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SOLID STATE CHEMISTRY

CONTENTS

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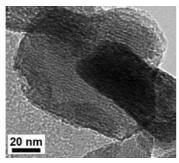
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Regular Articles

Mesoporous mixed metal oxides derived from P123-templated Mg-Al layered double hydroxides

Jun Wang, Jideng Zhou, Zhanshuang Li, Yang He, Shuangshuang Lin, Qi Liu, Milin Zhang and Zhaohua Jiang

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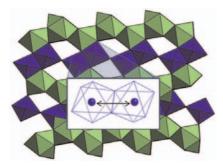


Ordered mesoporous Mg–Al MMOs can be obtained through the calcination of P123-templated Mg–Al–CO₃ LDHs. The pore diameter is 2.2 nm. At the presence of ibuprofen, the Mg–Al MMOs can recover to Mg–Al–IBU LDHs, based on its "remember effect".

The energetics of lanthanum tantalate materials

Tori Z. Forbes, May Nyman, Mark A. Rodriguez and Alexandra Navrotsky

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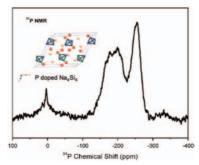


The energetics of three lanthanum tantalates were investigated by the high-temperature oxide melt solution calorimetry. The enthalpies of formation from the oxides were calculated from the enthalpies of drop solution to be $-87.1\pm9.6,\,-94.9\pm8.8,\,\mathrm{and}\,-93.1\pm8.7\,\,\mathrm{kJ/mol}$ for $La_2Ta_2O_7(\mathrm{OH})_2,\,LaTaO_4$ (850 °C), and $LaTaO_4$ (1200 °C), respectively. These results indicate that the intermediate phase, $LaTaO_4$ (850 °C), is the most stable in energy.

Regular Articles—Continued

Synthesis and spectroscopic characterization of P-doped Na_4Si_4

Jialing Wang, Sabyasachi Sen, Ping Yu, Nigel D. Browning and Susan M. Kauzlarich *Page 2522*

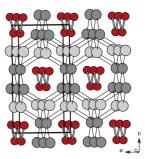


P-doped Na₄Si₄ has been prepared and Raman spectroscopy and ²⁹Si, ²³Na, and ³¹P multinuclear NMR show that P dopes into both crystallographic sites for Si.

A new phase in the system lithium-aluminum: Characterization of orthorhombic Li₂Al

Kati Puhakainen, Magnus Boström, Thomas L. Groy and Ulrich Häussermann

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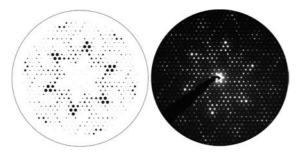


A new phase, Li₂Al, has been discovered in the binary Li–Al system. The structure of orthorhombic Li₂Al is closely related to that of the established monoclinic phase Li₉Al₄.

The new ternary pnictides $Er_{12}Ni_{30}P_{21}$ and $Er_{13}Ni_{25}As_{19}$: Crystal structures and magnetic properties

Stepan Oryshchyn, Volodymyr Babizhetskyy, Olga Zhak, Mariya Zelinska, Jean-Yves Pivan, Viola Duppel, Arndt Simon and Lorenz Kienle

Page 2534

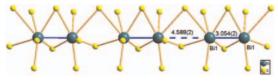


The new ternary pnictides $E_{12}Ni_{30}P_{21}$ and $Er_{13}Ni_{25}As_{19}$ have been synthesized from the elements. They crystallize with hexagonal structures determined from single-crystal X-ray data. The compounds belong to a large family of structures with a metal–metalloid ratio of 2:1. HRTEM investigations were conducted to probe for local ordering of the disordered structure at the nanoscale.

$Bi_3In_4S_{10}$ and $Bi_{14.7}In_{11.3}S_{38}$: Two new bismuth sulfides with interesting Bi-Bi bonding

Wenlong Yin, Dajiang Mei, Jiyong Yao, Peizhen Fu and Yicheng Wu

Page 2544

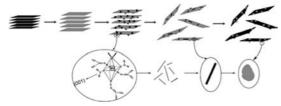


Two new bismuth sulfides $Bi_3In_4S_{10}$ and $Bi_{14.7}In_{11.3}S_{38}$ have been synthesized and characterized. The figure is the arrangement of Bil atoms along the b direction with alternating short and long distances (Å) in $Bi_3In_4S_{10}$.

Facile solvothermal synthesis of graphene-MnOOH nanocomposites

Sheng Chen, Junwu Zhu, Huajie Huang, Guiyu Zeng, Fude Nie and Xin Wang

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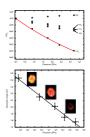


Manganese oxyhydroxide nanocrystals have been successfully attached onto the graphene sheets via an oriented attachment and dissolution-crystallization process, forming a nanocomposite with unusual catalytic capabilities.

Pressure-induced transition in Tl₂MoO₄

Denis Machon, Karen Friese, Tomasz Breczewski and Andrzej Grzechnik

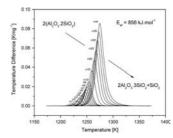
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(up) Structural evolutions of Tl_2MoO_4 in the low-pressure phase. (Down) Optical properties of the high-pressure phase as a function of pressure.

The kinetics of Al-Si spinel phase crystallization from calcined kaolin

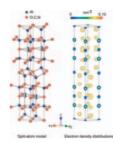
Petr Ptáček, František Šoukal, Tomáš Opravil, Magdaléna Nosková, Jaromír Havlica and Jiří Brandštetr Page 2565



Kinetics of crystallization of Al–Si spinel from calcined kaolin was investigated by the DTA using the Kissinger kinetic approach. The apparent activation energy and morphology parameter of the process is $856\pm2~kJ~mol^{-1}$ and $3.08\pm0.03,$ respectively.

Synthesis and structural characterization of a new aluminum oxycarbonitride, Al₅(O, C, N)₄

Haruya Inuzuka, Motoaki Kaga, Daisuke Urushihara, Hiromi Nakano, Toru Asaka and Koichiro Fukuda *Page 2570*



A new oxycarbonitride discovered in the Al–O–C–N system, $Al_5(O_{1.4}C_{2.1}N_{0.5})$. The crystal is an inversion twin, and hence the structure is represented by a split-atom model. The three-dimensional electron density distributions are determined by the maximum-entropy methods-based pattern fitting, being consistent with the disordered structural model.

Hydrothermal synthesis and electrochemical performance of NiO microspheres with different nanoscale building blocks

Ling Wang, Yanjing Hao, Yan Zhao, Qiongyu Lai and Xiaoyun Xu

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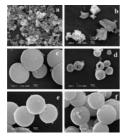


Fig. 5 is the SEM image of NiO that was prepared in the different hydrothermal reaction temperatures. It showed that reaction temperature played a crucial role for the morphology of products.

Series of compositions $Bi_2(M'_xM_{1-x})_4O_9$ (M', M=Al, Ga, Fe; $0 \le x \le 1$) with mullite-type crystal structure: Synthesis, characterization and $^{18}O/^{16}O$ exchange experiment

T. Debnath, C.H. Rüscher, P. Fielitz, S. Ohmann and G. Borchardt

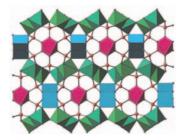
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Fig. Perspective view of the mullite-type ${\rm Bi_2}(M'_xM_{1-x})_4{\rm O_9}$ unit cell $(M',M\!=\!{\rm Al},{\rm Ga},{\rm Fe}).$

Synthesis, structural characterization and Li⁺ ion conductivity of a new vanado-molybdate phase, LiMg₃VMo₂O₁₂

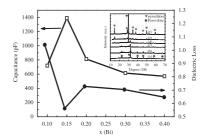
Lisa J. Gillie, Sharon A. de Souza, Denis Sheptyakov, Nik Reeves-McLaren, Denis Pasero and Anthony R. West *Page 2589*



A new vanado-molybdate LiMg $_3$ VMo $_2$ O $_{12}$ has been synthesized and the crystal structure determined. Ionic conductivity measurements show the presence of a phase transition, at 500–600 °C. A large decrease in activation energy for Li $^+$ ion conductivity occurs at the phase transition and the high temperature structure is a good Li $^+$ ion conductor.

Effect of biphase on dielectric properties of Bi-doped lead strontium titanate thin films

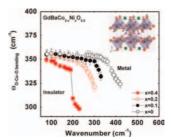
X.T. Li, P.Y. Du, Y.L. Zhao, Y. Tu, J.L. Dai, W.J. Weng, G.R. Han and C.L. Song *Page 2598*



The Bi-doped $Pb_{0.4}Sr_{0.6}TiO_3$ (PST) thin films prepared by the sol-gel method showed a $PST/Bi_2Ti_2O_7$ biphase structure for 0.2 < x < 0.4, and had the low dielectric capacitance and dielectric loss.

Infrared spectroscopic study of the local structural changes across the metal insulator transition in nickel-doped $GdBaCo_2O_{5.5}$

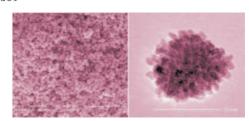
P. Yasodha, M. Premila, A. Bharathi, M.C. Valsakumar, R. Rajaraman and C.S. Sundar *Page 2602*



Softening of the bending mode across $T_{\rm MIT}$.

Controllable fabrication of platinum nanospheres with a polyoxometalate-assisted process

Guoying Sun, Qiuyu Li, Rui Xu, Jianmin Gu, Mingliang Ju and Enbo Wang *Page 2609*

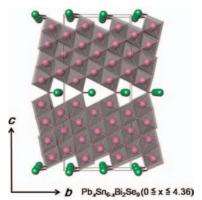


Large-scale Pt nanospheres were synthesized through a polyoxometalate-assisted process, and exhibited good electrocatalytic activity towards the oxidation of methanol, making them promising for applications in fuel cells.

Synthesis and phase width of new quaternary selenides $Pb_xSn_{6-x}Bi_2Se_9$ (x = 0-4.36)

Kuei-Bo Chen and Chi-Shen Lee

Page 2616

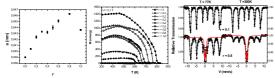


SYNOPSIS TOC New quaternary selenides, $Pb_xSn_{6-x}Bi_2Se_9$ (x = 0–4.36), were synthesized and their structure consisting layers of seven octahedra wide slabs expanding along the direction [0 1 0].

Magnetic dilution of the iron sublattice in $CoFe_{2-x}Sc_xO_4$ $(0 \le x \le 1)$

C. Lefevre, F. Roulland, N. Viart, J.M. Greneche and G. Pourroy

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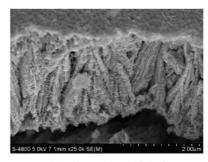


Evolution of the cell parameters, the magnetic properties and the Mössbauer spectra in $CoFe_{2-r}Sc_rO_4$ ($0 \le r \le 1$).

Two-step synthesis of Bi₂Te₃-Te nanoarrays with sheet-rod multiple heterostructure

Yuan Deng, Zhiwei Zhang, Yao Wang, Meng Yang and Rongmin Wang

Page 2631

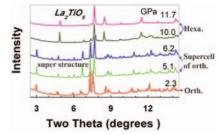


 Bi_2Te_3 —Te arrays with sheet–rod multiple heterostructure were obtained in a large scale using Te nanorod arrays as the in-situ templates under the solvothermal process.

Pressure-induced structural transformations in lanthanide titanates: La₂TiO₅ and Nd₂TiO₅

F.X. Zhang, J.W. Wang, M. Lang, J.M. Zhang and R.C. Ewing

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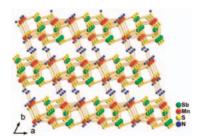


At high pressures, La₂TiO₅ and Nd₂TiO₅ transform from the orthorhombic phase to an $a \times b \times 2c$ superlattice of the orthorhombic structure and then to a hexagonal high-pressure phase.

Hydrazine-hydrothermal method to synthesize threedimensional chalcogenide framework for photocatalytic hydrogen generation

Yi Liu, Pushkar D. Kanhere, Chui Ling Wong, Yuefeng Tian, Yuhua Feng, Freddy Boey, Tom Wu, Hongyu Chen, Tim J. White, Zhong Chen and Qichun Zhang

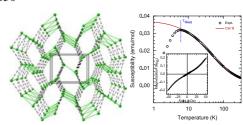
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A novel chalcogenide, $[Mn_2Sb_2S_5(N_2H_4)_3]$ (1), synthesized by hydrazine-hydrothermal method, has a band gap of about $\sim\!2.09$ eV and displays photocatalytic behaviors under visible light irradiation.

Crystal structure and magnetic properties of Na₂Ni^{II}(HPO₃)₂

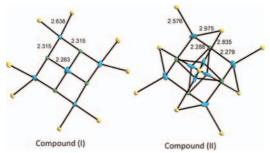
Wassim Maalej, Serge Vilminot, Zakaria Elaoud, Tahar Mhiri and Mohamedally Kurmoo *Page 2650*



The structure of $Na_2Ni(HPO_3)_2$ consists of zig-zag chains of NiO_6 octahedra bridged by two HPO_3^{2-} and the chains are further connected through HPO_3^{2-} to four nearest chains to form a three dimensional framework, delimiting intersecting tunnels in which the sodium ions are located. It orders antiferromagnetically at 6 K.

Dual graphs realized in the compounds di- μ_3 -4-mercaptopyridine catena-di- μ_2 -iodo-di- μ_3 -iodo- μ_4 -iodo penta copper(I) and di- μ_3 -4-mercaptopyridine-di-catena-iodo-di- μ_3 -iodo tri copper(I)

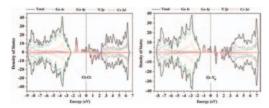
Ehsan Jalilian and Sven Lidin *Page 2656*



A comparison of the central core in both compounds.

Nitrogen vacancy and ferromagnetism in Cr-doped GaN: First-principles calculations

Yanlu Li, Weiliu Fan, Honggang Sun, Xiufeng Cheng, Pan Li, Xian Zhao and Minhua Jiang Page 2662

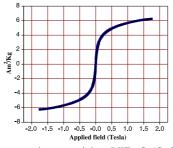


Nitrogen defects and their effect on the ferromagnetism in Cr-doped GaN were investigated by first-principles. Given are the PDOS of $Ga_{36}N_{36}$ with one Cr–Cr pair and one complex of Cr– V_N .

In-situ synthesis of magnetic (NiFe₂O₄/CuO/FeO) nanocomposites

Manish Srivastava, Animesh K. Ojha, S. Chaubey and Jay Singh

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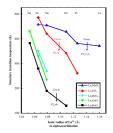
Magnetic nanocomposites containing (NiFe₂O₄/CuO/FeO) phases having particle size ~ 17 nm were synthesized by a sol–gel method. The synthesized nanocomposites exhibit ferromagnetic nature with small value of coercivity.

Hydrothermal crystal growth of the potassium niobate and potassium tantalate family of crystals

Matthew Mann, Summer Jackson and Joseph Kolis *Page 2675*



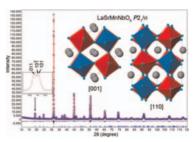
Magnetic properties and structural transitions of orthorhombic fluorite-related compounds Ln_3MO_7 (Ln=rare earths, M=transition metals) Makoto Wakeshima and Yukio Hinatsu Page~2681



Magnetic properties and structural transitions of ternary rare-earth transition-metal oxides Ln_3MO_7 (Ln= rare earths, M= transition metals) were investigated. In this study, we prepared a series of molybdates Ln_3MoO_7 (Ln= La \sim Gd). These compounds show a phase transition from the space group $P2_12_12_1$ to Pnma in the temperature range between 370 and 710 K. Their magnetic properties were characterized by magnetic susceptibility and specific heat measurements from 0.4 to 400 K. The results of Ln_3MoO_7 were compared with the magnetic properties and structural transitions of Ln_3MO_7 (M= Nb, Ru, Sb, Ta, Re, Os, or Ir).

B-site ordered perovskite LaSrMnNbO₆: Synthesis, structure and antiferromagnetism

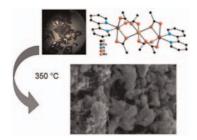
Tao Yang, Tyché Perkisas, Joke Hadermann, Mark Croft, Alexander Ignatov and Martha Greenblatt *Page 2689*



An ordered double perovskite, LaSrMnNbO₆ has been synthesized in the monoclinic space group $P2_1/n$. The Mn²⁺ and Nb⁵⁺ ions, whose valence states are confirmed by X-ray absorption near-edge spectroscopy, are ordered over the *B*-site. The magnetic susceptibility data indicate long-range antiferromagnetic ordering at $T_N = 8$ K.

Heterometallic M/Mn (M = Cu, Co, Zn) acetate complexes as precursors for binary oxides

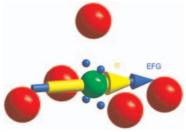
Valeriya G. Makhankova, Oleksiy V. Khavryuchenko, Vladyslav V. Lisnyak, Vladimir N. Kokozay, Viktoriya V. Dyakonenko, Oleg V. Shishkin, Brian W. Skelton and Julia Jezierska *Page 2695*



The novel heterometallic complexes $[M_2Mn(OAc)_6(bpy)_2]$ (M = Cu, Co, Zn, bpy = 2,2'-bipyridyl) were isolated and used as precursors for low-temperature synthesis of binary oxides. Single crystal X-ray diffraction, FTIR, TG/DTA/DTG, TPD-MS, PXRD, SEM/EDX analysis was performed on complexes and powders.

$NdBaFe_2O_{5+\textit{w}}$ and steric effect of Nd on valence mixing and ordering of Fe

J. Lindén and P. Karen *Page 2703*

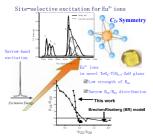


Mössbauer spectrum detects ordering of d_{xz} orbitals of Fe^{II}O₅ via the electric-field gradient (EFG) of the orbital, which makes the main component of the total EFG parallel with the magnetic moment B.

Fluorescence line narrowing spectroscopy of Eu³⁺ in zinc-thallium-tellurite glass

V.P. Tuyen, T. Hayakawa, M. Nogami, J.R-. Duclère and P. Thomas

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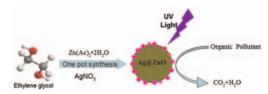


Crystal fields parameters B_{nm} of Eu³⁺ ions (strength, distribution) in novel TeO₂-TlO_{0.5}-ZnO glass system.

One pot synthesis of Ag nanoparticle modified ZnO microspheres in ethylene glycol medium and their enhanced photocatalytic performance

Chungui Tian, Wei Li, Kai Pan, Qi Zhang, Guohui Tian, Wei Zhou and Honggang Fu

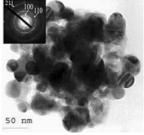
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A "one-pot" strategy was developed for preparing the Ag/ZnO microspheres in ethylene glycol. The composites exhibited superior photocatalytic performance for photodegradation of Rhodamine B dye in water.

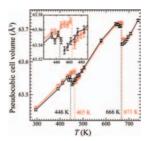
A simple and general route for the preparation of pure and high crystalline nanosized lanthanide silicates with the structure of apatite at low temperature

Stanislav Ferdov, Protima Rauwel, Zhi Lin, Rute A. Sá Ferreira and Augusto Lopes *Page 2726*



A simple one step process for the preparation of the rare earth silicates with the structure of apatite under a mild condition (230 $^{\circ}$ C) is presented. The process is based on the hydrothermal synthesis and the obtained powder materials are pure, high crystalline and with nanosize.

Structural evolution of Na_{0.5}K_{0.5}NbO₃ at high temperatures Nobuo Ishizawa, Jun Wang, Terutoshi Sakakura, Yumi Inagaki and Ken-ichi Kakimoto Page 2731



Changes in pseudocubic cell volume of an $Na_{0.5}N_{0.5}NbO_3$ as a function of temperature; the inset is an enlargement near the transition between the orthorhombic and tetragonal forms.

Corrigendum

Corrigendum to "Synthesis, structures, and phase transitions of barium bismuth iridium oxide perovskites Ba₂BiIrO₆ and Ba₃BiIr₂O₉" [J. Solid State Chem. 183 (2010) 727–735] Chris D. Ling, Brendan J. Kennedy, Qingdi Zhou, Jarrah R. Spencer and Maxim Avdeev *Page 2739*

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