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Regular Articles

Structural characterization, thermal, dielectric, vibrational properties and molecular motions in $[C_3N_2H_5]_6[Bi_4Br_{18}]$ A. Piecha, R. Jakubas, A. Pietraszko, J. Baran, W. Medycki and D. Kruk *Page 2949*



 $[C_3N_2H_3]_6[Bi_4Br_{18}]$ has been synthesized and characterized by the X-ray (at 293 and 110 K), calorimetric, dilatometric and dielectric measurements. A crystal structure consists of disordered imidazolium cations and ordered discrete tetramers of $[Bi_4Br_{18}]^{6-}$.

Spin-state transition of iron in $(Ba_{0.5}Sr_{0.5})(Fe_{0.8}Zn_{0.2})O_{3-\delta}$ perovskite

Armin Feldhoff, Julia Martynczuk, Mirko Arnold, Maxym Myndyk, Ingo Bergmann, Vladimir Šepelák, Wolfgang Gruner, Ulrich Vogt, Angelika Hähnel and Jörg Woltersdorf

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At room temperature, the iron in a high-performance perovskite for ceramic oxygen separation membranes is in a mixed valence state of 75% Fe⁴⁺ in the high-spin state and 25% Fe³⁺ predominantly in the low-spin state. When heated to 900 °C, a slight reduction of iron is observed that increases the quantity of Fe³⁺ species. However, the dominant occurrence is a gradual transition in the spin-state of trivalent iron from a mixed low-spin/high-spin to a pure high-spin configuration.

Regular Articles—Continued

 TiO_2 nanoparticles incorporated with $CuInS_2$ clusters: preparation and photocatalytic activity for degradation of 4-nitrophenol

Shi-Zhao Kang, Yi-Kai Yang, Wenbo Bu and Jin Mu Page 2972



Kinetic curves of 4-nitrophenol $(1.44\times 10^{-4}\,mol\,L^{-1})$ degradation under UV irradiation.

Crystal chemistry of anhydrous Li uranyl phosphates and arsenates. II. Tubular fragments and cation-cation interactions in the 3D framework structures of $Li_6[(UO_2)_{12}(PO_4)_8(P_4O_{13})]$, $Li_5[(UO_2)_{13}(AsO_4)_9(As_2O_7)]$, $Li[(UO_2)_4(AsO_4)_3]$ and $Li_3[(UO_2)_7(AsO_4)_5O)]$ Evgeny V. Alekseev, Sergey V. Krivovichev and Wulf Depmeier *Page 2977*



The crystal structures of $Li_5[(UO_2)_{13}(AsO_4)_9(As_2O_7)]$ separated into tubular units and intertubular complexes.

Hydrothermal synthesis of yttria stabilized ZrO₂ nanoparticles in subcritical and supercritical water using a flow reaction system

Hiromichi Hayashi, Akiko Ueda, Atsuko Suino, Kyoko Hiro and Yukiya Hakuta *Page 2985*



Nanoparticles of YSZ can be synthesized in subcritical and supercritical water using a hydrothermal flow reaction system. Given is the TEM image of YSZ nanoparticles.

Heterometallic clusters arising from cubic $Ni_3M'O_4$ (M' = K and Na) entity: Solvothermal synthesis with/without the assistance of microwave

Shu-Hua Zhang, Yan-Ling Zhou, Xiao-Jun Sun, Lian-Qiang Wei, Ming-Hua Zeng and Hong Liang *Page 2991*



Solvothermal reaction assisted with microwave leads to two heterometallic cubic clusters with 6-metallacrown-3 structure $[Ni_3O_3(OH)]$ acting as a host for a K⁺ or Na⁺ ion. The $\{Ni_3M'O_4\}$ (M' = K, Na) cores display dominant ferromagnetic interactions.

Swelling, intercalation, and exfoliation behavior of layered ruthenate derived from layered potassium ruthenate

Katsutoshi Fukuda, Hisato Kato, Jun Sato, Wataru Sugimoto and Yoshio Takasu *Page 2997*



Layered protonic ruthenate derived from a potassium form was directly reacted with bulky tetrabutylammonium ions to trigger exfoliation into nanosheets as long as it is highly hydrated.

Crystal structure, spectroscopy and thermodynamic properties of $M^{I}VWO_{6}(M^{I} - Li, Na)$

Aleksandr V. Knyazev, Miroslaw Maczka, Nataliya N. Smirnova, Lucyna Macalik, Nataliya Yu. Kuznetsova and Irene A. Letyanina *Page 3003*



Fragment of the structure of Li(Na)VWO₆.

Synthesis, thermal stability and magnetic properties of the $Lu_{1-x}La_xMn_2O_5$ solid solution

C. Ma, J.-Q. Yan, K.W. Dennis, R.W. McCallum and X. Tan

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2,4,6-Trimethylpyridinium perchlorate: Polar properties and correlations with molecular structure of organic–inorganic hybrid crystal

M. Wojtaś, A. Gągor, O. Czupiński, A. Pietraszko and R. Jakubas

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A novel organic–inorganic hybrid material, simple ionic salt: 2,4,6trimethylpyridinium perchlorate, $[(CH_3)_3C_5H_2NH][ClO_4]$ has been synthesized. In this paper we report singlecrystal X-ray, powder X-ray, calorimetric, dilatometric, dielectric and pyroelectric studies of this compound over a wide temperature range. A possible mechanism of the structural phase transitions in $[(CH_3)_3C_5H_2NH]$ $[ClO_4]$ is discussed with particular attention focused on unusually strong pyroelectric properties. Structural, magnetic, and thermal characteristics of the phase transitions in $Gd_5Ga_xGe_{4-x}$ magnetocaloric materials Sumohan Misra, Yurij Mozharivskyj,

Alexandra O. Tsokol, Deborah L. Schlagel, Thomas A. Lograsso and Gordon J. Miller *Page 3031*



Phase transformations in $Gd_5Ga_xGe_{4-x}$ magnetocaloric materials as a function of temperature.

Pressure-induced coordination changes in LiBO₂

Li Lei, Duanwei He, Kai He, Jiaqian Qin and Shanmin Wang

Page 3041



Constructing the pressure-temperature phase diagram for LiBO2.

Formation of helix-containing rods in a hybrid inorganic–organic material

Zhanhui Yuan, William Clegg and Martin P. Attfield *Page 3049*



Helical chains of corner-shared *cis*-AlO₄F₂ octahedra form the core of well-separated anionic [Al₂(O₃PCH₂CH₂PO₃)₂F₂]⁴⁻ rods in the novel hybrid aluminum diphosphonate material, (H₄tren)[Al₂ (O₃PCH₂CH₂PO₃)₂F₂]•(H₂O). The incorporation of the organic components into this hybrid material has aided the adoption of a uni-dimensional structure and a specific structural aspect, the helical pitch, within the resulting material, which indicates the potential of this approach to form particular structural features within hybrid materials.

Crystal growth and magnetic behavior of $R_6T_{13-x}Al_xM_y$ phases (R = La, Nd; T = Mn, Fe; M = main group) grown from lanthanide-rich eutectic fluxes

Evan M. Benbow, Naresh S. Dalal and Susan E. Latturner *Page 3055*



 $R_6T_{13-x}Al_xM_y$ phases with the La₆Co₁₁Ga₃ structure type crystallize from La/Ni and Nd/Fe eutectics. Transition metal slabs in La₆Fe_{13-x}Al_xM_y and La₆(Mn/Ni)₁₀Al₃ order antiferromagnetically (T_N 150 K) and ferromagnetically (T_C 200 K), respectively.

Synthesis, structure characterization and fluorescence property of a new fluoride borate crystal, CdZn₂KB₂O₆F Zhi-Wei Jiao, Fan Zhang, Qing-Feng Yan, De-Zhong Shen and Guang-Qiu Shen

Page 3063



Preparation, structure and fluorescence property of a new fluoride borate crystal, $CdZn_2KB_2O_6F$ are descripted. The crystal represents a new structure type in which $ZnBO_3$ layers are connected through bridging fluorine and cadmium atoms alternately to form a 3D open framework.

A 3D porous indium(III) coordination polymer involving *in-situ* ligand synthesis

Zheng-Bo Han, Yong-Juan Song, Jian-Wei Ji, Wei Zhang and Guang-Xi Han

Page 3067



The hydrothermal reaction of In^{3+} and 1,2,4-benzenetricarboxylic acid with the presence of piperazine leads to the generation of a novel 3D porous coordination polymer, $[H_3O][In_2(btc)(bdc)(OH)_2] \cdot 5.5H_2O$, (btc = 1,2,4-benzenetricarboxylate, bdc = 1,4-benzenedicarboxylate).

$Eu_3F_4S_2$: Synthesis, crystal structure, and magnetic properties of the mixed-valent europium(II,III) fluoride sulfide $EuF_2 \cdot (EuFS)_2$

Hagen Grossholz, Ingo Hartenbach, Gunter Kotzyba, Rainer Pöttgen, Henning Trill, Bernd D. Mosel and Thomas Schleid

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Crystal structure and $^{151}\mbox{Eu-M\"ossbauer}$ spectra of mixed-valent $\mbox{Eu}_3\mbox{F}_4\mbox{S}_2.$

Preparation and characterization of mesoporous N-doped and sulfuric acid treated anatase TiO₂ catalysts and their photocatalytic activity under UV and Vis illumination Robert Kun, Sándor Tarján, Albert Oszkó,

Torben Seemann, Volker Zöllmer, Matthias Busse and Imre Dékány

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High pressure induced coordination evolution in chain compound Li_2CuO_2

Shujie You, Zhi Li, Liuxiang Yang, Cheng Dong, Liangcheng Chen, Changqing Jin, Jingzhu Hu, Guoyin Shen and Hokwang Mao *Page 3085*



Li₂CuO₂ undergoes a first-order transition from the ambient orthorhombic to a monoclinic phase at above 5.4 GPa with coordination change from four-square to six-octahedron.

Syntheses and characterization of two oxoborates, $(Pb_3O)_2(BO_3)_2MO_4$ (M = Cr, Mo)

Xuean Chen, Fangping Song, Xinan Chang, Hegui Zang and Weiqiang Xiao *Page 3091*



 $(Pb_3O)_2(BO_3)_2MO_4$ (M=Cr, Mo) are characterized by 1D $^1_{\infty}[Pb_3O]^{4+}$ chains formed by corner-sharing OPb₄ tetrahedra. BO₃ and CrO₄ (MoO₄) groups are located around the chains to hold them together via Pb–O bonds.

Direct low-temperature synthesis of RB_6 (R = Ce, Pr, Nd) nanocubes and nanoparticles

Maofeng Zhang, Xiaoqing Wang, Xianwen Zhang, Pengfei Wang, Shenglin Xiong, Liang Shi and Yitai Qian *Page 3098*



FESEM images of CeB₆ nanocubes prepared at 500 $^{\circ}$ C for 12h using B₂O₃ as boron resource.

Interpenetrating metal-organic frameworks formed by selfassembly of tetrahedral and octahedral building blocks Yong-Ming Lu, Ya-Qian Lan, Yan-Hong Xu, Zhong-Min Su, Shun-Li Li, Hong-Ying Zang and Guang-Juan Xu Page 3105



A series of three-dimensional interpenetrating metal-organic frameworks based on different polygons or polyhedra has been synthesized. The crystal structures and topological analysis of these compounds, along with a systematic investigation of the relationship between topological types and molecular building blocks, will be discussed.

A new material for hydrogen storage; ScAl_{0.8}Mg_{0.2}

Martin Sahlberg, Premysl Beran, Thomas Kollin Nielsen, Yngve Cerenius, Krisztina Kadás, Marko P.J. Punkkinen, Levente Vitos, Olle Eriksson, Torben R. Jensen and Yvonne Andersson

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Hydrogen absorption in ScAl_{0.8}Mg_{0.2} studied by *in situ* synchrotron radiation powder X-ray diffraction. The hydrogen absorption properties were studied by neutron diffraction and quantum mechanical calculations.

Preparation, crystal structure and luminescent properties of the (6,3) type network supramolecular lanthanide picrate complexes with 2,2'-[(1,2-naphthalene)bis(oxy)]bis [N-(phenylmethyl)]acetamide

Qin Wang, Kuan-Zhen Tang, Wei-Sheng Liu, Yu Tang and Min-Yu Tan *Page 3118*



The (6,3) type network supramolecular luminescent lanthanide picrate complexes $\{Ln_2L_3(\text{Pic})_6\}_n$ (L=2,2'-[(1,2-naphthalene)bis(oxy)] bis[N-(phenylmethyl)]acetamide) displaying a two-dimensional honeycomb-like framework have been designed and prepared.

Novel building units with bimetallic rings in inorganic/ organic hybrid chains and layers

Thushitha Mahenthirarajah, Yang Li and Philip Lightfoot *Page 3125*



Hydrothermal synthesis is used to prepare hybrid mixed metal oxides and oxyfluorides with novel extended connectivities.

$Ba_5Ti_{12}Sb_{19+x}$, a polar intermetallic compound with a stuffed γ -brass structure

Haiying Bie and Arthur Mar *Page 3131*



A $\gamma\text{-}\text{brass}$ substructure built up of Ba–Sb clusters is stuffed with planar Ti_9 clusters.

Fabrication and thermoelectric properties of fine-grained TiNiSn compounds

Minmin Zou, Jing-Feng Li, Bing Du, Dawei Liu and Takuji Kita

Page 3138



Nearly single-phased TiNiSn-based half-Heusler compound polycrystalline materials with fine grains were fabricated by combining mechanical alloying (MA) and spark plasma sintering (SPS). A high ZT value for undoped TiNiSn was obtained because of the reduced thermal conductivity.

Flux synthesis of (3,4)-connected zinc phosphites with different framework topologies

Zhien Lin and Stefanie Dehnen Page 3143



Two three-dimensional open-framework zinc phosphites have been synthesized by a phosphorous acid flux method. The two compounds are constructed from $Zn_3(HPO_3)_4$ clusters and have noz and pcu topologies, respectively.

Continued

The effects of doping ferromagnetic spinel $CdCr_2Se_4$ with $Sb^{3\,+}$ ions

E. Malicka, A. Waśkowska, D. Skrzypek, R. Sitko and D. Kaczorowski

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Temperature dependent evolution of the ESR spectrum for the $(Cd_{0.56}Sb_{0.44})[Cr_2]Se_4$ single-crystal showing inhomogeneous nature of the ferromagnetic ordered state below $T_c = 130$ K. At temperature 127 K a fraction of the paramagnetic phase can still be observed.

Synthesis and characterization of copper 4-carboxyphenylphosphonates

Vítězslav Zima, Jan Svoboda, Ludvík Beneš,

Klára Melánová, Miroslava Trchová and Aleš Růžička Page 3155



Three new copper carboxyphenylphosphonates were synthesized. Layered structure of one of them, $CuH(OOCC_6H_4PO_3)$, is composed of CuO_6 octahedra arranged hexagonally around two phosphonate groups, which have their carboxyphenyl groups extending into the space above and below the copper–phosphonate layer.

The d^{10} metal-sulfosalicylate complexes: Herring-bone, ladder and double-stranded chain frameworks with green luminescences

Chun-Feng Yan, Fei-Long Jiang, Lian Chen, Rui Feng, Ming Yang and Mao-Chun Hong *Page 3162*



Reactions of 5-sulfosalicylic acid (H_3L) and d^{10} metal ions (Cd^{II}, Ag^I) produce five new complexes. Complexes **1–4** all display green luminescences at room temperature.

Phase separation in the spin-state transition system of $La_{1-x}Ba_xCoO_3$

Wanju Luo and Fangwei Wang Page 3171



 \boldsymbol{x} dependence of the calculated results from a phase separation model.

Porous cobalt oxide (Co₃O₄) nanorods: Facile syntheses, optical property and application in lithium-ion batteries Rui Xu, Jiawei Wang, Qiuyu Li, Guoving Sun,

Enbo Wang, Siheng Li, Jianmin Gu and Mingliang Ju Page 3177



The porous Co_3O_4 nanorods synthesized via a microemulsionbased method in combination with subsequent calcination were applied in the negative electrode materials for lithium-ion batteries and exhibited high electrochemical performance.

Electronic structure and magnetic properties of RuFe₃N nitride

A.V. dos Santos and C.A. Kuhnen *Page 3183*



Total energy curves, versus lattice spacing for the $RuFe_3N$ nitride. It is observed an energy difference between ferromagnetic and paramagnetic states, which provides high critic pressure.

Carbon-assisted morphological manipulation of CdS nanostructures and their cathodoluminescence properties Meng Zhang, Tianyou Zhai, Xi Wang, Qing Liao, Ying Ma and Jiannian Yao *Page 3188*



A facile and effective carbon-assisted thermal evaporation method is explored to synthesize CdS multipods, nanobrushes and nanocups. These CdS nanostructures display very different optical properties.

Rapid Communications

Density functional study on electronic and optical properties of C (or N)-doped cubic cerium dioxide Yufen Zhang and Xian Zhao Page 3207



By first-principles calculations, it is predicted that substitutional doping of C (or N) in *c*-CeO₂ lowers E_g and also O 2*p*-Ce 4*f* gap, and increases O 2*p*-Ce 4*f* transition intensity.

Structural studies of the phases in Ba₂LaIrO₆—New light on an old problem

Qingdi Zhou, Brendan J. Kennedy, Maxim Avdeev, Lisa Giachini and Justin A. Kimpton *Page 3195*



Variable temperature neutron and synchrotron X-ray powder diffraction methods have been used to resolve the long standing question regarding the symmetry and structure of the cation-ordered perovskite Ba₂LaIrO₆. We show this is monoclinic in I2/m at room temperature, with the sequence of phases $I\overline{1}I2/mR\overline{3}Fm\overline{3}m$.

Synthesis of nanosized silicon particles by a rapid metathesis reaction

C.W. Won, H.H. Nersisyan, H.I. Won and H.H. Lee *Page 3201*



Silicon nanoparticles 37.75 nm in mean diameter was obtained by rapid metathesis reaction performed in Na₂SiF₆ + 4NaN₃ powder bed diluted with NaF.

Three-dimensional (3-D) metal-organic frameworks with 3-pyridin-4-yl-benzoate defining new (3,6)-connected net topologies

Xiu-Juan Jiang, Miao Du, Yan Sun, Jian-Hua Guo and Jin-Shan Li

Page 3211



This work presents a series of 3-D metal-organic frameworks with 3-pyridin-4-yl-benzoate, which display new (3,6)-connected net topologies of $(3.4.5)(3^2.4^4.5^5.6^2.7^2)$ for $Mn^{II}/Zn^{II}/Cd^{II}$ and $(4^2.6)_2(4^4.6^2.8^9)$ for Pb^{II} species.

Corrigendum

Corrigendum to "Polymorphism of the iron doped strontium aluminate SrAl_{1.5}Fe_{0.5}O₄" [Journal of Solid State Chemistry 182 (2009) 1806–1820]

H. Desmoulins, S. Malo, S. Boudin, V. Caignaert and M. Hervieu *Page 3215*

Author inquiries

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