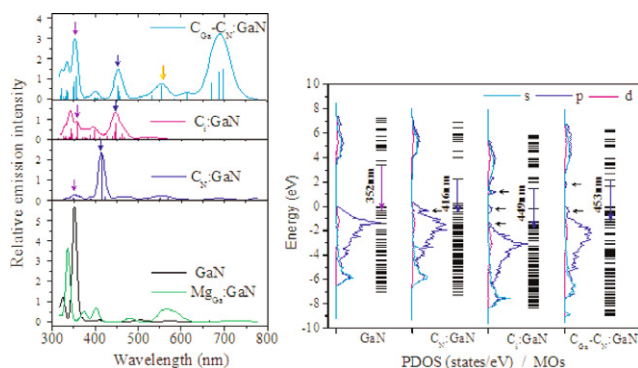
## CONTENTS

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### Regular Articles

#### Density functional theory predictions for blue luminescence and nonlinear optical properties of carbon-doped gallium nitride

XiaoLin Hu, YongFan Zhang, NaiFeng Zhuang and JunQian Li  
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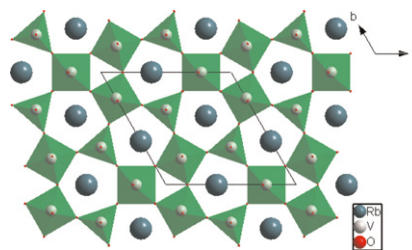


Carbon dopant may introduce the different acceptor or donor level. The blue luminescence of C:GaN are considerable in the region of 400–480 nm, especially that of C<sub>N</sub>:GaN.

### Regular Articles—Continued

#### Synthesis, crystal structure and nonlinear optical property of Rb<sub>3</sub>V<sub>5</sub>O<sub>14</sub>

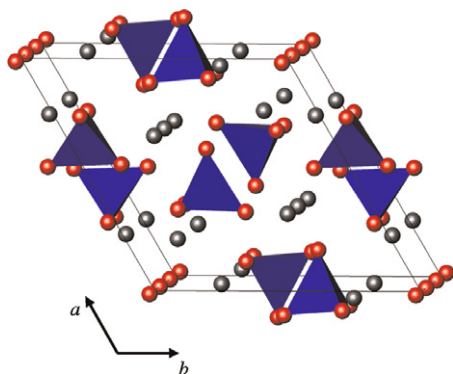
Jianguo Pan, Yuebao Li, Yuejie Cui, Lingyan Zhao, Xing Li and Lei Han  
page 2759



The new nonlinear optical crystal Rb<sub>3</sub>V<sub>5</sub>O<sub>14</sub> has been synthesized by solid state reaction and characterized by single-crystal X-ray diffraction, IR and thermogravimetric analysis. The crystal Rb<sub>3</sub>V<sub>5</sub>O<sub>14</sub> crystallizes in the trigonal system with space *P*31*m* (No. 157), *a* = *b* = 8.7134(12) Å, *c* = 5.2807(11) Å and *α* = 90°, *β* = 90°, *γ* = 120°, *Z* = 1, *ρ* = 3.516 g/cm<sup>3</sup>. It is a layered structure that is very flat and strongly parallel to *c*. The Kurtz powder SHG measurement, using 1064 nm radiation, showed that the second-harmonic generation efficiency of Rb<sub>3</sub>V<sub>5</sub>O<sub>14</sub> is about two times that of KDP.

#### Investigation of the stability of Co-doped apatite ionic conductors in NH<sub>3</sub>

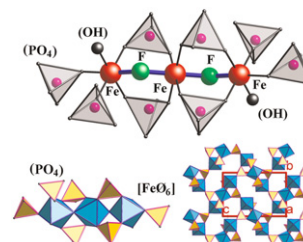
D.A. Headspith, A. Orera, P.R. Slater, N.A. Young and M.G. Francesconi  
page 2746



In reactions between the apatites La<sub>9.67</sub>Si<sub>5</sub>CoO<sub>26</sub> and La<sub>10</sub>(Si/Ge)<sub>5</sub>CoO<sub>26.5</sub> and NH<sub>3</sub> (g) at temperatures *T* > 500 °C, the partial substitution of the Si and Ge by Co seems to discourage O<sup>2-</sup>/N<sup>3-</sup> substitution in favour of the reduction of the metal.

#### Synthesis and crystal structure of a new open-framework iron phosphate (NH<sub>4</sub>)<sub>4</sub>Fe<sub>3</sub>(OH)<sub>2</sub>F<sub>2</sub>[H<sub>3</sub>(PO<sub>4</sub>)<sub>4</sub>]: Novel linear trimer of corner-sharing Fe(III) octahedra

Jin-Xiao Mi, Cheng-Xin Wang, Ning Chen, Rong Li and Yuanming Pan  
page 2763



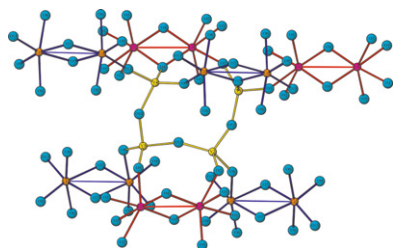
The three-dimensional open-framework structure of (NH<sub>4</sub>)<sub>4</sub>Fe<sub>3</sub>(OH)<sub>2</sub>F<sub>2</sub>[H<sub>3</sub>(PO<sub>4</sub>)<sub>4</sub>] is built from a novel isolated, linear (FeO<sub>4</sub>)<sub>3</sub>(OH)<sub>2</sub>F<sub>2</sub> trimer of corner-sharing Fe(III) octahedra linked by PO<sub>4</sub> tetrahedra.

Continued

### Crystal structure, thermal and magnetic properties of $\text{Cr}_2\text{V}_4\text{O}_{13}$

S.J. Patwe, S.N. Achary, J. Manjanna, R.M. Kadam, H.G. Salunke and A.K. Tyagi

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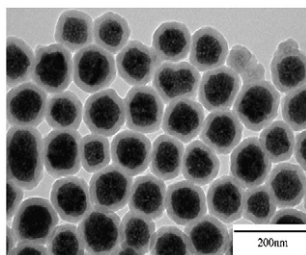


A tetravanadate of chromium ( $\text{Cr}_2\text{V}_4\text{O}_{13}$ ) is prepared characterized in detail. The crystal structure of this compound is formed by the U shaped  $\text{V}_4\text{O}_{13}$  (tetravanadates) and  $\text{Cr}_2\text{O}_{10}$  (dimer) units.

### Solvothermal synthesis and luminescence properties of monodisperse $\text{Gd}_2\text{O}_3:\text{Eu}^{3+}$ and $\text{Gd}_2\text{O}_3:\text{Eu}^{3+}@\text{SiO}_2$ nanospheres

Yu Wang, Xue Bai, Tong Liu, Biao Dong, Lin Xu, Qiong Liu and Hongwei Song

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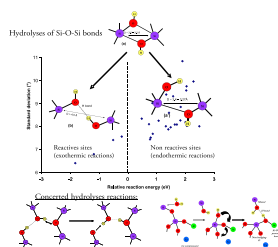


Uniform and monodisperse  $\text{Gd}_2\text{O}_3:\text{Eu}^{3+}$  and  $\text{Gd}_2\text{O}_3:\text{Eu}^{3+}@\text{SiO}_2$  monodisperse were synthesized by annealed relative parent's  $\text{Gd}(\text{OH})_3:\text{Eu}^{3+}$  and  $\text{Gd}(\text{OH})_3:\text{Eu}^{3+}@\text{SiO}_2$ , respectively. Their morphology and luminescence properties all strongly depended on the iron concentration.

### Water solubility in calcium aluminosilicate glasses investigated by first principles techniques

Frédéric Bouyer, Grégory Geneste, Simona Ispas, Walter Kob and Patrick Ganster

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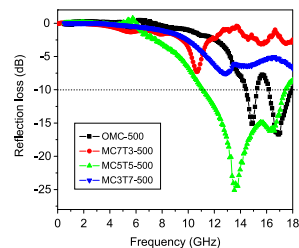


Reactivity within glass bulk: structures obtained after hydrolyses reactions (endothermic and exothermic processes) and mechanisms involving Si-OH, Al-OH, Si-OH-Al groups within aluminosilicates glasses (through ab initio molecular dynamics): formation of the Si-OH-Al entity coupled with an H exchange—Frédéric Bouyer and Grégory Geneste.

### Microwave absorption properties and infrared emissivities of ordered mesoporous C-TiO<sub>2</sub> nanocomposites with crystalline framework

Tao Wang, Jianping He, Jianhua Zhou, Jing Tang, Yunxia Guo, Xiaochun Ding, Shichao Wu and Jianqing Zhao

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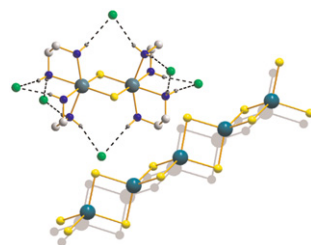


Ordered mesoporous C-TiO<sub>2</sub> nanocomposite with crystalline framework possess excellent microwave absorbing properties with the maximum reflection loss of -25.4 dB and the bandwidth lower than -10 dB is 6.6 GHz.

### Zero- and one-dimensional thioindates synthesized under solvothermal conditions yielding $\alpha\text{-In}_2\text{S}_3$ , $\beta\text{-In}_2\text{S}_3$ or $\text{MgIn}_2\text{S}_4$ as thermal decomposition products

E. Quiroga-González, L. Kienle, C. Näther, V.S.K. Chakravadhanula, H. Lühmann and W. Bensch

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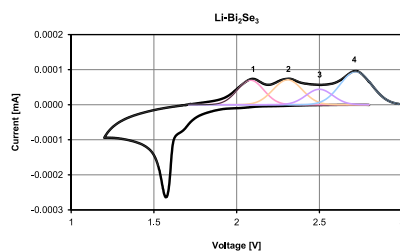


The structure of  $[\text{In}(\text{en})_2\text{S}]_2 \cdot 2\text{Cl}$  contains a cationic core and  $[\text{Mg}(\text{en})_3][\text{In}_2\text{S}_4]$  is the first thioindate with a charge compensating  $\text{Mg}^{2+}$  complex. Thermal decomposition yields  $\alpha$ - or  $\beta$ - $\text{In}_2\text{S}_3$  resp. spinel-type nanocrystalline  $\text{MgIn}_2\text{S}_4$ .

### Lithium ions in the van der Waals gap of $\text{Bi}_2\text{Se}_3$ single crystals

J. Bludská, I. Jakubec, S. Karamazov, J. Horák and C. Uher

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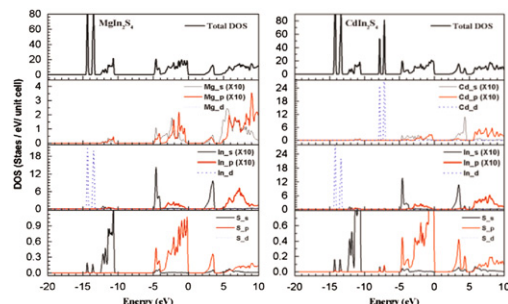


Insertion/extraction of lithium ions into/from  $\text{Bi}_2\text{Se}_3$  layered crystals was investigated by cyclic voltammetry. The extraction of  $\text{Li}^+$  results in the appearance of four bands on the voltammograms. The first two bands have a character of a reversible process. A part of  $\text{Li}^+$  ions is bound firmly in the crystal due to the formation of negatively charged clusters of the  $(\text{LiBiSe}_2\text{Bi}_3\text{Se}_4^-)$  type. Their extraction needs higher voltage due to the negative charge.

## Full potential study of the elastic, electronic, and optical properties of spinels $\text{MgIn}_2\text{S}_4$ and $\text{CdIn}_2\text{S}_4$ under pressure effect

F. Semari, R. Khenata, M. Rabah, A. Bouhemadou, S. Bin Omran, Ali H. Reshak and D. Rached

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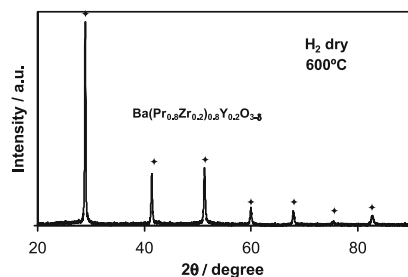


Calculated total and partial densities of states for  $\text{MgIn}_2\text{S}_4$  and  $\text{CdIn}_2\text{S}_4$ .

## Stability of $\text{Ba}(\text{Zr},\text{Pr},\text{Y})\text{O}_{3-\delta}$ materials for potential application in electrochemical devices

I. Antunes, G.C. Mather, J.R. Frade, J. Gracio and D.P. Fagg

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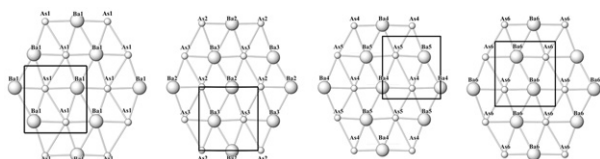


The stability of  $\text{Ba}(\text{Pr}_{1-x}\text{Zr}_x)_{0.9}\text{Y}_{0.1}\text{O}_{3-\delta}$  and  $\text{Ba}(\text{Pr}_{1-x}\text{Zr}_x)_{0.8}\text{Y}_{0.2}\text{O}_{3-\delta}$  systems has been assessed in various atmospheres for  $0 \leq x \leq 1$ . The figure shows that, by correct compositional selection, stability in reducing conditions can even extend to compositions containing high levels of Pr, such as  $\text{Ba}(\text{Pr}_{0.8}\text{Zr}_{0.2})_{0.8}\text{Y}_{0.2}\text{O}_{3-\delta}$ .

## A new polymorph of $\text{Ba}(\text{AsO}_3\text{OH})$ : Synthesis, crystal structure and vibrational spectra

Tamara Đorević and Ljiljana Karanović

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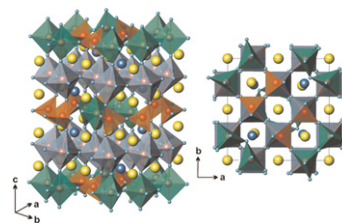


Mesh type and topological structure of the cation layers seen along  $[0 0 1]$ ;  $a$ -axis vertical,  $b$ -axis horizontal. A trace of the unit cell is drawn for reference.

## Coupled anion and cation ordering in $\text{Sr}_3\text{RFe}_4\text{O}_{10.5}$ ( $R = \text{Y}, \text{Ho}, \text{Dy}$ ) anion-deficient perovskites

Artem M. Abakumov, Hans D'Hondt, Marta D. Rossell, Alexander A. Tsirlin, Olga Gutnikova, Dmitry S. Filimonov, Walter Schnelle, Helge Rosner, Joke Hadermann, Gustaaf Van Tendeloo and Evgeny V. Antipov

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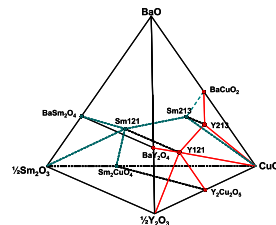


The  $\text{Sr}_3\text{RFe}_4\text{O}_{10.5}$  ( $R = \text{Y}, \text{Ho}, \text{Dy}$ ) anion-deficient perovskites with a complete ordering of the  $A$ -cations and oxygen vacancies have been prepared using a solid-state reaction in evacuated sealed silica tubes. Oxygen vacancies reside in the  $(\text{FeO}_{5/4} \text{ }_{3/4})$  layers, comprising corner-sharing  $\text{FeO}_4$  tetrahedra and  $\text{FeO}_5$  tetragonal pyramids, which are sandwiched between the layers of the  $\text{FeO}_6$  octahedra. Smaller  $R$  atoms occupy the 9-fold coordinated position, whereas the 10-fold coordinated positions are occupied by larger Sr atoms.

## Phase equilibria of the $\text{Ba-Sm-Y-Cu-O}$ system for coated conductor applications

G. Liu, W. Wong-Ng, Z. Yang, J.A. Kaduk and L.P. Cook

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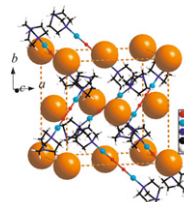


Phase diagram overview of the  $\text{Ba-Sm-Y-Cu-O}$  system in the BaO-poor region prepared in  $p_{\text{O}_2} = 22 \text{ kPa}$ ,  $950^\circ\text{C}$ .

## A series of new supramolecular structures constructed from triethylenediamine and different polyoxometalates

Yan Wang, Cheng-Ling Pan, Li-Na Xiao, Feng-Qing Wu, Hong Ding, Ya-Bing Liu, Zhong-Min Gao, Da-Fang Zheng, Tie-Gang Wang, Guang-Di Yang, Xiao-Bing Cui and Ji-Qing Xu

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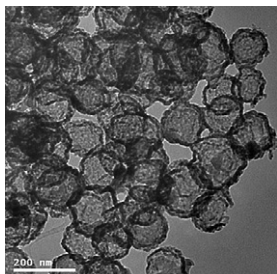


Three new supramolecular compounds based on triethylenediamine and different polyoxometalates have been hydrothermally synthesized and characterized by IR, XPS, TG, elemental analysis and X-ray diffraction analysis.

Continued

### Porous $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> hollow microspheres and their application for acetone sensor

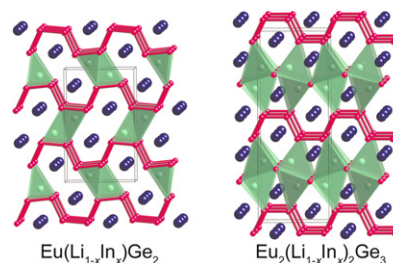
Shurong Wang, Liwei Wang, Taili Yang, Xianghong Liu, Jun Zhang, Baolin Zhu, Shoumin Zhang, Weiping Huang and Shihua Wu  
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HRTEM images of the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> hollow microspheres.

### *cis-trans* Germanium chains in the intermetallic compounds $ALi_{1-x}In_xGe_2$ and $A_2(Li_{1-x}In_x)_2Ge_3$ ( $A = Sr, Ba, Eu$ )—experimental and theoretical studies

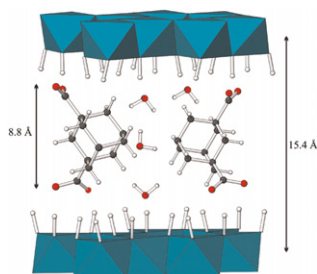
Tae-Soo You and Svilen Bobev  
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Presented are the single-crystal structures of two types of closely related intermetallics, as well as their band structures, calculated using tight-binding linear muffin-tin orbital (TB-LMTO-ASA) method.

### The intercalation of bicyclic and tricyclic carboxylates into layered double hydroxides

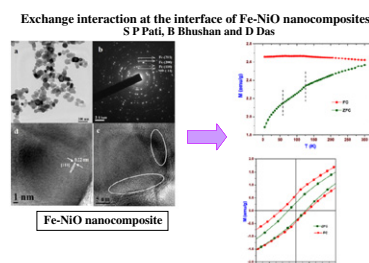
Aamir I. Khan, Gareth R. Williams, Gang Hu, Nicholas H. Rees and Dermot O'Hare  
page 2877



Twenty-four novel nanocomposites built from layered double hydroxides and bicyclic and tricyclic carboxylates have been synthesised and fully characterised. *In situ* X-ray diffraction was used to study reaction mechanisms and kinetics.

### Exchange interaction at the interface of Fe–NiO nanocomposites

S.P. Pati, B. Bhushan and D. Das  
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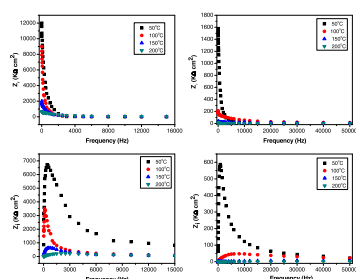


Fe–NiO nanocomposites exhibited some structural disordered region at the interface as revealed by HRTEM. A prominent shift in the hysteresis loops in field cooled condition confirmed the presence of exchange bias at Fe–NiO interfaces. The irreversibility observed in  $M$ – $T$  measurements also points to exchange bias effect.

### Investigation of structural, morphological, luminescent and thermal properties of combusted aluminium-based iron oxide

S.S. Shinde and K.Y. Rajpure

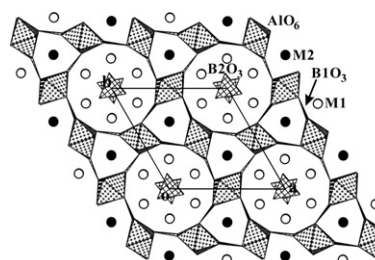
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Frequency and temperature dependent interparticle interactions like grains, grain boundary effects using complex impedance spectroscopy of pure and 10 at% Al:Fe<sub>2</sub>O<sub>3</sub> have been studied.

### Synthesis, crystal structure, spectrum properties, and electronic structure of a novel non-centrosymmetric borate, BiCd<sub>3</sub>(AlO<sub>3</sub>)<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>

Xuean Chen, Hui Yin, Xinan Chang, Hegui Zang and Weiqiang Xiao  
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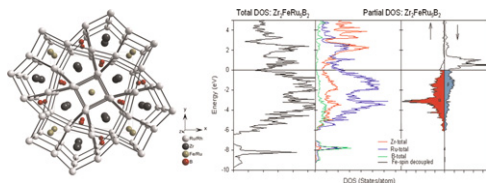
BiCd<sub>3</sub>(AlO<sub>3</sub>)<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> has a 3D network formed by stitching 1D chains of edge-sharing AlO<sub>6</sub> octahedra *via* BO<sub>3</sub> groups. There are channels occupied by Bi<sup>3+</sup>/Cd<sup>2+</sup> only or by Bi<sup>3+</sup>/Cd<sup>2+</sup> with BO<sub>3</sub> groups.



## Structure, bonding, and magnetic response in two complex borides: $\text{Zr}_2\text{Fe}_{1-\delta}\text{Ru}_{5+\delta}\text{B}_2$ and $\text{Zr}_2\text{Fe}_{1-\delta}(\text{Ru}_{1-x}\text{Rh}_x)_{5+\delta}\text{B}_2$

Jakoah Brgoch, Steven Yeninas, Ruslan Prozorov and Gordon J. Miller

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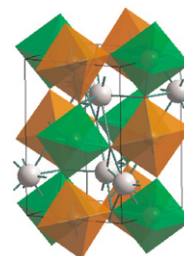


$\text{Zr}_2\text{FeRu}_{5-x}\text{Rh}_x\text{B}_2$  ( $x=0, 1$ ) crystallizes with magnetic atoms forming chains which have been shown to order magnetically depending on the total valence electron count. Magnetic measurements and tight-binding electronic structure calculations are employed to investigate the ordering.

## Structure distortion and magnetism in double perovskites $\text{Ca}_{2-x}\text{La}_x\text{FeReO}_6$ ( $0 \leq x \leq 0.8$ )

Minfeng Lü, Junjie Li, Heng Zou, Zhijian Wu and Jian Meng

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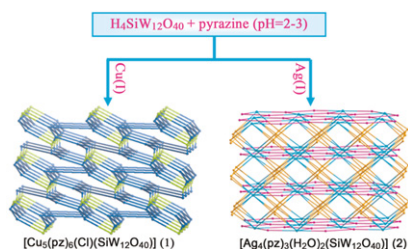


The crystal structures of  $\text{Ca}_{2-x}\text{La}_x\text{FeReO}_6$  transform from monoclinic to orthorhombic; meanwhile, high degree of anti-site disorder was present at B/B' position, which promotes AFM correlations as an La increases.

## Two new organic-inorganic hybrid compounds based on metal-pyrazine coordination polymers and Keggin polyoxometalates: effect of metal ions on the structure

Feng-Yun Cui, Xiao-Yu Ma, Cong Li, Tao Dong, Yuan-Zhe Gao, Zhan-Gang Han, Ying-Nan Chi and Chang-Wen Hu

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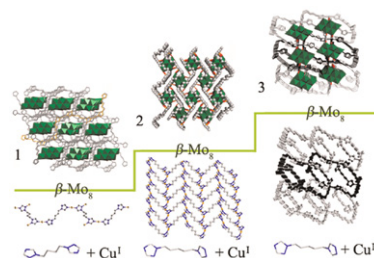


Two new highly connected Keggin POMs-based hybrids have been synthesized by changing metal ions under hydrothermal conditions and the effect of metal ions on the final structure and topology of the POMs-based hybrid compounds was discussed.

## Three 3D hybrid networks based on octamolybdates and different $\text{Cu}^{\text{I}}/\text{Cu}^{\text{II}}$ -bis(triazole) motifs

Chun-Jing Zhang, Hai-Jun Pang, Qun Tang, Hui-Yuan Wang and Ya-Guang Chen

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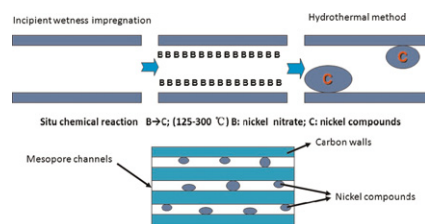


Three 3D compounds based on  $\beta\text{-}[\text{Mo}_8\text{O}_{26}]^{4-}$  clusters with different  $\text{Cu}^{\text{I}}/\text{Cu}^{\text{II}}$ -bis(triazole) motifs were synthesized by regularly tuning flexible ligand spacer length and metal coordination preferences.

## The electrochemical performance of ordered mesoporous carbon/nickel compounds composite material for supercapacitor

Jicheng Feng, Jiachang Zhao, Bohejin Tang, Ping Liu and Jingli Xu

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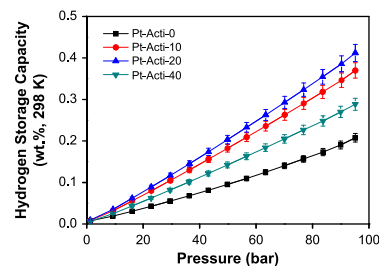


A series of high performance nickel compound/ordered mesoporous carbon composites were synthesized by a combination of incipient wetness impregnation and hydrothermal method for the first time.

## Influence of $\text{CO}_2$ activation on hydrogen storage behaviors of platinum-loaded activated carbon nanotubes

Seul-Yi Lee and Soo-Jin Park

page 2951

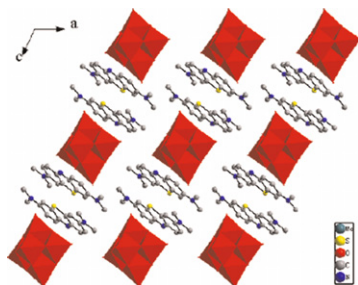


The hydrogen storage capacities of the Pt-loaded activated MWNTs as a function of  $\text{CO}_2$  flow time are described.

Continued

## Two inorganic–organic hybrid materials based on polyoxometalate anions and methylene blue: Preparations, crystal structures and properties

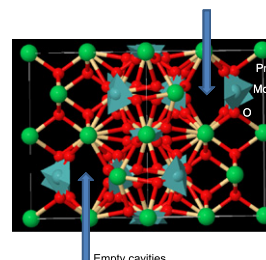
Shanshan Nie, Yaobin Zhang, Bin Liu, Zuoxi Li, Huaiming Hu, Ganglin Xue, Feng Fu and Jiwu Wang  
page 2957



Their crystal structures present that the layers of organic molecules and inorganic anions array alternatively, and there exist strong  $\pi \cdots \pi$  stacking interactions between dimeric MB cations.

## Preparation and structural study from neutron diffraction data of $\text{Pr}_5\text{Mo}_3\text{O}_{16}$

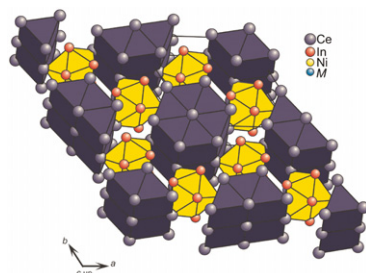
M.J. Martínez-Lope, J.A. Alonso, D. Sheptyakov and V. Pomjakushin  
page 2974



Formerly formulated as  $\text{Pr}_2\text{MoO}_6$ , the title compound is a cubic superstructure of fluorite ( $a = 11.0897(1)$  Å, space group  $Pn\bar{3}n$ ) due to the long-range ordering of  $\text{PrO}_8$  scalenohedra and  $\text{MoO}_4$  tetrahedral units, showing noticeable shifts of the oxygen positions in order to provide a tetrahedral coordination for Mo ions. A mixed valence  $\text{Mo}^{5+}\text{--}\text{Mo}^{6+}$  is identified, which could account for the excellent catalytic properties of this material.

## Crystal structure and magnetic properties of $\text{Ce}_7\text{Ni}_{5\pm x}\text{Ge}_{3\pm x}\text{In}_6$ and $\text{Pr}_7\text{Ni}_{5\pm x}\text{Ge}_{3\pm x}\text{In}_6$

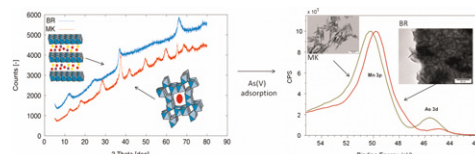
Nataliya Chumalo, Galyna P. Nychporuk, Volodymyr V. Pavlyuk, Rainer Pöttgen, Dariusz Kaczorowski and Vasyľ I. Zaremba  
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Packing of the polyhedra in the  $\text{Ce}_7\text{Ni}_{4.73}\text{Ge}_{3.27}\text{In}_6$  structure.

## Synthesis, characterization and study of arsenate adsorption from aqueous solution by $\alpha$ - and $\delta$ -phase manganese dioxide nanoadsorbents

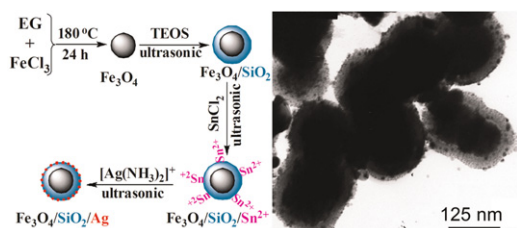
Mandeep Singh, Dong Nguyen Thanh, Pavel Ulbrich, Nina Strnadová and František Štěpánek  
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$\alpha$ - $\text{MnO}_2$  ( $2 \times 2$  tunnel structure) nanorods and  $\delta$ - $\text{MnO}_2$  (2-D layered structure) nano-fiber clumps were synthesized in a facile way in an aqueous solution and characterized by TEM, FE-SEM, XRD and BET- $\text{N}_2$  adsorption techniques. The structural analysis shows that  $\alpha$ - $\text{MnO}_2$  is needle shaped nanorods and  $\delta$ - $\text{MnO}_2$  consists of 2-D platelets of fine needle-like fibers arranged in ball-like aggregates. Further batch experiments confirmed that both nanoadsorbents are potential candidates for the adsorption of  $\text{As(V)}$  with a capacity of 19.41 and 15.33  $\text{mg g}^{-1}$  for  $\alpha$ - $\text{MnO}_2$  and  $\delta$ - $\text{MnO}_2$ , respectively. The presence of  $\text{As}3d$  peak in XPS study indicates that arsenic on the surface of nanoadsorbents is in the stable form of  $\text{As(V)}$  with a percentage of arsenate onto  $\alpha$ - $\text{MnO}_2$  is 0.099% as compared to 0.021% onto  $\delta$ - $\text{MnO}_2$ , clearly indicating the higher adsorption of  $\text{As(V)}$  in case of  $\alpha$ - $\text{MnO}_2$  as compared to  $\delta$ - $\text{MnO}_2$ , which is in good agreement with the adsorption studies results.

## Synthesis of $\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{Ag}$ nanoparticles and its application in surface-enhanced Raman scattering

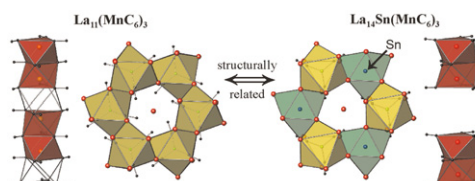
Baoliang Lv, Yao Xu, Hong Tian, Dong Wu and Yuhua Sun  
page 2968



$\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{Ag}$  particles, a recyclable surface-enhanced Raman scattering (SERS) material, were designed and synthesized via a simple ultrasonic route.

## Structural relationships between new carbide $\text{La}_{14}\text{Sn}(\text{MnC}_6)_3$ and fully ordered $\text{La}_{11}(\text{MnC}_6)_3$

Julia V. Zaikina, Haidong Zhou and Susan E. Lattner  
page 2987

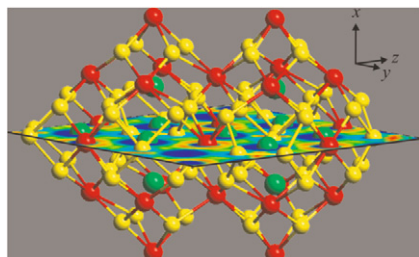


$\text{La}_{11}(\text{MnC}_6)_3$  with fully ordered superstructure and a new carbide  $\text{La}_{14}\text{Sn}(\text{MnC}_6)_3$  were obtained from La/Ni eutectic flux.

### 3D [Ag–Mg] polyanionic frameworks in the $\text{La}_4\text{Ag}_{10}\text{Mg}_3$ and $\text{La}_4\text{Ag}_{10.3}\text{Mg}_{12}$ new ternary compounds

Pavlo Solokha, Serena De Negri, Volodymyr Pavlyuk, Bernhard Eck, Richard Dronskowski and Adriana Saccone

page 2995

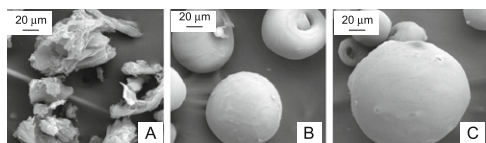


An independent fragment of the 3D [Ag–Mg] framework in  $\text{La}_4\text{Ag}_{10}\text{Mg}_3$  together with an ELF section (1/2 0 0 basal plane).

### Solubility and release of fenbufen intercalated in Mg, Al and Mg, Al, Fe layered double hydroxides (LDH): The effect of Eudragit® S 100 covering

M. del Arco, A. Fernández, C. Martín and V. Rives

page 3002

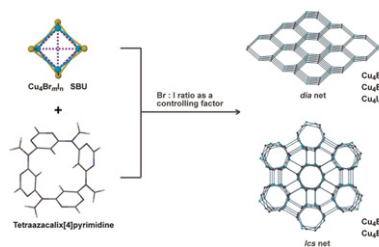


LDHs containing Mg, Al, Fe increase fenbufen solubility, release takes place through ionic exchange with phosphate anions from the medium. Spherical solids with homogeneous, smooth surface are formed when using Eudragit® S 100, efficiently covering the LDH surface.

### Synthesis and structural characterization of different topological coordination polymers based on tunable $\text{Cu}_4\text{Br}_{4-m}\text{I}_m$ secondary building units and macrocyclic azacalixaromatics

Li-Xia Wang, Liang Zhao, De-Xian Wang and Mei-Xiang Wang

page 3010

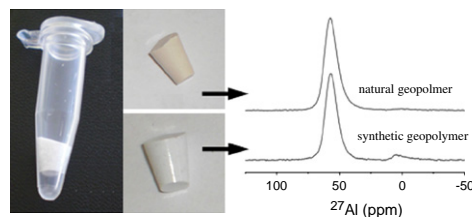


Five luminescent coordination polymers **1–5** were obtained via the reaction of tetrahedral  $\text{Cu}_4\text{Br}_{4-m}\text{I}_m$  SBUs and a flexible macrocyclic ligand tetraazacalix[4] pyrimidine (TAPM), wherein the Br/I ratio serves as a controlling factor to fine-tune the geometries of  $\text{Cu}_4\text{Br}_{4-m}\text{I}_m$  and induce the conformation variation of TAPM, thus constructing two different *dia* and *lcs* topological nets.

### Solid-state NMR study of geopolymer prepared by sol–gel chemistry

Yi-Ling Tsai, John V. Hanna, Yuan-Ling Lee, Mark E. Smith and Jerry C.C. Chan

page 3017

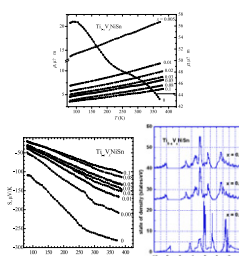


Geopolymer prepared by the sol–gel route has the same spectroscopic properties as the sample prepared from the natural kaolinite.

### Crystal, electronic structure and electronic transport properties of the $\text{Ti}_{1-x}\text{V}_x\text{NiSn}$ ( $x = 0\text{--}0.10$ ) solid solutions

Yu. Stadnyk, A. Horyn', V.V. Romaka, Yu. Gorelenko, L.P. Romaka, E.K. Hlil and D. Fruchart

page 3023

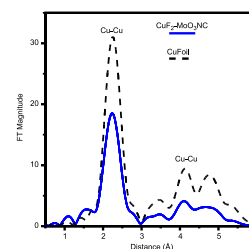


Both approaches experimental and calculations point to the same conclusions. Resistivity, power factor and thermopower estimations indicate that doping of  $\text{TiNiSn}$  based compound by the V induces insulator–metal transition without change of the negative sign of  $S$  thermopower. Vanadium is revealed as donor impurity.

### In situ X-ray absorption spectroscopic investigation of the electrochemical conversion reactions of $\text{CuF}_2\text{--MoO}_3$ nanocomposite

A.N. Mansour, F. Badway, W.-S. Yoon, K.Y. Chung and G.G. Amatucci

page 3029



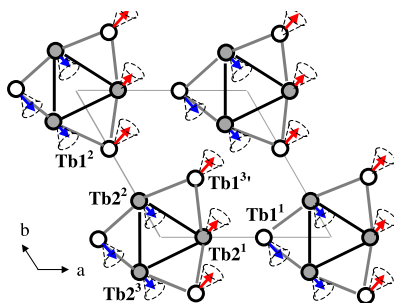
Comparison of Fourier transform of in situ Cu K-edge EXAFS spectra for a fully discharged  $\text{CuF}_2\bullet\text{MoO}_3$  nanocomposite in a nonaqueous Li cell with that of a Cu foil. Quantitative analysis of the Fourier transforms confirmed that the discharge mechanism for the nanocomposite proceeds via the reaction  $\text{CuF}_2 + 2\text{Li} \rightarrow \text{Cu} + 2\text{LiF}$ . The discharge product of Cu is in the form of highly dispersed nanoparticles.

Continued

### Magnetic properties of Fe<sub>2</sub>P-type Tb<sub>6</sub>FeTe<sub>2</sub>, Tb<sub>6</sub>CoTe<sub>2</sub>, Tb<sub>6</sub>NiTe<sub>2</sub> and Er<sub>6</sub>FeTe<sub>2</sub> compounds

A.V. Morozkin, Yu. Mozharivskiy, V. Svitlyk, R. Nirmala and A.K. Nigam

page 3039

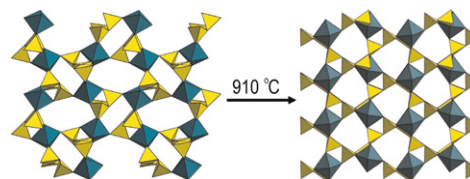


The novel Fe<sub>2</sub>P-type Tb<sub>6</sub>{Fe, Co, Te}Te<sub>2</sub> and Er<sub>6</sub>FeTe<sub>2</sub> phases (space group *P62m*) show the complex magnetic ordering below 18–228 K. The magnetocaloric effect for Tb<sub>6</sub>NiTe<sub>2</sub> in terms of the isothermal entropy change,  $-\Delta S_m$ , has the maximum value of 4.86 J/kg K at 229 K for the 0–5 T field change.

### Novel microporous zirconium silicate (K<sub>2</sub>ZrSi<sub>3</sub>O<sub>9</sub> · 2H<sub>2</sub>O) from high temperature phase transformation

Artur Ferreira, Zhi Lin, Maria R. Soares and João Rocha

page 3067

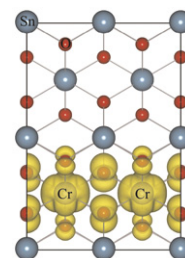


A new microporous zirconosilicate has been prepared by high temperature phase transformation at 910 °C. Its structure has been determined *ab initio* from powder X-ray diffraction data. The water molecules in this material are lost below 125 °C in a way typical of zeolites and molecular sieves.

### Effects of oxygen vacancy on the magnetic properties of Cr-doped SnO<sub>2</sub>: Density functional investigation

Wei Wei, Ying Dai, Meng Guo, Zhenkui Zhang and Baibiao Huang

page 3073

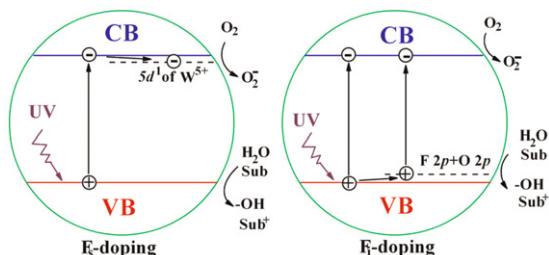


We studied the magnetic properties in Cr-doped SnO<sub>2</sub> by means of the first-principles calculations. It indicated that introduction of oxygen vacancy obviously weakened the ferromagnetic coupling, which could give a rational explanation for the discrepancies in experimental observations.

### Origin of the improved photo-catalytic activity of F-doped ZnWO<sub>4</sub>: A quantum mechanical study

Honggang Sun, Weiliu Fan, Yanlu Li, Xiufeng Cheng, Pan Li and Xian Zhao

page 3052

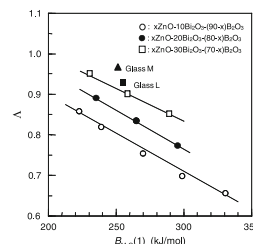


DFT calculations are used to investigate the origin of the improved photo-activity of monoclinic ZnWO<sub>4</sub> induced by the substituted and interstitial F-doping. Two possible mechanisms are tentatively put forward according to the F-doping types.

### Approach to thermal properties and electronic polarizability from average single bond strength in ZnO–Bi<sub>2</sub>O<sub>3</sub>–B<sub>2</sub>O<sub>3</sub> glasses

Taisuke Inoue, Tsuyoshi Honma, Vesselin Dimitrov and Takayuki Komatsu

page 3078

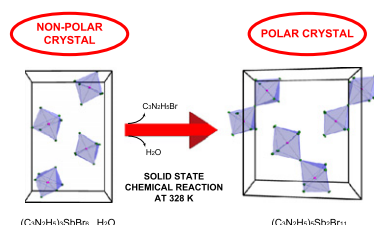


This figure shows the correlation between optical basicity  $\Lambda$  and average single bond strength  $B_{M-O}$  in ZnO–Bi<sub>2</sub>O<sub>3</sub>–B<sub>2</sub>O<sub>3</sub> glasses. A good correlation is observed, proposing that the average single bond strength is a good parameter for understanding optical properties of ZnO–Bi<sub>2</sub>O<sub>3</sub>–B<sub>2</sub>O<sub>3</sub> glasses.

### Unprecedented solid-state chemical reaction—from (C<sub>3</sub>N<sub>2</sub>H<sub>5</sub>)<sub>3</sub>SbBr<sub>6</sub> · H<sub>2</sub>O to (C<sub>3</sub>N<sub>2</sub>H<sub>5</sub>)<sub>5</sub>Sb<sub>2</sub>Br<sub>11</sub>. From centrosymmetric to non-centrosymmetric crystal structure

A. Piecha, A. Gągor, A. Pietraszko and R. Jakubas

page 3058

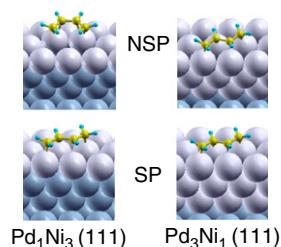


Chemical reaction taking place in (C<sub>3</sub>N<sub>2</sub>H<sub>5</sub>)<sub>3</sub>SbBr<sub>6</sub> · H<sub>2</sub>O at 328 K.



### The adsorption of 1,3-butadiene on Pd/Ni multilayers: The interplay between spin polarization and chemisorption strength

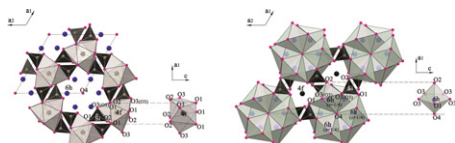
Guillermina Gómez, Patricia G. Belelli, Gabriela F. Cabeza and Norberto J. Castellani  
page 3086



The adsorption of 1,3-butadiene on Pd/Ni(1 1 1) multilayers was theoretically studied. The most stable adsorption site depends on the substrate composition and on the inclusion of spin polarization.

### Study of the cation distributions in Eu doped $\text{Sr}_2\text{Y}_8(\text{SiO}_4)_6\text{O}_2$ by X-ray diffraction and photoluminescent spectra

Yiqiang Shen, Rui Chen, Fen Xiao, Handong Sun, Alfred Tok and Zhili Dong  
page 3093

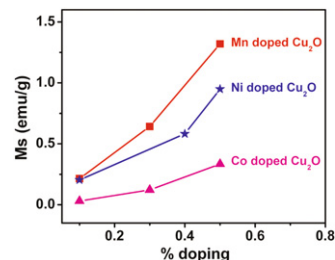


The crystal structures of Eu doped  $\text{Sr}_2\text{Y}_8(\text{SiO}_4)_6\text{O}_2$  especially the distributions of  $\text{Eu}^{3+}$  cations between  $4f$  and  $6h$  sites were studied by X-ray diffraction, Rietveld refinement and photoluminescent spectra.

### Rapid Communication

#### Room temperature ferromagnetism in Mn, Ni and Co ions doped $\text{Cu}_2\text{O}$ nanorods

Asar Ahmed and Namdeo S. Gajbhiye  
page 3100



Room temperature ferromagnetism was observed in the  $\text{Cu}_2\text{O}$  nanorods doped with Mn, Ni and Co ions. The origin seems to be the defects of cation vacancies created by the dopant ions.

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