



# **JOURNAL OF** SOLID STATE CHEMISTRY

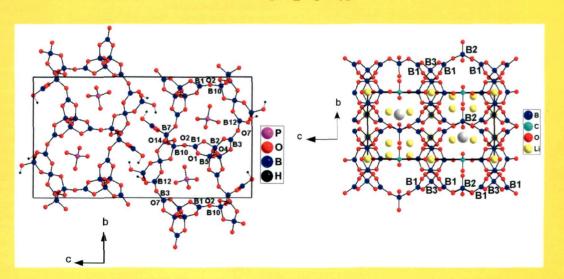
M.G. KANATZIDIS

**Associate Editors** I. LI W. TREMEL S.I. CLARKE

H.-C. ZUR LOYE

#### IN THIS ISSUE:

Hydrothermal synthesis and structural analysis of new mixed oxyanion borates:  $Ba_{11}B_{26}O_{44}(PO_4)_2(OH)_6$ ,  $Li_9BaB_{15}O_{27}(CO_3)$ and Ba<sub>3</sub>Si<sub>2</sub>B<sub>6</sub>O<sub>16</sub>



Carla Heyward, Colin D. McMillen and Joseph Kolis

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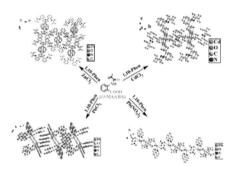
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#### Regular Articles

Synthesis, structures of four coordination compounds constructed from o-methacrylamidobenzoic acid and their relationship between structure and solid state luminescence Hong-Xia Chen, Yong Ma, Feng Zhou, Bing Wu, Qing-Feng Xu, Jian-Mei Lu, Jian-Feng Ge page 1

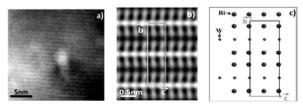


Four coordination compounds constructed by o-methacrylamidobenzoic, phenanthroline and metal ions are reported. The photoluminescent properties is studied, which is affected by the molecular stacking and LMCT.

### Electron microscopy analyses and electrical properties of the layered $Bi_2WO_6$ phase

A. Taoufyq, H. Ait Ahsaine, L. Patout, A. Benlhachemi, M. Ezahri, F. Guinneton, A. Lyoussi, G. Nolibe, J.-R. Gavarri

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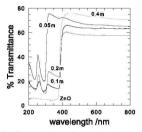
High resolution transmission electron microscopy: inverse fast Fourier transform giving the layered structure of the  $Bi_2WO_6$  phase, with a representation of the cell dimensions (b and c vectors). The  $Bi_2O_2^{2+}$  and  $WO_4^{2-}$  sandwiches are visible in the IFFT image.

#### Regular Articles—Continued

## Synthesis and controlled release properties of 2,4-dichlorophenoxy acetate—zinc layered hydroxide nanohybrid

Abbas M. Bashi, Mohd Zobir Hussein, Zulkarnain Zainal, Didier Tichit

page 19



The phenomenon indicates that the optical energy gap is enlarged with the increase of molar concentrations in 2,4-dichlorophenoxy acetate anion content into ZnO to create a ZLH–24D nanohybrid

### Thermoelectric properties of composites made of Ni<sub>0.05</sub>Mo<sub>3</sub>Sb<sub>5.4</sub>Te<sub>1.6</sub> and fullerene

Nagaraj Nandihalli, Ali Lahwal, Daniel Thompson, Tim C. Holgate, Terry M. Tritt, Véronique Dassylva-Raymond, László I. Kiss, Elisabeth Sellier, Stéphane Gorsse, Holger Kleinke

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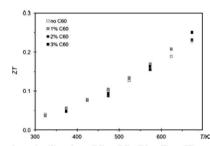
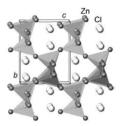


Figure-of-merit of various Ni<sub>0.05</sub>Mo<sub>3</sub>Sb<sub>5.4</sub>Te<sub>1.6</sub>/C composites.

### Synthesis and single-crystal structure determination of the zinc nitride halides $Zn_2NX$ (X = Cl, Br, I)

Xiaohui Liu, Claudia Wessel, Fangfang Pan, Richard Dronskowski

page 31

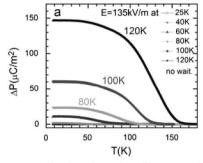


Zn<sub>2</sub>NCl, Zn<sub>2</sub>NBr, and Zn<sub>2</sub>NI have been synthesized, and their crystal structures (Cl and Br phases: *Pna*2<sub>1</sub>; I phase: *Pnma*) have been determined from XRD; the direct band gap of Zn<sub>2</sub>NCl is theoretically (HSE06 hybrid functional) predicted as 3.7 eV.

## From spin induced ferroelectricity to spin and dipolar glass in a triangular lattice: The $CuCr_{1-x}V_xO_2$ ( $0 \le x \le 0.5$ ) delafossite

S. Kumar, K. Singh, M. Miclau, Ch. Simon, C. Martin, A. Maignan

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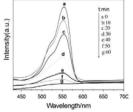
The P(T) curves evidencing the aging effect on polarization in  $\text{CuCr}_{0.5}\text{V}_{0.5}\text{O}_2$ :  $E=135\ \text{kV/m}$  is applied during cooling at different temperatures. The P values and the inflection point of the transition depend on the poling temperature suggesting a relaxor behaviour. This effect related to the spin glass state is not observed for the lowest vanadium content.

### Self-assembled cabbage-like NaInS<sub>2</sub> microstructures with efficient visible light photocatalytic performance

Yuanhao Gao, Xuezhen Zhai, Yange Zhang, Zhihong Xu, Pinjiang Li, Zhi Zheng

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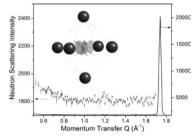




Cabbage-like NaInS<sub>2</sub> microstructures were facilely synthesized *via* simple hydrothermal reaction. The cabbage-like NaInS<sub>2</sub> architectures exhibit the superiority of photocatalytic performance for the photodegradation of RhB irradiation under visible light irradiation.

### Investigation of an unusual low-temperature phase transformation in RbBH<sub>4</sub> by neutron diffraction

Brian B. Kitchen, Nina Verdal, Terrence J. Udovic, John J. Rush, Michael R. Hartman, Daniel J. DeVries *page 51* 



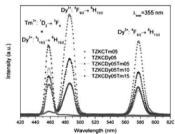
The neutron powder diffraction pattern of RbBD<sub>4</sub> below the phase transition temperature (shown here in black) is indistinguishable from that collected above the phase transition temperature. The inset depicts the cubic structure that fits the data at both temperatures.

### Effect of co-doping ${\rm Tm}^{3+}$ ions on the emission properties of ${\rm Dy}^{3+}$ ions in tellurite glasses

T. Sasikala, L. Rama Moorthy, A. Mohan Babu,

T. Srinivasa Rao

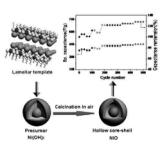
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The graphical abstract shows the emission spectra of  $Dy^{3+}$ ,  $Tm^{3+}$  and  $Dy^{3+}/Tm^{3+}$  co-doped TZKC glasses recorded by exciting at 355 nm wavelength.

### Facile approach to prepare hollow coreshell NiO microspherers for supercapacitor electrodes

Dandan Han, Pengcheng Xu, Xiaoyan Jing, Jun Wang, Dalei Song, Jingyuan Liu, Milin Zhang page 60

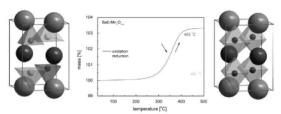


The hollow coreshell NiO was prepared with a facile lamellar template method. The prepared NiO show higher capacitance, lower ion diffusion resistance and better electroactive surface utilization for Faradaic reactions.

### Synthesis, crystal structure and electrical properties of A-site cation ordered BaErMn<sub>2</sub>O<sub>5</sub> and BaErMn<sub>2</sub>O<sub>6</sub>

Konrad Świerczek, Alicja Klimkowicz, Kun Zheng, Bogdan Dabrowski

page 68

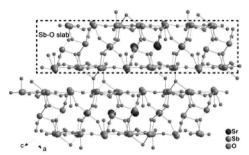


Structure and oxygen storage properties of  $BaErMn_2O_{5+\delta}$ .

### A new strontium antimonate<sup>III</sup> Sr<sub>5</sub>Sb<sub>22</sub>O<sub>38</sub>: Synthesis, crystal structure and characterizations

Lei Geng, Chang-Yu Meng, Chen-Sheng Lin, Wen-Dan Cheng

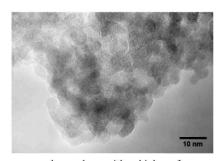
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The 2D SbO slabs are stacked through sharing oxygen atoms to form the 3D network structure of the new strontium antimonate  $^{\rm III}$  Sr<sub>5</sub>Sb<sub>22</sub>O<sub>38</sub>.

### Hydrothermal synthesis and characterization of zirconia based catalysts

T. Caillot, Z. Salama, N. Chanut, F.J. Cadete Santos Aires, S. Bennici, A. Auroux page 79

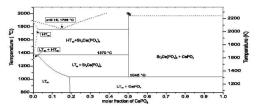


Mesoporous amorphous phase with a high surface area of titania zirconia mixed oxide obtained by hydrothermal preparation.

## Study of phase relationships in the $\rm Sr_3(PO_4)_2CePO_4$ system. Phase diagram and thermal characteristics of phases

Aleksandra Matraszek

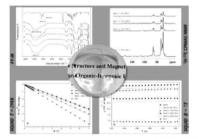
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The phase diagram of  $Sr_3(PO_4)_2CePO_4$  system showing the stability ranges of limited solid solution and  $Sr_3Ce(PO_4)_3$  phases.

### Structure and magnetic properties of SiO<sub>2</sub>/PCL novel solgel organicinorganic hybrid materials

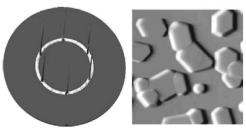
Michelina Catauro, Flavia Bollino, Maria Cristina Mozzati, Chiara Ferrara, Piercarlo Mustarelli page 92



Characterization and magnetic properties of SiO<sub>2</sub>/PCL organic-inorganic hybrid materials synthesized via solgel. FT-IR, Fourier transform infrared spectroscopy; solid-state NMR: solid-state nuclear magnetic resonance; SQUID: superconducting quantum interference device.

### Oriented Y-type hexagonal ferrite thin films prepared by chemical solution deposition

J. Buršík, R. Kužel b, K. Knížek, I. Drbohlav page 100



XRD pole figure and AFM patterns of  $Ba_2Zn_2Fe_{12}O_{22}$  thin film epitaxially grown on  $SrTiO_3(1\ 1\ 1)$  single crystal using seeding layer templating.

# Diverse assemblies of the (4,4) grid layers exemplified in Zn (II)/Co(II) coordination polymers with dual linear ligands Guang-Zhen Liu, Xiao-Dong Li, Ling-Yun Xin,

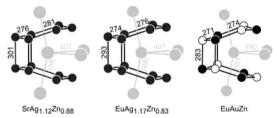
Xiao-Ling Li, Li-Ya Wang page 106



Diverse assemblies of the (4,4) grid layers with different network nodes forms five coordination polymers that are well characterized by IR, TGA, element analysis, fluorescent and magnetic measurement.

# SrAgZn and EuAgZn with KHg<sub>2</sub>-type structure—Structure, magnetic properties, and <sup>151</sup>Eu Mössbauer spectroscopy Birgit Gerke, Ute Ch. Rodewald, Oliver Niehaus, Rainer Pöttgen

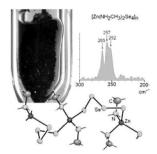
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The near neighbor coordination of the strontium and europium atoms in  $SrAg_{1.12}Zn_{0.88}$ ,  $EuAg_{1.17}Zn_{0.83}$ , and EuAuZn.

#### 1D coordination polymers with polychalcogenides as linkers between metal atoms

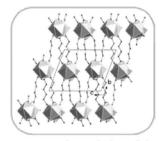
Oleksandr Kysliak, Johannes Beck page 120



The reaction of Zn and Se in liquid methylamine yields dark red  $[Zn(NH_2CH_3)Se_4]$ , a 1D coordination polymer consisting of helical Zn–Se<sub>4</sub>–Zn– chains.

#### Topological aspects of lanthanide-adipate-aqua compounds: Close packed and open framework structures

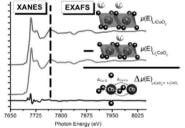
Durga Sankar Chowdhuri, Swapan Kumar Jana, Debdoot Hazari, Ennio Zangrando, Sudipta Dalai page 128



A survey of structures and topologies of lanthanide adipate compounds is presented. A newly synthesized lanthanium adipate complex  $\{[La_2(adip)_3(H_2O)_2]\ (adipH_2=adipic\ acid)\ is\ also\ reported.$ 

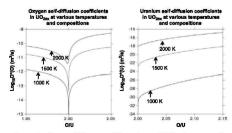
### *In-situ* X-ray absorption spectroscopy analysis of capacity fade in nanoscale-LiCoO<sub>2</sub>

Christopher J. Patridge, Corey T. Love, Karen E. Swider-Lyons, Mark E. Twigg, David E. Ramaker page 134



Electrochemical cycling of Li-ion batteries has strong impact on the structure and integrity of the cathode active material particularly near the surface/electrolyte interface. In developing a new method, we have used *in-situ* X-ray absorption spectroscopy during electrochemical cycling of nanoscale LiCoO<sub>2</sub> to track changes during charge and discharge and between subsequent cycles. Using difference spectra, several small changes in Co-O bond length, Co-O and Co-Co coordination, and site exchange between Co and Li sites can be tracked. These methods show promise as a new technique to better understand processes which lead to capacity fade and loss in Li-ion batteries.

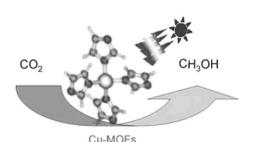
#### Diffusion model of the non-stoichiometric uranium dioxide Emily Moore, Christine Guéneau, Jean-Paul Crocombette page 145



Complete description of OxygenUranium diffusion as a function of composition at various temperatures according to the developed Dictra model.

## Copper(II) imidazolate frameworks as highly efficient photocatalysts for reduction of $CO_2$ into methanol under visible light irradiation

Jingtian Li, Deliang Luo, Chengju Yang, Shiman He, Shangchao Chen, Jiawei Lin, Li Zhu, Xin Li page 154

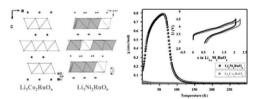


Carbon dioxide was reduced into methanol with water over copper (II) imidazolate frameworks under visible light irradiation.

### New rock salt-related oxides $\text{Li}_3M_2\text{RuO}_6$ (M = Co, Ni): Synthesis, structure, magnetism and electrochemistry

S. Laha, E. Morán, R. Sáez-Puche, M.Á. Alario-Franco, A.J. Dos santos-Garcia, E. Gonzalo, A. Kuhn, F. García-Alvarado, T. Sivakumar, S. Tamilarasan, S. Natarajan, J. Gopalakrishnan

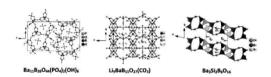
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Two new rock salt related oxides of formula,  $\text{Li}_3M_2\text{RuO}_6$ , (M=Co,Ni) have been prepared. The M=Co oxide adopts the  $\text{LiCoO}_2$  (R-3m) structure and the M=Ni oxide adopts a similar layered structure related to  $\text{Li}_2\text{TiO}_3$ , monoclinic (C2/c), with partial mixing of Li and Ni/Ru atoms. For  $\text{Li}_3\text{Co}_2\text{RuO}_6$ , oxidation state for Ru is 4+ and antiferromagnetic (AFM) order is found below 10 K while for the analogous  $\text{Li}_3\text{Ni}_2\text{RuO}_6$ , Ru oxidation state is 5+ and a ferrimagnetic (FM) behavior with a Curie temperature of 100 K is found. Electrochemical studies correlate well with both magnetic properties and crystal structure.

## Hydrothermal synthesis and structural analysis of new mixed oxyanion borates: $Ba_{11}B_{26}O_{44}(PO_4)_2(OH)_6$ , $Li_9BaB_{15}O_{27}(CO_3)$ and $Ba_3Si_2B_6O_{16}$

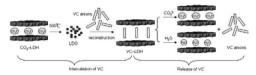
Carla Heyward, Colin D. McMillen, Joseph Kolis page 166



### Intercalation and controlled release properties of vitamin C intercalated layered double hydroxide

Xiaorui Gao, Lixu Lei, Dermot O'Hare, Juan Xie, Pengran Gao, Tao Chang

page 174

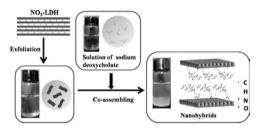


Vitamin C anions have been intercalated in the interlayer space of layered double hydroxide and released in  $CO_3^{2-}$  solution and deionised water.

### Facile synthesis of deoxycholate intercalated layered double hydroxide nanohybrids via a coassembly process

Xiaowen Wu, Shuang Wang, Na Du, Renjie Zhang, Wanguo Hou

page 181

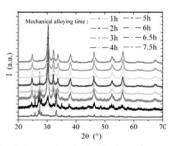


Deoxycholate intercalated layered double hydroxide nanohybrids were successfully synthesized via a coassembly strategy. In this strategy, the interlayer spaces of LDHs can be efficiently used for the intercalation of guest species.

### Direct synthesis of BiCu*Ch*O-type oxychalcogenides by mechanical alloying

Vincent Pele, Celine Barreteau, David Berardan, Lidong Zhao, Nita Dragoe

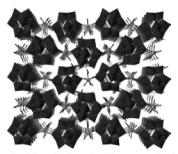
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BiCuSeO synthesis by mechanical alloying: phase pure after 7.5h.

## Open frameworks based on mono-lanthanide-substituted polyoxometaloaluminate building units: Syntheses, structures and properties

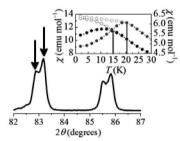
Xin-Xiong Li, Lin Cheng, Guo-Yu Yang page 193



A series of lanthanide-substituted polyoxometaloaluminates have been hydrothermally made and their photoluminescence, nonlinear optical and ferroelectricity properties have also been investigated, respectively.

### Oxygen miscibility gap and spin glass formation in the pyrochlore Lu<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub>

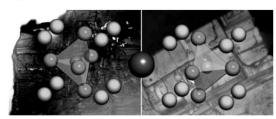
L. Clark, C. Ritter, A. Harrison, J.P. Attfield page 199



The cubic  $\text{Lu}_2\text{Mo}_2\text{O}_{7-x}$  system exhibits a miscibility gap between coexisting pyrochlore phases at 1600 °C. Neutron powder diffraction refinement and chemical analysis shows that the gap separates stoichiometric x=0 and oxygen-deficient  $x\approx 0.4$  phases.  $\text{Lu}_2\text{Mo}_2\text{O}_{7-x}$  has a frustrated spin glass ground state that is sensitive to the oxygen content.

### A new oxytelluride: Perovskite and CsCl intergrowth in Ba<sub>3</sub>Yb<sub>2</sub>O<sub>5</sub>Te

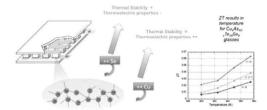
J.B. Whalen, T. Besara, R. Vasquez, F. Herrera, J. Sun, D. Ramirez, R.L. Stillwell, S.W. Tozer, T.D. Tokumoto, S.A. McGill, J. Allen, M. Davidson, T. Siegrist page 204



Optical images of Ba<sub>3</sub>Yb<sub>2</sub>O<sub>5</sub>Te in transmission (left) and reflected (right) light, with atomic unit cell overlay.

### Thermal stability and thermoelectric properties of $Cu_xAs_{40-x}Te_{60-y}Se_y$ semiconducting glasses

J.B. Vaney, A. Piarristeguy, A. Pradel, E. Alleno, B. Lenoir, C. Candolfi, A. Dauscher, A.P. Gonçalves, E.B. Lopes, G. Delaizir, J. Monnier, M. Ribes, C. Godart *page 212* 



Effect of substitution of Te by Se and As by Cu on thermal stability and thermoelectric properties of  $Cu_xAs_{40-x}Te_{60-y}Se_y$  semiconducting glasses.

### Synthesis, structural and magnetic characterisation of the fluorinated compound 15R-BaFeO<sub>2</sub>F

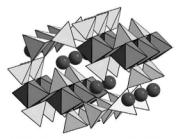
Oliver Clemens, Frank J. Berry, Jessica Bauer, Adrian J. Wright, Kevin S. Knight, Peter R. Slater page 218



The crystal and magnetic structure of the perovskite phase 15R-BaFeO<sub>2</sub>F.

## Phase formation in the $Li_2MoO_4$ -Rb<sub>2</sub> $MoO_4$ -Fe<sub>2</sub>( $MoO_4$ )<sub>3</sub> system and crystal structure of a novel triple molybdate $LiRb_2Fe(MoO_4)_3$

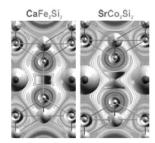
Klara M. Khal'baeva, Sergey F. Solodovnikov, Elena G. Khaikina, Yuliya M. Kadyrova, Zoya A. Solodovnikova, Olga M. Basovich page 227



Exploring the Li<sub>2</sub>MoO<sub>4</sub>–Rb<sub>2</sub>MoO<sub>4</sub>–Fe<sub>2</sub>(MoO<sub>4</sub>)<sub>3</sub> system showed its partial non-quasiternarity and revealed a new compound LiRb<sub>2</sub>Fe(MoO<sub>4</sub>)<sub>3</sub> which was structurally studied.

### Synthesis, structure and chemical bonding of $CaFe_{2-x}Rh_xSi_2$ ( $x=0,\,1.32,\,$ and 2) and $SrCo_2Si_2$

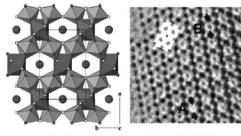
Viktor Hlukhyy, Andrea V. Hoffmann, Thomas F. Fässler page 232



The  $SrCo_2Si_2$  and  $CaFe_{2-x}Rh_xSi_2$  (x=0, 1.32, and 2) crystallize in the  $ThCr_2Si_2$ -type. The structure of  $SrCo_2Si_2$  contains isolated  $[Co_2Si_2]^{2-}$  layers in the ab-plane, whereas the  $[T_2Si_2]$  layers in  $CaFe_{2-x}Rh_xSi_2$  are interconnected along the c-axis via Si-Si bonds resulting in a  $[T_2Si_2]^{2-}$  network.

### New high pressure rare earth tantalates $RE_xTa_2O_{5+1.5x}$ (RE = La, Eu, Yb)

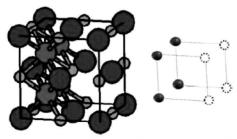
Igor P. Zibrov, Vladimir P. Filonenko, Nikolai D. Zakharov, Peter Werner, Dmitrii V. Drobot, Elena E. Nikishina, Elena N. Lebedeva page 240



The structure of  $RE_xTa_2O_{5+1.5x}$  and its HRTEM image ("A" arrows show empty channel, "B" arrows show filled channel).

### Phase separation and antisite defects in the thermoelectric TiNiSn half-Heusler alloys

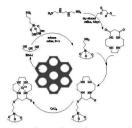
K. Kirievsky, Y. Gelbstein, D. Fuks *page 247* 



Phase separation and antisite defects in the thermoelectric TiNiSn alloy, are covered as methods for nanostructuring and thereby enhancement of the thermoelectric potential.

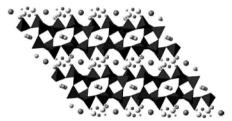
### Grafted chromium 13-membered dioxo-macrocyclic complex into aminopropyl-based nanoporous SBA-15

Aliakbar Tarlani, Monika Joharian, Khashayar Narimani, Jacques Muzart, Mahtab Fallah page 255



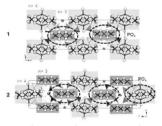
Chromium (III) tetraaza dioxo ligand was grafted onto functionalized SBA-15 using coordinating ability of anchored amino functionalized SBA-15. Preparation of the catalyst is depicted in Scheme 1

A new naturally-occurring nanoporous copper sheet-silicate with 6<sup>4</sup>8<sup>2</sup> cages related to synthetic "CuSH" phases Mark D. Welch, Michael S. Rumsey page 260



Projection onto (010) of the structure of the natural nanoporous sheet silicate  $Na_2CaCu_2Si_8O_{20} \cdot H_2O$  showing the double sheet of corner-linked  $SiO_4$  tetrahedra, intralayer Na and interlayer Na, Ca Cu and  $H_2O$ . Small green sphere Cu, large blue spheres Ca, orange purple and yellow small spheres Na, large grey sphere  $H_2O$  molecules. Bonds from inter/intralayer species to sheets have been omitted for clarity.

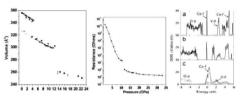
Bi<sub>2</sub>O<sub>3</sub>-CuO-P<sub>2</sub>O<sub>5</sub> system: Two novel compounds built from the intergrowths oxocentered polycationic 1D-ribbons Marie Colmont, Diana Endara, Almaz Aliev, Christine Terryn, Marielle Huvé, Olivier Mentré page 266



This paper reports the crystal structure of two new bismuth oxophosphate compounds. Both are built on the association of n=3 and 4 building unit ribbons surrounded by isolated PO4 tetrahedra and tunnels hosting  $\text{Cu}^{2+}$  cations. They come in addition to the numerous Bi-based compounds already pointed out. Once more, this is the proof of the richness of this crystal system.

### Phase transition and possible metallization in $\mbox{CeVO}_4$ under pressure

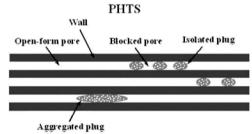
Alka B. Garg, K.V. Shanavas, B.N. Wani, Surinder M. Sharma *page 273* 



Pressure induced structural phase transition in  $CeVO_4$  as observed by x-ray diffraction (pressure vs. volume) and possible metallization in  $CeVO_4$  through electrical resistance and first principles electronic structure calculations.

## Direct synthesis of Al-SBA-15 containing aluminosilicate species plugs in an acid-free medium and structural adjustment by hydrothermal post-treatment

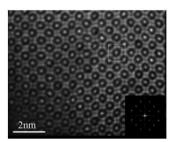
Lei Shi, Yan Xu, Na Zhang, Sen Lin, Xiangping Li, Peng Guo, Xuebing Li page 281



The plugs-containing structures can be interpreted as the distribution of individual isolated plugs along the mesoporous channel.

## Observation of atomic scale compositional and displacive modulations in incommensurate melilite electrolytes

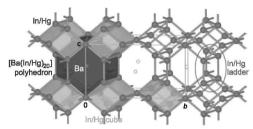
Fengxia Wei, Tim Williams, Tao An, Tom Baikie, Christian Kloc, Jun Wei, Tim White *page 291* 



HAADF image for melilite composition  $[Nd_{1.5}Ca_{0.5}]_2[Ga]_2\\ [Ga_2O_{7.25}]_2.$ 

The new Hg-rich barium indium mercurides  $BaIn_xHg_{7-x}$  (x = 3.1) and  $BaIn_xHg_{11-x}$  (x = 0-2.8) Synthesis, crystal and electronic structure

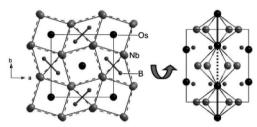
Marco Wendorff, Michael Schwarz, Caroline Röhr page 297



BaIn<sub>2.6</sub>Hg<sub>4.4</sub>: distorted cubes [(In/Hg)<sub>8</sub>] (green, like in BaHg<sub>11</sub>), folded ladders (violet, like in BaIn, BaHg<sub>2</sub> and BaIn<sub>2</sub>) and Ba coordination polyhedra [Ba(In/Hg)<sub>20</sub>] (blue, like in BaHg<sub>11</sub>).

Nb<sub>2</sub>OsB<sub>2</sub>, with a new twofold superstructure of the U<sub>3</sub>Si<sub>2</sub> type: Synthesis, crystal chemistry and chemical bonding Mohammed Mbarki, Rachid St. Touzani, Boniface P.T. Fokwa

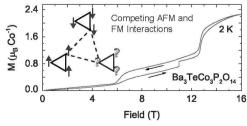
page 304



 ${\rm Nb_2OsB_2}$  is, to the best of our knowledge, the first fully characterized phase in the ternary Nb–Os–B system. It crystallizes (space group P4/mnc, 128) with a new twofold superstructure of the  ${\rm U_3Si_2}$  structure type (space group P4/mbm, 127), and is therefore the first boride in this structure family crystallizing with a superstructure of the  ${\rm U_3Si_2}$  structure type. We show that the distortions leading to this superstructure occurs mainly in the Nb-layer, which tries to accommodate the large osmium atoms. The consequence of this puckering is the building osmium dumbbells instead of chains along [001].

## Crystal structure and magnetic properties of the $Ba_3TeCo_3P_2O_{14}$ , $Pb_3TeCo_3P_2O_{14}$ , and $Pb_3TeCo_3V_2O_{14}$ langasites

J.W. Krizan, C. dela Cruz, N.H. Andersen, R.J. Cava page 310

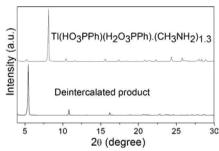


Ba<sub>3</sub>TeCo<sub>3</sub>P<sub>2</sub>O<sub>14</sub>, Pb<sub>3</sub>TeCo<sub>3</sub>P<sub>2</sub>O<sub>14</sub> and Pb<sub>3</sub>TeCo<sub>3</sub>V<sub>2</sub>O<sub>14</sub> exhibit a triangles-of-triangles arrangement of the magnetic cations. Despite the Pb-induced crystallographic distortion, all of these materials exhibit competing antiferromagnetic and ferromagnetic interactions that lead to complex high field magnetism.

Monovalent metal phenylphosphonates and phenylarsonates: Single crystal X-ray structures of  $A(HO_3PPh)(H_2O_3PPh)$  (A = K, Rb, Cs, Tl) and Na( $HO_3AsPh)(H_2O_3AsPh)$  and methylamine intercalation of  $A(HO_3PPh)(H_2O_3PPh)$  (A = Li, Na, K, Tl)

Nitin Balkrushna Padalwar, Chekka Pandu, Kanamaluru Vidyasagar

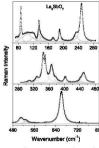
page 321



Amongst  $A(HO_3PPh)(H_2O_3PPh)$  (A= alkali metal, Tl) phenylphosphonates of four structure types, lithium, sodium, potassium and thallium compounds undergo methylamine intercalation.

## Crystal structure of fluorite-related $Ln_3SbO_7$ (Ln = LaDy) ceramics studied by synchrotron X-ray diffraction and Raman scattering

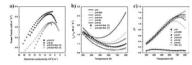
K.P.F. Siqueira, R.M. Borges, E. Granado, L.M. Malard, A.M. de Paula, R.L. Moreira, E.M. Bittar, A. Dias *page 326* 



Raman spectrum for La<sub>3</sub>SbO<sub>7</sub> ceramics showing their 22 phonon modes adjusted through Lorentzian lines. According to synchrotron X-ray diffraction and Raman scattering, this material belongs to the space group *Cmcm*.

### High figure of merit and thermoelectric properties of Bi-doped Mg<sub>2</sub>Si<sub>0.4</sub>Sn<sub>0.6</sub> solid solutions

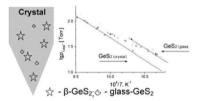
Wei Liu, Qiang Zhang, Kang Ying, Hang Chi, Xiaoyuan Zhou, Xinfeng Tang, Ctirad Uher page 333



- (a) The relationship between electrical conductivity and power factor for Sb/Bi-doped  $Mg_{2.16}(Si_{0.4}Sn_{0.6})_{1-y}(Sb/Bi)_y$  (0 < y = 0.03) solid solutions.
- (b) The correlation between temperature and the combination of the lattice and the bipolar terms of thermal conductivity of  $Mg_{2.16}(Si_{0.4}Sn_{0.6})_{1-y}Bi_y$  (0=y=0.03) solid solutions.
- (c) Temperature dependent dimensionless figure of merit ZT of  $Mg_{2.16}(Si_{0.4}Sn_{0.6})_{1.y}Bi_y$  (0 = y = 0.03) solid solutions.

### A new way of phase identification, of $AgGaGeS_4 \cdot nGeS_2$ crystals

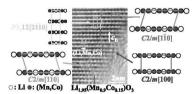
R.E. Nikolaev, I.G. Vasilyeva *page 340* 



 $\lg p-1/T$  dependences of as-grown AgGaGeS<sub>4</sub> · nGeS<sub>2</sub> crystals.

### Electron diffraction and high-resolution electron microscopy studies on layered $\text{Li}_{2-\delta}(Mn_{1-x}Co_x)_{1+\delta}O_3$

Hiroki Fujii, Kiyoshi Ozawa, Takashi Mochiku page 345



An HREM image for  $\text{Li}_{1.95}(\text{Mn}_{0.9}\text{Co}_{0.15})\text{O}_3$  and schematic drawings of C2/m and  $P3_112~\text{Li}_2\text{MnO}_3$  projected along the various zone axes. Each projected unit cell is indicated by rectangles and parallelograms

### Corrigendum

Corrigendum to "Mixed oxides of sodium, antimony (5+) and divalent metals (Ni, Co, Zn or Mg)" [J. Solid State Chem. 183 (2010) 684691]

V.V. Politaev, V.B. Nalbandyan, A.A. Petrenko, I.L. Shukaev, V.A. Volotchaev, B.S. Medvedev *page 192* 

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