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Regular Articles

Synthesis of morphology-controllable mesoporous Co_3O_4 and CeO_2

Yangang Wang, Yanqin Wang, Jiawen Ren, Yan Mi, Fengyuan Zhang, Changlin Li, Xiaohui Liu, Yun Guo, Yanglong Guo and Guanzhong Lu *Page 277*



Mesoporous Co_3O_4 and CeO_2 with different morphologies, such as micrometer-sized rod, hollow sphere, saucer-like sphere, and solid sphere were synthesized by nanocasting.

$UTa_2O(S_2)_3Cl_6$: A ribbon structure containing a heterobimetallic 5*d*-5*f* M₃ cluster

Daniel M. Wells, George H. Chan, Donald E. Ellis and James A. Ibers *Page 285*



The UTa2O(S2)3Cl6 cluster with completed coordination sphere around uranium.

Regular Articles—Continued

Alkyl group dependence on structure and magnetic properties in layered cobalt coordination polymers containing substituted glutarate ligands and 4,4'-bipyridine Joseph H. Nettleman, Ronald M. Supkowski and Robert L. LaDuca *Page 291*



Five two-dimensional divalent cobalt coordination polymers containing 4,4'-bipyridine (bpy) and substituted or unsubstituted glutarate ligands have been prepared and structurally characterized by single-crystal X-ray diffraction. Three contain dimeric $\{Co_2(CO_2)_2\}$ units, while two manifest $\{Co(CO_2)_n$ chains, depending on the steric bulk of the substituent. The magnetic properties of the complexes were analyzed successfully with a recently developed phenomenological chain model accounting for both magnetic coupling (*J*) and zero-field splitting effects (*D*).

Synthesis and structural characterization of two cobalt phosphites: 1-D (H₃NC₆H₄NH₃)Co(HPO₃)₂ and 2-D (NH₄)₂Co₂(HPO₃)₃

Chi-Chang Cheng, Wei-Kuo Chang, Ray-Kuang Chiang and Sue-Lein Wang

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The 2-D structure of $(NH_4)_2Co_2(HPO_3)_3$ comprises anionic complex sheets with ammonium cations present between them. An anionic complex sheet contains three-deck phosphite units, which are interconnected by dimmeric Co_2O_9 to form complex layers.

Ionothermal syntheses of three transition-metal-containing polyoxotungstate hybrids exhibiting the photocatalytic and electrocatalytic properties

Wei-Lin Chen, Bao-Wang Chen, Hua-Qiao Tan, Yang-Guang Li, Yong-Hui Wang and En-Bo Wang *Page 310*



Three new transition-metal-containing polyoxotungstate hybrids were synthesized successfully under the ionothermal condition, which proves that the ionothermal synthesis is a suitable synthetic method for different kinds of polyoxometalates.

Raman characterization of α - and β -LiFe₅O₈ prepared through a solid-state reaction pathway W. Cook and M. Manley *Page 322*



The disordered, β -phase of lithium ferrite is sustained by air quenching from 900 °C. Shown is a SEM image of β -LiFe₅O₈ exhibiting even particle sizes less than 300 nm.

Non-stoichiometric Fe_xWN_2 : Leaching of Fe from layerstructured $FeWN_2$

Akira Miura, Xiao-Dong Wen, Hideki Abe, Grace Yau and Francis J. DiSalvo *Page 327*



Non-stoichiometric Fe_xWN₂ ($x \sim 0.72$) was synthesized via leaching of Fe from layer-structured stoichiometric FeWN₂ by soaking in sulfuric acid at ca. 50 °C.

Hydrothermal synthesis, structure and properties of a new arsenotungstate

Zhifeng Zhao, Baibin Zhou, Zhanhua Su and Chuncheng Zhu *Page 332*



We report the synthesis, crystal structure and electrochemical and magnetic properties of the new lacunary arsenotungstate substituted simultaneously arsenide fragment and copper complexes.

New oxypnictide superconductors: $PrOFe_{1-x}Co_xAs$ J. Prakash, S.J. Singh, D. Das, S. Patnaik and A.K. Ganguli *Page 338*



Cobalt doping at the iron site in PrOFeAs (semimetal) compound suppresses structural distortion and spin density wave with the evolution of superconductivity. The Seebeck and Hall coefficient (R_H) indicate electron type charge carriers in these compounds and charge carrier density increases with increase in Co-doping. Temperature dependence of resistivity (ρ) for (a) PrOFeAs, (b) PrOFe_{0.95}Co_{0.05}As, (c) PrOFe_{0.9}Co_{0.1}As, (d) PrOFe_{0.85}Co_{0.15}As, (e) PrOFe_{0.8}Co_{0.2}As and (f) PrOFe_{0.7}Co_{0.3}As.

Spin-driven ferroelectricity in the delafossite $CuFe_{1-x}Rh_xO_2$ ($0 \le x \le 0.15$)

E. Pachoud, C. Martin, B. Kundys, Ch. Simon and A. Maignan

Page 344



Polycrystalline samples of the delafossite solid solution Cu-Fe_{1-x}Rh_xO₂ were synthesized and characterized. Polarization has been observed in the range $0.02 < x \le 0.15$ with characteristic temperatures in coincidence with magnetic transition temperatures.

Magnetic relaxation behavior of lanthanide substituted Dawson-type tungstoarsenates

Lizhen Liu, Fengyan Li, Lin Xu, Xizheng Liu and Guanggang Gao

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Two polyoxometalate compounds $[(CH_3)_4N]_8[Ln(H_2O)_8]_2[(\alpha_2-As_2W_{17}O_{61})Ln(H_2O)_2]_2 \cdot nH_2O$ (Ln = Er (1), Dy (2)) have been prepared. The dynamic magnetic measurements for 2 display a slow relaxation of magnetization, showing a frequency-dependent susceptibility.

Solvothermal indium fluoride chemistry: Syntheses and crystal structures of $K_5In_3F_{14}$, β -(NH₄)₃InF₆ and [NH₄]₃[C₆H₂₁N₄]₂[In₄F₂₁]

Anil C.A. Jayasundera, Richard J. Goff, Yang Li, Adrian A. Finch and Philip Lightfoot *Page 356*



Solvothermal synthesis has been used to prepare three indium fluorides, including a novel hybrid material containing a unique $[In_3F_{15}]$ trimer templated by *tren*.

Synthesis, crystal structure, and photocatalytic activity of the new three-layer aurivillius phases, $Bi_2ASrTi_2TaO_{12}$ (A = Bi, La)

Dong Wang, Kaibin Tang, Zhenhua Liang and Huagui Zheng Page 361





Two new three-layer Aurivillius phases $Bi_2ASrTi_2TaO_{12}$ (A=Bi, La) have been synthesized by a conventional solid state reaction method. And this is the crystal structure of the three-layer Aurivillius phases, $Bi_2ASrTi_2TaO_{12}$.

Hydrogenation of palladium rich compounds of aluminium, gallium and indium

H. Kohlmann Page 367



In situ differential scanning calorimetry of the hydrogenation of tetragonal $InPd_3$ (ZrAl₃ type) at 1.3 MPa hydrogen pressure.

A high temperature superionic phase of $CsSn_2F_5$

P. Berastegui, S. Hull and S.G. Eriksson *Page 373*



 $CsSn_2F_5$ is shown to undergo a first order phase transition at $510(2)\,K$ to a superionic phase in which the specific electronic configuration of the Sn^{2+} plays a key role in promoting extensive disorder of the anions.

Structural refinement of $T_2Mo_3O_8$ (T=Mg, Co, Zn and Mn) and anomalous valence of trinuclear molybdenum clusters in $Mn_2Mo_3O_8$

Hideki Abe, Akira Sato, Naohito Tsujii, Takao Furubayashi and Masahiko Shimoda *Page 379*



Trinuclear Mo₃ clusters in Mn₂Mo₃O₈ adopt an anomalous valence of $12-\cong (\cong >0)$ unlike the Mo₃¹²⁺ clusters that are usually recognized for Mo₃-containing inorganic compounds including T_2 Mo₃O₈ (T=Mg, Co or Zn).

Fabrication and electron transport properties of epitaxial films of electron-doped 12CaO · 7Al₂O₃ and 12SrO · 7Al₂O₃ Masashi Miyakawa, Hidenori Hiramatsu, Toshio Kamiya, Masahiro Hirano and Hideo Hosono *Page 385*



Reciprocal space maps around the 408 and the 709 diffractions show the films were grown epitaxially with the orientation relationship of (001)[100] 12SrO·7Al₂O₃ || (001)[100] 12CaO·7Al₂O₃ || (001)[100] Y₃Al₅O₁₂.

Neutron diffraction study of the crystal structure and structural phase transition of $La_{0.7}Ca_{0.3-x}Sr_xCrO_3$ ($0 \le x \le 0.3$) The relationship between thermodynamic behavior and crystal structure changes at the phase transition Kazuki Omoto, Stefan T. Norberg, Steve Hull, Akimitsu Aoto and Takuya Hashimoto *Page 392*



Temperature dependence of parameter, Φ , representing the extent of distortion from the ideal cubic perovskite structure, for La_{0.7}Ca_{0.3}CrO₃ (diamonds) and La_{0.7}Ca_{0.15}Sr_{0.15}CrO₃ (circles) calculated from neutron diffraction patterns.

High-pressure crystal growth and magnetic and electrical properties of the quasi-one dimensional osmium oxide Na₂OsO₄

Y.G. Shi, Y.F. Guo, S. Yu, M. Arai, A.A. Belik, A. Sato, K. Yamaura, E. Takayama-Muromachi, T. Varga and J.F. Mitchell *Page 402*



 Na_2OsO_4 crystals were grown by a NaCl flux method under high pressure. It crystallizes in the Ca_2IrO_4 -type structure comprising infinite $Os^{6+}O_6$ octahedra ($5d^2$) chains. The crystal growth, the crystal structure, and the magnetic and electrical properties are reported.

$LiZnNb_4O_{11.5}$: A novel oxygen deficient compound in the Nb-rich part of the $Li_2O-ZnO-Nb_2O_5$ system

Vladimir A. Morozov, Alla V. Arakcheeva, Vera V. Konovalova, Philip Pattison, Gervais Chapuis, Oleg I. Lebedev, Valery V. Fomichev and Gustaaf Van Tendeloo *Page 408*



LiZnNb₄O_{11.5} with an original α -PbO₂ related structure has been found in the Nb-rich part of Li₂O–ZnO–Nb₂O₅ system and characterized by X-ray diffraction and transition electron microscopy (TEM). Using synchrotron powder diffraction data, the structure has been solved and refined by means of both commensurate modulation and supercell models.

On the symmetry and crystal structures of Ba₂LaIrO₆ W.T. Fu, R.J. Götz and D.J.W. IJdo *Page 419*



Observed (crosses) and calculated (continuous line) profiles of Ba_2LaIrO_6 at some selected temperature showing the region containing the basic (222), (321) and (400) reflections. Tick marks below indicate the positions of the allowed Bragg's reflections.

Cooperative effect of monoclinic distortion and sinusoidal modulation in the martensitic structure of Ni_2FeGa

J.B. Lu, H.X. Yang, H.F. Tian, L.J. Zeng, C. Ma, L. Feng, G.H. Wu, J.Q. Li and J. Jansen

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The structural model of the "5M" Ni₂FeGa martensite viewed along the $[001]_c$ (i.e. $[010]_m$) zone axis, demonstrating the cooperative effect of monoclinic distortion and sinusoidal modulation along the $[110]_c$ direction.

NaAlF₄: Preparation, crystal structure and thermal stability Sergei D. Kirik and Julia N. Zaitseva Page 431



The compound NaAlF₄ was for the first time described 55 years ago, but until now it was not properly studied. Meantime the phase is responsible for the most low-melting part of the NaF–AlF₃ system, which is the great importance for the aluminum production. The lack of information about NaAlF₄ is due to narrow interval of stability which is close to liquid part of the system.

Structural, electronic and optical properties of orthorhombic CdGeO₃ from first principles calculations

C.A. Barboza, J.M. Henriques, E.L. Albuquerque, E.W.S. Caetano, V.N. Freire and J.A.P. da Costa *Page 437*



Different views of the unit cell of orthorhombic CdGeO₃ (left, top). The electronic band structure near the main gap and the partial density of states (PDOS) are shown also (right), as well as the optical absorption for different polarizations of incident light (left, bottom).

Synthesis, structure and theoretical studies of a new ternary non-centrosymmetric β -LaGaS₃

Peng Li, Long-Hua Li, Ling Chen and Li-Ming Wu Page 444



New non-centrosymmeteic ternary lanthanum gallium sulfide, β -LaGaS₃, features the wavy GaS₄ tetrahedron chains that are separated by La³⁺ cations has been synthesized by a solid state reaction. Such an orthorhombic β -LaGaS₃ is isomeric with the monoclinic α -LaGaS₃. Detailed structural differences between the title compound and its isomer, monoclinic α -LaGaS₃, are discussed. The absorption spectra and electronic structures of both types of LaGaS₃ have been calculated with the aid of WIEN2k package as well as the refractive indexes, absorption coefficients and reflectivities. The calculated band gap and absorption edge of β -LaGaS₃ agree well with the experimental measurements. And a weak NLO response of β -LaGaS₃ has been detected.

Homogeneous one-dimensional structured Tb(OH)₃:Eu³⁺ nanorods: Hydrothermal synthesis, energy transfer, and tunable luminescence properties

Jun Yang, Guogang Li, Chong Peng, Chunxia Li, Cuimiao Zhang, Yong Fan, Zhenhe Xu, Ziyong Cheng and Jun Lin *Page 451*





The colors of $Tb(OH)_3$: xEu^{3+} phosphors can be easily tuned from green, yellow, orange, to red due to different energy transfer occurs from Tb^{3+} to Eu^{3+} .

Crystal growth, crystal structure of new polymorphic modification, β -Bi₂B₈O₁₅ and thermal expansion of α -Bi₂B₈O₁₅

R.S. Bubnova, J.V. Alexandrova, S.V. Krivovichev, S.K. Filatov and A.V. Egorysheva *Page 458*



Typical Bi_2O_2 unit in crystal structure of α - and β - $Bi_2B_8O_{15}$.

Crystal growth, structure and magnetic properties of the double perovskites Ln_2 MgIrO₆ (Ln = Pr, Nd, Sm–Gd) Samuel J. Mugavero III, Adam H. Fox, Mark D. Smith and Hans-Conrad zur Loye *Page 465*



A SEM image of a typical crystal of Ln_2 MgIrO₆, which forms in the monoclinic double perovskite structure, is shown.

$Gd_4B_4O_{11}F_2$: Synthesis and crystal structure of a rare-earth fluoride borate exhibiting a new "fundamental building block" in borate chemistry

Almut Haberer, Reinhard Kaindl and Hubert Huppertz Page 471



A new gadolinium fluoride borate $Gd_4B_4O_{11}F_2$ could be synthesized via high-pressure/high-temperature synthesis (multianvil technique). The crystal structure exhibits a structural motif not yet reported from borate chemistry: two BO_4 -tetrahedra (\Box) and two BO_3 -groups (Δ) are connected via common corners, leading to the fundamental building block $2\Delta 2 \Box : \Delta \Box \Box \Delta$.

A novel nanocomposite material prepared by intercalating photoresponsive dendrimers into a layered double hydroxide Toshiyuki Tanaka, Shunsuke Nishimoto, Yoshikazu Kameshima, Junpei Matsukawa, Yasuhiko Fujita, Yutaka Takaguchi, Motohide Matsuda and Michihiro Miyake Page 479



A novel inorganic–organic nanocomposite material, a layered double hydroxide (LDH) containing photoresponsive dendrimers in the interlayer space, was successfully prepared through an ionexchange reaction. The resulting material exhibited unique photochemical properties, compared to those of the bare photoresponsive dendrimer molecule.

Author inquiries

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Multiband orange-red photoluminescence of Eu³⁺ ions in new "114" *Ln*BaZn₃GaO₇ and *Ln*BaZn₃AlO₇ oxides M.P. Saradhi, B. Raveau, V. Caignaert and U.V. Varadaraju *Page 485*



The projected structure consists of alternate stacked layers of Kagomé and Triangular type with statistical distribution of Zn and Ga atoms between two tetrahedral sites. Ba^{2+} present in anticuboctahedron coordinating with 12 oxygen atoms. The Eu^{3+} present in octahedral coordination with 3-fold rotational symmetry.