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Regular Articles

Electromagnetic transport properties and magnetoresistance of $La_{0.7}Ca_{0.2}Sr_{0.1}MnO_3$ -Ag composites prepared by electroless process

C.S. Xiong, Y.F. Cui, Y.H. Xiong, H.L. Pi, X.C. Bao, Q.P. Huang, Y. Zeng, F.F. Wei, C.F. Zheng and J. Zhu *Page 2123*



Magnetic field dependence of the MR for the composites at 298 K. The inset is the different silver-plating time dependence of the variation of MR at 2 T.

Hydrothermal synthesis of antimony oxychloride and oxide nanocrystals: $Sb_4O_5Cl_2$, $Sb_8O_{11}Cl_2$, and Sb_2O_3 Xiang Ying Chen, Hyun Sue Huh and Soon W. Lee *Page 2127*



We described herein a facile solution-phase route to three nanocrystals of antimony oxychlorides and oxides $(Sb_4O_5Cl_2, Sb_8O_{11}Cl_2, and Sb_2O_3)$. In particular, the solvent composition controlled the selective preparation of cubic Sb_2O_3 (senarmontite) and orthorhombic Sb_2O_3 (valentinite).

Regular Articles—Continued

Wet chemical synthesis and photocatalytic activity of potassium niobate $K_6Nb_{10.8}O_{30}$ powders

Gaoke Zhang, Yanjun Hu, Xinmiao Ding, Jin Zhou and Junwei Xie

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The $K_6Nb_{10.8}O_{30}$ powders with TB-type structure were synthesized by a wet chemical method at lower temperature. The particle size of the as-prepared powders is much smaller than that of the sample by obtained solid-state method and its photocatalytic activity is much higher than that of the latter and slightly higher than that of P25-TiO₂.

The effect of nitrogen on the cycling performance in thin-film $Si_{1-x}N_x$ anode

Donggi Ahn, Chunjoong Kim, Joon-Gon Lee and Byungwoo Park *Page 2139*



The Si_{0.76}N_{0.24} thin films showed negligible initial capacity, but an abrupt capacity increase to ~2300 mA h/g after ~650 cycles, followed by excellent cycle-life performance. This abnormal electrochemical behavior was demonstrated to be correlated with the formation of Li₃N and Si₃N₄.

Precipitation of $ALn(CO_3)_2$, xH_2O and $Dy_2(CO_3)_3$, xH_2O compounds from aqueous solutions for $A^+ = Li^+$, Na^+ , K^+ , Cs^+ , NH_4^+ and $Ln^{3+} = La^{3+}$, Nd^{3+} , Eu^{3+} , Dy^{3+} Violaine Philippini, Thomas Vercouter, Annie Chaussé and Pierre Vitorge

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Linear relationships between the ionic radii of the lanthanides and the unit cell parameters of the corresponding $NaLn(CO_3)_2$, xH_2O compounds, extracted from three different studies (our experimental data (black) are compared with those of Mochizuki et al. (red) and Runde et al. (blue)).

Synthesis and study of the crystallographic and magnetic structure of DyFeMnO₅: A new ferrimagnetic oxide M.J. Martínez-Lope, M. Retuerto, J.A. Alonso and V. Pomjakushin *Page 2155*



DyFeMnO₅ is orthorhombic (*Pbam*) as the parent DyMn₂O₅ oxide. The crystal structure contains infinite chains of edge-sharing $Mn^{4+}O_6$ octahedra, interconnected by dimer units of Fe³⁺O₅ square pyramids. It is ferrimagnetic below $T_C \approx 178$ K; a NPD study indicated an antiferromagnetic coupling of the Mn⁴⁺ and Fe³⁺ spins, with Dy³⁺ magnetic moments parallel to those of Fe.

Photoluminescence of Eu^{3+} -doped triple phosphate $Ca_8MgR(PO_4)_7$ (R = La, Gd, Y)

Yanlin Huang, Wanxue Zhao, Yonggang Cao, Kiwan Jang, Ho Sueb Lee, Eunjin Cho and Soung-Soo Yi *Page 2161*



The RT luminescence spectra of Ca₈Mg*R*(PO₄)₇ (*R*=La, Gd, Y) under 254 nm excitation using lamp source with the same conditions. The red emission lines at 612 nm originating from the electric dipole transition ${}^{5}\text{D}_{0}{}^{-7}\text{F}_{2}$ is the dominant luminescence in the spectrum. It is found that the emission intensity of Eu³⁺ ions in Ca₈Mg*R*(PO₄)₇ (*R*=La, Gd, Y) decreases in the sequence of R = Gd > Y > La.

A sodium gadolinium phosphate with two different types of tunnel structure: Synthesis, crystal structure, and optical properties of Na₃GdP₂O₈

M. Fang, W.-D. Cheng, H. Zhang, D. Zhao, W.-L. Zhang and S.-L. Yang *Page 2165*



Projection of the structure of $Na_3GdP_2O_8$ with a unit cell edge along the *b*-axis. The Na–O bonds are omitted for clarity.

Structure and morphology controllable synthesis of Ag/ carbon hybrid with ionic liquid as soft-template and their catalytic properties

Shu Ying Wu, Yun Sheng Ding, Xiao Min Zhang, Hai Ou Tang, Long Chen and Bo Xuan Li *Page 2171*



Monodisperse carbon hollow nanospheres encapsulating Ag nanoparticles and Ag/carbon nanocables were selectively prepared with ionic liquids as the soft-template. The controllable synthesis of Ag/C nano-hybrids was realized by varying the concentration of ionic liquids, reaction temperature, reaction time and the mole ratio of silver nitrate to glucose. The catalysis of Ag/C nano-hybrid in the oxidation of 1-butanol by H_2O_2 was also investigated.

Syntheses, crystal structures and properties of two 1-D cadmium(II) coordination polymers based on 1,1'-(1,3-propanediyl)bis-1H-benzimidazole

Huaixia Yang, Xiangru Meng, Yun Liu, Hongwei Hou, Yaoting Fan and Xiaoqing Shen



Two new Cd(II)-containing complexes have been synthesized and characterized by single-crystal X-ray diffraction. The antimicrobial activity and the non-isothermal kinetics of the thermal decomposition of the polymers were also investigated.

Synthesis and structural investigation of a new oxide fluoride of composition $Ba_2SnO_{2.5}F_3 \cdot xH_2O$ ($x \approx 0.5$) Frank J. Berry, Elaine Moore, Michael Mortimer, Xiaolin Ren, Richard Heap, Peter Slater and Michael F. Thomas

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The K₂NiF₄-type phase Ba₂SnO₄ has been fluorinated at 240 °C using ZnF₂ to give a new oxide fluoride of composition Ba₂SnO_{2.5}F₃ · xH₂O ($x \approx 0.5$). A model in which fluorine occupies both interstitial and apical substitutional sites in the structure of the precursor oxide is supported by spectroscopic and diffraction information, combined with atomistic computer modelling studies.

The role of intermolecular interactions in the assemblies of Fe^{II} and Co^{II} tetrakis-isothiocyanatometalates with tris(1,10-phenanthroline)-Ru^{II}: Crystal structures of two dual-metal assemblies featuring octahedral cationic and tetrahedral anionic modules

Mohamed Ghazzali, Vratislav Langer and Lars Öhrström Page 2191



Side projection in **2** showing the crankshaft caused by $S \cdots S$ interactions in $[Co(NCS)_4]^{2-}$ in-between $[Ru^{II}(phen)_3]^{2+}$ helices. Only isothiocyanates arms of $[Co(NCS)_4]^{2-}$ that are part of $S \cdots S$ interactions are shown and $[Ru^{II}(phen)_3]^{2+}$ are presented as polyhedra.

Synthesis and structure of $[C_6H_{14}N_2][(UO_2)_4(HPO_4)_2(PO_4)_2(H_2O)] \cdot H_2O$: An expanded open-framework amine-bearing uranyl phosphate Travis H. Bray, John D. Gorden and Thomas E. Albrecht-Schmitt *Page 2199*



Packing diagram of the three-dimensional channels and occluded $DABCOH_2^{2^+}$ and water molecules found in $[C_6H_{14}N_2][(UO_2)_4 (HPO_4)_2(PO_4)_2(H_2O)] \cdot H_2O$.

0-D and 1-D inorganic-organic composite polyoxotungstates constructed from in-situ generated monocopper^{II}-**substituted Keggin polyoxoanions and copper**^{II}-**organoamine complexes** Jun-Wei Zhao, Shou-Tian Zheng and Guo-Yu Yang *Page 2205*



A family of inorganic–organic composite polyoxotugstates have been harvested by combination of in-situ generated monocopper^{II}substituted Keggin polyoxoanions and copper^{II}–organoamine complexes based on di-/tri-/hexa-vacant polyoxoanion precursors, CuCl₂·2H₂O and organoamines under hydrothermal conditions and structurally characterized by the elemental analysis, IR spectroscopy, TGA and single-crystal X-ray crystallography.

Structural chemistry and magnetic properties of $Pr_{3-x}Sr_{1+x}CrNiO_8$

Siân E. Dutton, Mona Bahout, Peter D. Battle, Florent Tonus and Valérie Demange

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The n=1 Ruddlesden–Popper system $Pr_{3-x}Sr_{1+x}CrNiO_8$ ($(0.0 < x \le 1.0)$) has been characterized by diffraction methods and magnetometry. There is no evidence of Cr/Ni cation ordering in any composition. The atomic magnetic moments adopt a spin-glass-like state below a transition temperature that decreases from 52 K (x=0.1) to 13 K (x=1.0).

The role of orbital ordering in the tetragonal-to-cubic phase transition in $CuCr_2O_4$

Brendan J. Kennedy and Qingdi Zhou *Page 2227*



The first-order tetragonal–cubic phase transition in $CuCr_2O_4$ is accompanied by a noticeably reduction in cell volume associated with the loss of orbital ordering present in the low-temperature Jahn–Teller distorted tetragonal structure.

Synthesis of nanospherical Fe₃BO₆ anode material for lithium-ion battery by the rheological phase reaction method Xixi Shi, Caixian Chang, Jiangfeng Xiang, Yong Xiao, Liangjie Yuan and Jutang Sun *Page 2231*



Nanospherical Fe₃BO₆ anode material for lithium-ion battery has been synthesized by the rheological phase reaction method. The electrochemical properties of these Fe₃BO₆ nanospheres show that sample synthesized at 800 °C delivers a high reversible capacity above 500 mAh g⁻¹, and sample synthesized at 900 °C possesses relatively good cycleability with a capacity retaining of 376 mAh g⁻¹ after 10 cycles.

Hydrothermal assembly and luminescence property of lanthanide-containing Anderson polyoxometalates

Ying Liu, Shu-Xia Liu, Rui-Ge Cao, Hong-Mei Ji, Shi-Wei Zhang and Yuan-Hang Ren

Page 2237



Two compounds based on Anderson-type polyoxoanion building blocks and rare-earth ions have been synthesized under hydrothermal conditions. Compound 1 exhibits a 2D layer architecture constructed from $[TeMo_6O_{24}]^{6-}$ anions and rare-earth ions Ln^{3+} . Compound 2 displays a 1D chain structure and possesses the intense luminescence property.

Phase formation, structural and microstructural characterization of novel oxynitride-perovskites synthesized by thermal ammonolysis of (Ca,Ba)MoO₄ and (Ca,Ba)MoO₃

D. Logvinovich, M.H. Aguirre, J. Hejtmanek, R. Aguiar, S.G. Ebbinghaus, A. Reller and A. Weidenkaff *Page 2243*



Reactions of $AMoO_4$ and $AMoO_3$ ($A = Ca^{2+}$, Ba^{2+}) oxides with ammonia have been studied at T = 873-1123 K. Orthorhombic CaMoO_{1.7(1)}N_{1.3(1)} (*Pbnm*) and cubic BaMo(O,N)₃ (*Pm*³*m*) were prepared by thermal ammonolysis of the corresponding CaMoO₃ and BaMoO₃ precursors at T = 898 and 998 K, respectively.

The role of the coordination defect: A new structural description of four fluorite-related sesquioxide minerals, bixbyite (Mn_2O_3), braunite (Mn_7SiO_{12}), braunite II ($CaMn_{14}SiO_{24}$), parwelite ($Mn_{10}Sb_2As_2Si_2O_{24}$), and their structural relationships

D.J.M. Bevan and R.L. Martin *Page 2250*



The anion-deficient, fluorite-related structures of the manganesebased minerals bixbyite (Mn₂O₃), braunite (Mn₇SiO₁₂), braunite II (CaMn₁₄SiO₂₄) and parwelite (Mn₁₀Sb₂As₂Si₂O₂₄), are reinterpreted in terms of the Coordination Defect (CD) theory to gain new insights into their structural interrelationships. CDs are extended, defects centred by an anion vacancy and including its immediate atomic environment of 4 tetrahedrally coordinated metals and 6 octahedrally coordinated O atoms: it is represented as $\Box M_4O_6$, where the symbol \Box is the anion vacancy. The arrangement of $\Box M_4$ tetrahedra in bixbyite is shown in the [111] projection.

Polymorphism in PbBiOXO₄ compounds (X = V, P, As). Part I: Crystal structures of α - and β -PbBiOVO₄

Olfa Labidi, Pascal Roussel, Florence Porcher, Michel Drache, Rose-Noëlle Vannier and Jean-Pierre Wignacourt *Page 2260*



Polymorphism in PbBiOXO₄ compounds (X = V, P, As): Part II—PbBiOPO₄ and PbBiOAsO₄ structures and characterization of related solid solutions

Olfa Labidi, Pascal Roussel, Michel Drache, Rose-Noëlle Vannier and Jean-Pierre Wignacourt



 $\alpha \rightarrow \beta$ PbBiOV_{1-x}As_xO₄ composition dependence.

Fabrication and characterization of hexagonal boron nitride powder by spray drying and calcining-nitriding technology Xiaoliang Shi, Sheng Wang, Hua Yang, Xinglong Duan and Xuebin Dong Page 2274



hBN powder was fabricated prepared by spray drying and calcining–nitriding technology. The results indicated that spray drying and calcining–nitriding technology assisted with high-energy ball-milling process following calcined process was a hopeful way to manufacture hBN powder with high crystallinity in industrial scale.

Synthesis and properties of transparent luminescent nanocomposites with surface functionalized semiconductor nanocrystals

Junfang Gao, Yuqin Fu, Xiaodan Lü, Yaying Du, Changli Lü and Zhongmin Su *Page 2279*



Transparent luminescent nanocomposites with Aphen functionalized CdS nanocrystals were synthesized by ligand exchange and insitu bulk polymerization. The functionalized nanocrystals and their polymer nanocomposites possessed strong luminescent emission and can be potentially used to fabricate multifunctional devices with novel photoelectric properties.

Aluminium substitution in iron(II–III)-layered double hydroxides: Formation and cationic order

Christian Ruby, Mustapha Abdelmoula, Rabha Aissa, Ghouti Medjahdi, Michela Brunelli and Michel François *Page 2285*



(a) Crystallographical structure of sulphated green rust: SO_4^2 point to the Fe³⁺ cations (red) that form an ordered array with the Fe²⁺ cations (green). (b) Width and asymmetry of the synchrotron XRD peaks increase rapidly when some Al³⁺ species substitute the Fe³⁺ cations; *z* is molar ratio Al³⁺/Fe³⁺.

Neutron powder diffraction study of the magnetic and crystal structures of $SrFe_2(PO_4)_2$

Alexei A. Belik, Qingzhen Huang, Eiji Takayama-Muromachi and Jeffrey W. Lynn *Page 2292*



Temperature dependence of the intensities of representative magnetic reflections (-101) and $(-1,\frac{1}{2},\frac{1}{2})$ during cooling and heating in SrFe₂(PO₄)₂.

Characterization of CoMCM-41 mesoporous molecular sieves obtained by the microwave irradiation method Tingshun Jiang, Wei Shen, Qian Zhao, Mei Li, Jinyu Chu and Hengbo Yin

Page 2298



CoMCM-41 mesoporous molecular sieves with different amounts of cobalt were synthesized via the microwave irradiation method. The samples were characterized by X-ray diffraction (XRD), Fourier transform infrared (FT-IR), temperature programmed reduction (TPR), transmission electron microscopy (TEM) and N₂ adsorption–desorption technique, and thermal and hydrothermal stabilities of synthesized CoMCM-41 samples were also investigated. The results show that these synthesized materials have typical MCM-41 structure and highly thermal and hydrothermal stabilities.

Structure and phase composition of nanocrystalline $Ce_{1-x}Lu_xO_{2-y}$

Małgorzata A. Małecka, Leszek Kępiński and Mirosław Mączka



Phase separation in nanocrystalline $Ce_{1-x}Lu_xO_{2-y}$ mixed oxide heated in air at 1100 °C.

Crystal structures and polymorphism in compounds $Bi_{6+x}T_{1-x}P_2O_{15+y}$, T = first row transition metals and PbNachiappan Arumugam, Vincent Lynch and Hugo Steinfink Page 2313



View of Bi_{6.24}Cr_{0.09}P₂O_{14.4} perpendicular to [010].

Synthesis and structural investigation of the compounds containing HF_2^- anions: Ca(HF₂)₂, Ba₄F₄(HF₂)(PF₆)₃ and Pb₂F₂(HF₂)(PF₆)

Tina Bunič, Melita Tramšek, Evgeny Goreshnik and Boris Žemva *Page 2318*



Three new compounds $Ca(HF_2)_2$, $Ba_4F_4(HF_2)(PF_6)_3$ and $Pb_2F_2(HF_2)(PF_6)$ were obtained in the system metal(II) fluoride and anhydrous HF acidified with excessive PF_5 and characterized by X-ray single crystal diffraction method and partly by Raman spectroscopy. $Ca(HF_2)_2$ represents the second known compound with homoleptic HF_2^- environment of the central atom.

Synthesis, structure and magnetic properties of A_2 Mn $B'O_6$ (A = Ca, Sr; B' = Sb, Ta) double perovskites

Tapas Kumar Mandal, Viktor V. Poltavets, Mark Croft and Martha Greenblatt

Page 2325



The M vs. H plots for the ordered Sr₂MnSbO₆. The magnetization data at 5K shows hysteresis loop (inset) with a Brillouin-like curvature indicating significant ferromagnetic correlations in the system.

Phase transformation and optical properties of Cu-doped ZnS nanorods

Anuja Datta, Subhendu K. Panda and Subhadra Chaudhuri *Page 2332*



ZnS nanorods doped with 0–15 mol% of Cu has been prepared by simple solvothermal route. Interestingly, phase transformation of the doped ZnS nanorods from wurtzite to cubic was observed with gradual increase in the Cu concentration. Doped ZnS nanorods showed luminescence over a wide range from UV to near IR, which is also a rare observation.



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A survey of more than 1000 of oxygen polyhedrons around caesium ions shows bond lengths ranging from 2.46 to 3.60 Å with 32% of the shortest bonds in the polyhedrons less than 3.00 Å. Coordination numbers from 1 to 12 are observed, in which the average bond lengths increase from 2.714 to 3.323 Å with the coordination, and with a preference for 8, 9 and 10-fold surrounding.

Flux growth and magnetic properties of FeVO₄ single crystals

Zhangzhen He, Jun-Ichi Yamaura and Yutaka Ueda Page 2346



FeVO₄ (I) single crystals are grown by the flux method using V_2O_5 as the self-flux. Magnetic properties are investigated by means of magnetic susceptibility, magnetization, and heat capacity measurements, showing two magnetic phase transitions at ~13 and ~20 K.

Reactivity of metal oxides: Thermal and photochemical dissolution of MO and MFe_2O_4 (M=Ni, Co, Zn) Luis A. García Rodenas, Miguel A. Blesa and Pedro J. Morando

Page 2350



Linear relationships between k_{Me} and k_{-w} are observed. In ferrites, Fe(III) arrests more the reactivity of the more labile ions, thus producing a lower slope.

Direct synthesis of silver/polymer/carbon nanocables via a simple hydrothermal route

Mingshang Jin, Qin Kuang, Zhiyuan Jiang, Tao Xu, Zhaoxiong Xie and Lansun Zheng *Page 2359*



High-yield silver/polymer/carbon coaxial nanocables were synthesized via a one-step simple hydrothermal route by using silver chloride and glucose as precursors. Our experiments indicate that such novel nanostructures formed through the growth mechanism that the silver nanowires grow first, and then glycosidation of glucose occurs on the silver nanowire surfaces, and finally the partial carbonization occurs on the outmost surface of the polymer layer.

Temperature dependence of the cation distribution in $ZnFe_2O_4$ measured with high temperature neutron diffraction

F. Bræstrup, B.C. Hauback and K.K. Hansen *Page 2364*



High temperature in situ neutron powder diffraction, dilatometry and resistivity measurements was performed on the spinel-type oxide ZnFe₂O₄.

Solvothermal syntheses, and characterization of $[Ln(en)_4$ (SbSe₄)] (Ln = Ce, Pr) and $[Ln(en)_4]$ SbSe₄ · 0.5en (Ln = Eu, Gd, Er, Tm, Yb): The effect of lanthanide contraction on the crystal structures of lanthanide selenidoantimonates(V) Dingxian Jia, Aimei Zhu, Qinyan Jin, Yong Zhang and Wenqing Jiang

Page 2370



Two types of lanthanide selenidoantimonates $[Ln(en)_4(SbSe_4)]$ (Ln = Ce, Pr) and $[Ln(en)_4]SbSe_4 \cdot 0.5en$ (Ln = Eu, Gd, Er, Tm, Yb; en = ethylenediamine) have been synthesized under the mild solvothermal conditions, and a systematic investigation of the crystal structures reveals that two types of structural features of these lanthanide selenidoantimonates are related with lanthanides contraction across the lanthanide series.

Hydrothermal syntheses, crystal structures and properties of three coordination frameworks based on a new semirigid ligand and benzenedicarboxylate

Yao-Mei Fu, Ya-Hui Zhao, Ya-Qian Lan, Kui-Zhan Shao, Yong-Qing Qiu, Xiang-Rong Hao and Zhong-Min Su *Page 2378*



Three unprecedented complexes have been constructed from a new semirigid ligand 1,1'-bis(pyridin-3-ylmethyl)-2,2'-biimidazole (L) combined with benzenedicarboxylate isomers and different metal ions under hydrothermal conditions, which exhibit novel topologies. Luminescent properties of L ligand, compounds 1 and 3 are also determined.

Isomorphous substitution of europium for strontium in the structure of synthetic hydroxovanadate

E.I. Get'man, N.V. Yablochkova, S.N. Loboda, V.V. Prisedsky, V.P. Antonovich and N.A. Chivireva

Page 2386 La Pr Nd Sm Eu Gd





Continued

Phase relations in the $K_2W_2O_7$ - K_2WO_4 - KPO_3 - Bi_2O_3 system and structure of $K_{6.5}Bi_{2.5}W_4P_6O_{34}$

K.V. Terebilenko, I.V. Zatovsky, V.N. Baumer, I.V. Ogorodnyk, N.S. Slobodyanik and O.V. Shishkin *Page 2393*



Sandwich-like architecture of $K_{6.5}Bi_{2.5}W_4P_6O_{34}$ prepared during high-temperature investigation of $K_2W_2O_7\text{--}K_2WO_4\text{--}KPO_3$ system. It is organized from $\{K_7Bi_5W_8P_{12}O_{68}\}_\infty$ layers and potassium atom sheets.

One-step synthesis of hydrothermally stable mesoporous aluminosilicates with strong acidity

Dongjiang Yang, Yao Xu, Dong Wu and Yuhan Sun *Page 2401*



Based on the nonsurfactant method, a facile one-step synthesis route has been developed to prepare methyl-modified mesoporous aluminosilicates that possessed hydrothermal stability and strong acidity.

Two unprecedented 1D coordination polymer chains based on tetranuclear copper(II) building blocks

Gaijuan Li, Yan Xing, Shuyan Song, Ning Xu, Xianchun Liu and Zhongmin Su *Page 2406*



Two unprecedented Cu(II) coordination polymers have been prepared by using solvothermal method; they consist of tetrahedral tetranuclear clusters that are bridged by unique Cu(II) atom through the sulfate oxygen to form the infinite one-dimensional polymer chains (a) for complex **1** and (b) for complex **2**.

Computerized crystal-chemical classification of silicates and related materials with CRYSTANA and formula notation for classified structures

Hans-Joachim Klein and Friedrich Liebau Page 2412



The computer program CRYSTANA is described which implements a method for the crystal-chemical classification of silicates and related materials. The implementation is based upon a graphtheoretical formalization of the classification method. An extended notation of crystal-chemical formulas is introduced. The formulas can be derived from the output of the program.

Role of crystallite size on the photoluminescence properties of SrIn₂O₄:Eu³⁺ phosphor synthesized by different methods N. Lakshminarasimhan and U.V. Varadaraju *Page 2418*



Comparison of PL excitation and emission of Eu^{3+} in $SrIn_2O_4$ synthesized by solid state reaction (SSR) and combustion synthesis (CS) methods revealing a decrease in intensity for CS method.

Preparation and characterization of (SBA-15)–La₂O₃ host–guest composite materials

Hui Yu and Qing-Zhou Zhai *Page 2424*



Lanthanum oxide was successfully incorporated into SBA-15 mesoporous molecular sieve via the microwave-assisted synthesis method (MASM) for the first time. The results showed that the preparation of (SBA-15)–La₂O₃ host–guest composite materials by MASM has the advantages of simpler operation, higher efficiency and more plentiful lanthanum oxide can be incorporated into SBA-15 compared with other methods.

New germanates $RCrGeO_5$ (R = Nd-Er, Y): Synthesis, structure, and properties

Roman V. Shpanchenko, Alexander A. Tsirlin, Ekaterina S. Kondakova, Evgeny V. Antipov, Catherine Bougerol, Joke Hadermann, Gustaaf van Tendeloo, Hiroya Sakurai and Eiji Takayama-Muromachi *Page 2433*



Alternating Cr–Cr separations in the chain of edge-sharing CrO_6 octahedra and the constraining effect of the GeO₅ square pyramids in the structures of *R*CrGeO₅.

Consolidated silica glass from nanoparticles

Thomas G. Mayerhöfer, Zhijian Shen, Ekaterina Leonova, Mattias Edén, Antje Kriltz and Jürgen Popp *Page 2442*



We report the preparation of SiO_2 glass by consolidating a highly dispersed silicic acid powder with the Spark Plasma Sintering (SPS) technique. The glass was characterized by ellipsometry, transmission electron microscopy (TEM), infrared reflectance and transmittance spectroscopy, as well as by Raman-, UV–Vis–NIR- and solid-state nuclear magnetic resonance (NMR) spectroscopy.

Yb₃CoSn₆ and Yb₄Mn₂Sn₅: New polar intermetallics with 3D open-framework structures

Xiao-Wu Lei, Guo-Hua Zhong, Min-Jie Li and Jiang-Gao Mao

Page 2448



 Yb_3CoSn_6 and $Yb_4Mn_2Sn_5$ have been prepared and structurally characterized. Yb_3CoSn_6 features a 3D open-framework composed of novel [CoSn₃] layers interconnected by the zigzag Sn chains whereas the anionic substructure of $Yb_4Mn_2Sn_5$ is composed of parallel [Mn_2Sn_2] ladders interconnected by the unusual onedimensional (1D) chains formed by linear [Sn_3] trimers.

Influence of crystal structure on the Co^{II} diffusion behavior in the $Zn_{1-x}Co_xO$ system

M. Peiteado, D. Makovec, M. Villegas and A.C. Caballero *Page 2456*



Maximum diffusion distance for the $ZnO-CoO_x$ couple as a function of temperature. Dashed gray lines represent the temperature values at which the transformations between CoO and Co_3O_4 compounds take place.

Electronic structures and optical properties of wurtzite type LiBSe₂ (B = Al, Ga, In): A first-principles study Long-Hua Li, Jun-Qian Li and Li-Ming Wu Page 2462



The electronic structures and optical properties of wurtzite type $\text{Li}B\text{Se}_2$ (B = Al, Ga, In) have been studied by the DFT calculations. And the correlation of the electronegative of *B* element and the band gap decrease-trend are discussed. The comparison between different calculation methods and the experimental results is presented.

Fabrication of oriented zeolite L monolayer via covalent molecular linkers

Yige Wang, Huanrong Li, Binyuan Liu, Quanying Gan, Qinglin Dong, Gion Calzaferri and Zheng Sun *Page 2469*



1, 4-diisocyanatobutane (DICB) was used as the covalent molecular linker in this study to prepare the uniformly oriented zeolite L monolayer with a relatively high coverage degree and close packing degree. This could be ascribed to substantial amounts of DICB self-assemble and standing on the substrate surface instead of folding up into a U-shape. This point has been further verified by the quality of oriented zeolite L monolayers obtained from the procedure involving DICB, 1, 4-bis (triethoxysilyl) benzene (BTSEB) and 1,2-bis(trimethoxysilyl)ethane (BTMSE) as covalent molecular linkers.

Hyperfine interactions and lattice dynamics of $Sn_{21}O_6Cl_{16}(OH)_{14}$

M.T. Sougrati, S. Jouen, B. Hannoyer and B. Lefez Page 2473



In this study, the tin(II) oxy-hydroxychloride $\text{Sn}_{21}\text{O}_6\text{Cl}_{16}(\text{OH})_{14}$ has been synthesised. The Mössbauer parameters determined at various temperatures are reported and discussed for the first time. At room temperature, the isomer shift and the quadrupole splitting of $\text{Sn}_{21}\text{O}_6\text{Cl}_{16}(\text{OH})_{14}$ are, respectively, $\delta = 3.22 \,\text{mm s}^{-1}$ and $\Delta = 1.71 \,\text{mm s}^{-1}$ and the recoil-free fraction at 300 K is $f_{300} = 0.09 \pm 0.02$.

Structure, bonding and physical properties of tetragonal and orthorhombic SiS₂ from (hybrid) DFT calculations Martijn A. Zwijnenburg, Robert G. Bell and Furio Corà

Page 2480



Periodic DFT calculations were employed to study the (physical) properties of tetragonal and orthorhombic SiS_2 . The results obtained were compared with those for SiS_2 better studied oxide analog silica and demonstrate large changes in the materials' energy landscape, nature of bonding, flexibility and band gap, upon substitution of sulphur for oxygen.

Lanthanide complexes of the monovacant Dawson polyoxotungstate $[\alpha_2-As_2W_{17}O_{61}]^{10-}$ with 1D chain: Synthesis, structures, and photoluminescence properties Xin-Yu Zhao, Shu-Xia Liu, Yuan-Hang Ren, Jian-Fang Cao, Rui-Ge Cao and Kui-Zhan Shao *Page 2488*



Six new lanthanide complexes based on monovacant Dawson-type tungstoarsenates have been synthesized. These complexes are one-dimensional chain-like structures constructed by lanthanide cations and $[\alpha_2-As_2W_{17}O_{61}]^{10-}$ anions. There are three kinds of coordination environment for lanthanide cations. Photoluminescence measurement reveals that **4** and **5** exhibit orange and red fluorescent emission at room temperature, respectively.

Type A–B carbonate chlorapatite synthesized at high pressure

Michael E. Fleet and Xi Liu *Page 2494*



Defect cluster (blue) of A carbonate ion in apatite channel, Na $^+$ cation, and B carbonate ion replacing phosphate group, in carbonate chlorapatite synthesized at high pressure.

Structure and oxide anion conductivity in $Ln_2(TO_4)O$ (Ln = La, Nd; T = Ge, Si)

Laura León-Reina, José M. Porras-Vázquez, Enrique R. Losilla, Laureano Moreno-Real and Miguel A.G. Aranda *Page 2501*



 $Ln_2(TO_4)O$ oxy-silicates and oxy-germanates show ionic conductivities $\sim 10^{-4} \, \mathrm{S \, cm^{-1}}$ at 1173 K with p-type electronic contribution under oxidising conditions. Furthermore, the studied materials are not stable under strongly reducing conditions as shown in the attached figure.

Anchored thiol smectite clay—kinetic and thermodynamic studies of divalent copper and cobalt adsorption Denis Lima Guerra and Claudio Airoldi

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A natural smectite clay sample from Serra de Maicuru, Pará State, Brazil, had aluminum and zirconium polyoxycations inserted within the interlayer space. The precursor and pillarized smectites were organofunctionalized with the silyating agent 3-mercaptopropyltrimethoxysilane. These chemically immobilized clay samples adsorb divalent copper and cobalt cations from aqueous solutions of pH 5.0 at 298 ± 1 K. The Langmuir, Redlich–Peterson and Toth adsorption isotherm models have been applied to fit the experimental data with a nonlinear approach. Hierarchical chlorine-doped rutile TiO₂ spherical clusters of nanorods: Large-scale synthesis and high photocatalytic activity

Hua Xu, Zhi Zheng, Lizhi Zhang, Hailu Zhang and Feng Deng

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Hierarchical chlorine-doped rutile TiO₂ spherical clusters of nanorods photocatalyst were synthesized on a large scale via a soft interface approach. This catalyst showed much higher photocatalytic activity than the famous commercial titania (Degussa P25) under visible light (λ > 420 nm).

Crystal structures and chemistry of double perovskites $Ba_2M(II)M'(VI)O_6$ (M = Ca, Sr, M' = Te, W, U) W.T. Fu, Y.S. Au, S. Akerboom and D.J.W. IJdo *Page 2523*



Evolution of structures as function of temperature in Ba_2SrWO_6 (left) and Ba_2CaWO_6 (right). The existence of two phase region in Ba_2SrWO_6 can be clearly seen by the progressive increase of the rhombohedral $R\bar{3}$ phase marked by asterisk (*).

Structure and magnetic properties of $Ca_2Fe_{1-x}Mn_xAlO_{5+\delta}$ M.D. Carvalho, L.P. Ferreira, J.C. Waerenborgh, E. Tsipis, A.B. Lopes and M. Godinho *Page 2530*



Structure of the Ca₂Fe_{1-x}Mn_xAlO₅ compound and electron diffraction pattern obtained along the [$\overline{1}01$] zone axis (x=0.2), showing a brownmillerite structure.

Synthesis and characterization of a cadmium germanium phosphate CdGe(OH)₃PO₄ with an open framework

Yan Liu, Xiao-Li Yang, Gui-Li Wang, Jun Zhang, Yi-Zhi Li, Hong-Bin Du and Xiao-Zeng You *Page 2542*



A new three-dimensional framework cadmium germanium phosphate, $CdGe(OH)_3PO_4$ was synthesized by solvothermal methods. The framework of $CdGe(OH)_3PO_4$ is built by a mixed network of GeO_6 octahedra, CdO_6 octahedra and PO_4 tetrahedra and contains a network of one-dimensional 3 and 6-membered ring channels. It belongs to a class of metal germanium phosphates with an open framework.

Erratum

Erratum to "Cerium effect on the phase structure, phase stability and redox properties of Ce-doped strontium ferrates" [J. Solid State Chem. 179 (2006) 3406–3419] F. Deganello, L.F. Liotta, A. Longo, M.P. Casaletto and M. Scopelliti

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