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#### **Regular** Articles

Investigation of structural and magnetic properties of nanocrystalline manganese substituted lithium ferrites P.P. Hankare, R.P. Patil, U.B. Sankpal, S.D. Jadhav, P.D. Lokhande, K.M. Jadhav and R. Sasikala *Page 3217* 



The synthesized nanoparticles shapes, sizes and size dispersibilities were obtained from the transmission electron microscopy (TEM). The TEM micrographs of synthesized samples revealed that, spherical shape with average particle size 50 nm. Selected area electron diffraction pattern (SAED) suggests the polycrystallinity and also the formation of spinel ferrites.

#### **Regular** Articles—Continued

#### Composition and structure of acid leached $LiMn_{2-y}Ti_yO_4$ (0.2 $\leq y \leq$ 1.5) spinels

Georgi Avdeev, José Manuel Amarilla, José María Rojo, Kostadin Petrov and Rosa María Rojas *Page 3226* 



Schematic representation of the acid leaching of  $\text{LiMn}_{2-y}\text{Ti}_y\text{O}_4$  (0.2  $\leq$  y  $\leq$  1.0).

Crystal structures and magnetic properties of twodimensional antiferromagnets  $Co_{1-x}Zn_xTeMoO_6$ Yoshihiro Doi, Ryo Suzuki, Yukio Hinatsu and Kenji Ohoyama

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The metal telluromolybdates Co<sub>1-x</sub>Zn<sub>x</sub>TeMoO<sub>6</sub> have an orthorhombic structure with space group  $P2_12_12_2$ . In this structure, M ions form a pseudo-square-planer lattice in the *ab* plane. These compounds show a low-dimensional magnetism reflecting this structural feature. The magnetic transition observed in the CoTeMoO<sub>6</sub> is a canted antiferromagnetic ordering of Co<sup>2+</sup> ions, and the figure is the magnetic structure.

Crystal growth and anisotropic magnetic properties of  $V_3O_7$ C. Li, M. Isobe, H. Ueda, Y. Matsushita and Y. Ueda *Page 3222* 



The temperature dependence of the magnetic susceptibility of  $V_3O_7$  for (H||b) and  $(H\perp b)$ , respectively, at 0.1 T. The inset shows crystals of  $V_3O_7$  grown by using NH<sub>4</sub>Cl as the transport agent.

Continued

Preparation and characterization of Zr doped TiO<sub>2</sub> nanotube arrays on the titanium sheet and their enhanced photocatalytic activity

Haijin Liu, Guoguang Liu and Qingxiang Zhou Page 3238



Zr-doped TiO<sub>2</sub> nanotube arrays were prepared by two-step electrochemical process. The photocatalytic efficiency of  $Zr/TiO_2$  was much better than that of TiO<sub>2</sub> nanotubes under UV irradiation. Nanotube arrays prepared by this method could be reused for more than 20 times and maintained good photocatalytic activities.

Shape-controlled synthesis of gold icosahedra and nanoplates using Pluronic P123 block copolymer and sodium chloride Won-Ki Lee, Sang-Ho Cha, Ki-Hyun Kim, Byung-Woo Kim and Jong-Chan Lee Page 3243



PEO20-PPO70-PEO20, HAuCl4, Aqueous Solution

Gold icosahedra were prepared by heating an aqueous solution of Pluronic P123 and HAuCl<sub>4</sub>. When NaCl was added to this solution, gold nanoplates were produced.  $K_2Ca_6Si_4O_{15}\mbox{--}structural and spectroscopical studies on a mixed tetrahedral-octahedral framework}$ 

E. Arroyabe, R. Kaindl, D.M. Többens and V. Kahlenberg *Page 3254* 



Side view of the whole heteropolyhedral framework in K2Ca6-Si4O15.

### Crystal structure and magnetic properties of Li,Crcontaining molybdates $Li_3Cr(MoO_4)_3$ , $LiCr(MoO_4)_2$ and $Li_{1.8}Cr_{1.2}(MoO_4)_3$

A. Sarapulova, D. Mikhailova, A. Senyshyn and H. Ehrenberg

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Magnetic structure of  $\rm LiCr(MoO_4)_2.$  The orientation of the magnetic moments of  $\rm Cr^{3\,+}$  are shown by arrows.

Molten salt synthesis and localized surface plasmon resonance study of vanadium dioxide nanopowders Fu Wang, Yun Liu and Chun-yan Liu *Page 3249* 



Schematic illustration of the formation mechanism of  $VO_2(M)$  nanoparticles in molten salt, particles size can be controlled by choosing organic carbon sources with different chain length.

New thallium iodates—Synthesis, characterization, and calculations of  $Tl(IO_3)_3$  and  $Tl_4(IO_3)_6$ ,  $[Tl_3^+Tl^{3+}(IO_3)_6]$  Jeongho Yeon, Sang-Hwan Kim and P. Shiv Halasyamani *Page 3269* 



Visualization of the stereo-active lone-pair (purple) through ELFs for  $Tl_4(IO_3)_6$ . The spherical nature of the ELFs around the  $Tl^+$  cation indicates the lone-pair is inert.

### Structural distortions in the spin-gap regime of the quantum antiferromagnet $SrCu_2(BO_3)_2$

C. Vecchini, O. Adamopoulos, L.C. Chapon, A. Lappas, H. Kageyama, Y. Ueda and A. Zorko *Page 3275* 



We report the first crystallographic study within the low-temperature spin-gap region of the two-dimensional frustrated antiferromagnet  $SrCu_2(BO_3)_2$ . Subtle spin-lattice coupling was unveiled in the low-temperature region.

Low temperature molten-salt synthesis of nanocrystalline cubic  $\mathrm{Sr}_2\mathrm{SbMnO}_6$ 

Antara Baral and K.B.R. Varma *Page 3282* 



The as synthesized powders of  $Sr_2SbMnO_6$  calcined at 900 °C/10 h yielded a cubic phase (~60 nm sized crystallites). Centrosymmetric tetragonal (*I4/mcm*) phase was obtained by increasing the calcination temperature to 1000 °C.

## Theoretical investigation of structural stability and lattice vibrations of $U_6Fe_{16}Si_7$ and its interstitial carbide $U_6Fe_{16}Si_7C$

Ping Qian, Qing-Yu Hu and Jiang Shen Page 3289



It is seen from the figure that the first silicon atoms to enter the structure fill a high percentage of the 4a sites, after which, occupation of the 24d sites begin.

## Formation of apatite oxynitrides by the reaction between apatite-type oxide ion conductors, $La_{8+x}Sr_{2-x}(Si/Ge)_6 O_{26+x/2}$ , and ammonia

A. Orera, D. Headspith, D.C. Apperley, M.G. Francesconi and P.R. Slater

Page 3294



In this paper we show that heating the apatite-type electrolytes  $La_{8+x}Sr_{2-x}(Si/Ge)_6O_{26+x/2}$  in NH<sub>3</sub> at high temperatures leads to nitridation of the electrolyte, with the level of nitridation increasing with increasing *x*.

### Electronic structure and photoluminescence properties of $Eu^{2+}$ -activated $Ca_2BN_2F$

Y.Q. Li, C.M. Fang, Y. Fang, A.C.A. Delsing, G. de With and H.T. Hintzen

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Diffuse reflection spectrum, excitation and emission spectra of  $Ca_2BN_2F:Eu^{2+}$ , showing that only the ionic  $Eu^{2+}$  center offers deep blue emission at about 422 nm under excitation at 339 nm.

### Oxidation behaviour of uranium and neptunium in stabilised zirconia

Marcus Walter, Joseph Somers, Daniel Bouëxière, Piotr Gaczyński and Boris Brendebach





The O/U ratio in oxidised  $(Zr,Y,U)O_{2-x}$  depends on the Y/U ratio, whereas O/Np in  $(Zr,Y,Np)O_{2-x}$  correlates with the Y/(Zr + Np)ratio. This indicates that both Zr and Np compete for oxygen vacancies, which hinders the Np oxidation at low Y/Zr ratios.

Continued

## Structural characterization of C–S–H and C–A–S–H samples—Part I: Long-range order investigated by Rietveld analyses

Guillaume Renaudin, Julie Russias, Fabrice Leroux, Fabien Frizon and Céline Cau-dit-Coumes *Page 3312* 



The Tobermorite M model has been successfully used to perform Rietveld analyses on X-ray powder patterns from C–S–H samples. Refinement of the cationic site occupancies explains the evolution from the linear silicate chains to the isolated silicate dimers when increasing the C/S ratio.

# Structural characterization of C–S–H and C–A–S–H samples—Part II: Local environment investigated by spectroscopic analyses

Guillaume Renaudin, Julie Russias, Fabrice Leroux, Céline Cau-dit-Coumes and Fabien Frizon *Page 3320* 



The insertion of aluminum atoms into the C–S–H structure has been investigated by spectroscopic analyses ( $^{27}$ Al and  $^{1}$ H MAS NMR and Raman). The previously determined structural continuity, when increasing the C/S ratio from the C–S–H(I) type to the C–S–H(I) type, has been confirmed even in the presence of aluminum.

# Intercalation of stable organic radicals into layered inorganic host matrices: Preparation and structural characterization of $Cd_{1-x}PS_3(metaMPYNN)_{2x}$

Wilhelm L. Hemme, Wataru Fujita, Kunio Awaga and Hellmut Eckert

#### Page 3330



The orientation of a nitroxide radical relative to the CdPS<sub>3</sub> layers in the corresponding intercalation compound is inferred from x-ray diffraction and solid state NMR spectroscopy.

### Structural and spectroscopic characterization of $Mo_{1-x}W_xO_{3-\delta}$ mixed oxides

S. Morandi, M.C. Paganini, E. Giamello, M. Bini, D. Capsoni, V. Massarotti and G. Ghiotti *Page 3342* 



The combined use of different techniques provides new insight into structural, optical and electronic properties of semiconductor  $Mo_{1-x}W_xO_{3-\delta}$  mixed oxides.

#### Preparation and properties of antiperovskite-type nitrides: InNNi<sub>3</sub> and InNCo<sub>3</sub>

W.H. Cao, B. He, C.Z. Liao, L.H. Yang, L.M. Zeng and C. Dong

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Two ternary nitrides  $InNM_3$  (M=Ni, Co) were synthesized by solid–gas reactions of metal powders with NH<sub>3</sub>. Both InNNi<sub>3</sub> and InNCo<sub>3</sub> adopt the antiperovskite crystal structure, and measurements of magnetization indicate that they have spin-glass-like properties.

## Evidence of local defects in the oxygen excess apatite $La_{9.67}(SiO_4)_6O_{2.5}$ from high resolution neutron powder diffraction

Stéphanie Guillot, Sophie Beaudet-Savignat, Sébastien Lambert, Rose-Noelle Vannier, Pascal Roussel and Florence Porcher





Structural defect position and possible conduction mechanism along the *c*-axis (representation of two adjacent unit-cells).

### Yttrium-succinates coordination polymers: Hydrothermal synthesis, crystal structure and thermal decomposition

Zakariae Amghouz, Laura Roces, Santiago García-Granda, José R. García, Badredine Souhail, Luís Mafra, Fa-nian Shi and João Rocha

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In the field of coordination polymers or MOF's, few studies report on the polymorphs of Ln(III)-succinic acid. Here, we describe the hydrothermal synthesis and structural characterization of two novel yttrium-succinates coordination polymers, respectively 2D and 3D,  $Y_2(C_4H_4O_4)_3(H_2O)_4 \cdot 6H_2O$  and  $Y_2(C_4H_4O_4)_3(H_2O)_2$ .

## Order-disorder transition and valence state of ytterbium in $YbAu_xGa_{2-x}$ (0.26 $\le x \le 1.31$ )

R. Gumeniuk, E. Bischoff, U. Burkhardt, Yu. Prots, W. Schnelle, L. Vasylechko, M. Schmidt, Yu. Kuzma and Yu. Grin

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Ordering of the crystal structure in the YbAu<sub>x</sub>Ga<sub>2-x</sub> is accompanied by the change of valence of Yb atoms.

## Facile synthesis of PbTe nanoparticles and thin films in alkaline aqueous solution at room temperature

Y.Y. Wang, K.F. Cai and X. Yao *Page 3383* 



PbTe nanoparticles and films were fabricated at room temperature and ambient pressure in an alkaline aqueous solution by a chemical bath method.

## Efficient preparation of nanocrystalline anatase $TiO_2$ and $V/TiO_2$ thin layers using microwave drying and/or microwave calcination technique

H. Žabová, J. Sobek, V. Církva, O. Šolcová, Š. Kment and M. Hájek

Page 3387



This study has demonstrated that the synthesis of thin layers may be improved and extended if microwave energy is employed during the preparation process. Microwave processing has the potential to reduce the time, cost and energy input for the production of thin layers.

Enhancement mechanism of field electron emission properties in hybrid carbon nanotubes with tree- and wing-like features G.M. Yang, C.C. Yang, Q. Xu, W.T. Zheng and S. Li *Page 3393* 



Tree-like carbon nanotubes (CNTs) with branches and the winglike CNTs with graphitic-sheets were synthesized by using plasma enhanced chemical vapor deposition. The structural dependence of field electron emission property was also investigated.

### A twofold interpenetrating framework based on the α-metatungstates

Pengpeng Zhang, Jun Peng, Xiaoqing Shen, Zhangang Han, Aixiang Tian, Haijun Pang, Jingquan Sha, Yuan Chen and Min Zhu *Page 3399* 



The 3D + 3D structure representation of the first example of interpenetrating framework based on the isopolytungstate.

# Thermo-Raman spectroscopy *in situ* monitoring study of solid-state synthesis of NiO-Al<sub>2</sub>O<sub>3</sub> nanoparticles and its characterization

Anil Vithal Ghule, Kalyani Ghule, Shin-Hwa Tzing, Tushar H. Punde, Hua Chang and Yong Chien Ling *Page 3406* 



Hyphenation of thermogravimetric analyzer and thermo-Raman spectrophotometer for *in situ* monitoring of solid-state reaction at controlled heating rate and in oxygen atmosphere forming NiO-Al<sub>2</sub>O<sub>3</sub> catalyst nanoparticles is investigated.

#### **Rapid Communication**

## On the solid solution of the spinel phase in the system NiO-Al<sub>2</sub>O<sub>3</sub>

Magnus Rotan, Julian Tolchard, Erling Rytter, Mari-Ann Einarsrud and Tor Grande *Page 3412* 



The degree of inversion in the spinel solid solution in the system  $NiO-Al_2O_3$  has been investigated. The inversion was little influenced by the  $Al_2O_3$  content and decreases with increasing equilibrated temperature. At room temperature the spinel is close to inverse.

#### Author inquiries

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