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Regular Articles

Solution combustion synthesis of calcium zirconate, CaZrO₃, powders Robert Ianoș and Paul Barvinschi *Page 491*



Single-phase CaZrO₃ powder was prepared by low-temperature combustion synthesis. The resulting powder had a BET area of $21.5 \text{ m}^2/\text{g}$. After sintering at 1400 °C for 2 h 95% of the theoretical density was reached.

Regular Articles—Continued

Site preference and vibrational properties of $R_3T_{4+x}Al_{12-x}$ (R = Y, Ce, Gd, U, Th; T = Fe, Ru) Yi Chen, Jiang Shen and Nan-xian Chen *Page 504*



The crystal structure of $R_3T_4Al_{12}$ could be considered as two kinds of layer stacking up along the hexagonal *c* axis. Fe and Ru atoms preferentially substitute for Al atoms at 6*h* site.

Uniform Ln^{3+} (Eu³⁺, Tb³⁺) doped NaLa(WO₄)₂ nanocrystals: Synthesis, characterization, and optical properties

Jun Gu, Yongchun Zhu, Haibo Li, Xianwen Zhang and Yitai Qian

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Uniform shuttle-like $Ln^{3+}(Eu^{3+}, Tb^{3+})$ doped NaLa(WO₄)₂ nanocrystals have been solvothermally synthesized in the mixed solvent of ethylene glycol (EG) and water at 180 °C for 16 h.

Lattice distortions in layered type arsenides $LnTAs_2$ (Ln = La-Nd, Sm, Gd, Tb; T = Ag, Au): Crystal structures, electronic and magnetic properties

D. Rutzinger, C. Bartsch, M. Doerr, H. Rosner, V. Neu, Th. Doert and M. Ruck

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Synthesis, electronic transport and magnetic properties of $Zr_{1-x}Y_xNiSn$, (x = 0–0.25) solid solutions

E.K. Hlil, Yu. Stadnyk, Yu. Gorelenko, L. Romaka, A. Horyń and D. Fruchart *Page 521*



Both approaches experimental and calculations point to the same conclusions. Resistivity and thermopower measurements assert that doping of ZrNiSn based compound by the Y as acceptor impurity induces the insulator-metal transition and leads the *S* value sign reverse.

 $Ca_{3-x}La_xCo_4O_{9+\delta}$ (x=0, 0.3): New cobaltite materials as cathodes for proton conducting solid oxide fuel cell Hamdi Ben Yahia, Fabrice Mauvy and Jean Claude Grenier *Page 527*



Arrehnius plots of the ASR for $Ca_3Co_4O_{9+\delta}$ and $Ca_{2.7}La_{0.3}$ $Co_4O_{9+\delta}.$

On the ammonolysis of Ga_2O_3 : An XRD, neutron diffraction and XAS investigation of the oxygen-rich part of the system Ga_2O_3 -GaN

D. Roehrens, J. Brendt, D. Samuelis and M. Martin *Page 532*



The ammonolysis of β -Ga₂O₃ powders forming GaN at temperatures of 600–780 °C was monitored by means of XRD, neutron diffraction and X-ray absorption spectroscopy in order to identify the possible intermediates and the solubility limit of nitrogen in the oxide lattice.

The transformation of ferrihydrite in the presence of trace Fe(II): The effect of the ammonia, amine and the coordination ions of Fe(III)

Hui Liu, Lijuan Yang, Miaorui Ma, Ping Li and Yu Wei Page 542



Fe(II)-induced transformation of ferrihydrite in the presence of ammonia, amine and coordination ions of Fe(III) was studied. The introduction of the additives favors the formation of goethite.

Single-crystal structures of uranium and neptunium oxychalcogenides AnOQ (An = U, Np; Q = S, Se) Geng Bang Jin, Adam D. Raw, S. Skanthakumar, Richard G. Haire, L. Soderholm and James A. Ibers *Page 547*



View down [010] of the structure of AnOQ.

Single crystal growth and structure of La₄Cu₃MoO₁₂ James A. Enterkin, Paul A. Maggard, Shintaro Ishiwata, Laurence D. Marks, Kenneth R. Poeppelmeier, Masaki Azuma and Mikio Takano *Page 551*



Structural view of a single layer of the triangular lattice of $La_4Cu_3MoO_{12}$ perpendicular to the *b*-axis. The copper atoms are blue, the oxide ions are red and the MoO5 trigonal bipyramids are yellow. The isolated triangular clusters of Cu₃O are outlined by the thin blue lines.

The crystal structures of $Hf_{3\pm\delta}Nb_{4\pm\delta}As_3$ and $Hf_{7,2}Nb_{3,8}As_4$: Members of a homologous series combining W-type, Mg-type and AlB₂-type building blocks Igor Chumak, Piotr Warczok and Klaus W. Richter *Page 557*



 $Hf_{3\pm\delta}Nb_{4\pm\delta}As_3$ (*Pnma*, new structure type) is stabilized by differential fractional site occupation. Its structural relations within a homologous series based on W-type, Mg-type and Al₂B-type building blocks are discussed.

Ternary systems Sr-{Ni,Cu}-Si: Phase equilibria and crystal structure of ternary phases

Navida Nasir, Nataliya Melnychenko-Koblyuk, Andriy Grytsiv, Peter Rogl, Gerald Giester, Jaroslaw Wosik and Gerhard E. Nauer *Page 565*



The crystal structure of $\text{SrNi}_{9-x}\text{Si}_{4+x}$ (own-type, x=2.7, a=0.78998(3), c=1.1337(2) nm; space group P4/nbm) was determined from X-ray single crystal counter to be a low symmetry derivative of the cubic, parent NaZn₁₃-type and is related to CeNi_{8.5}Si_{4.5}-type.

Synthesis, crystal structures and photoluminescent properties of lanthanide supramolecular complexes with 4-oxo-1(4H)-quinolineacetate

Jun Wang, Jun Fan, LiangYu Guo, Xia Yin, ZhiHong Wang and WeiGuang Zhang *Page 575*



The hydrothermal reactions of the oqa molecules with varied lanthanide ions resulted in the formation of five new complexes, which exhibit three typical structure features.

Preparation and up-conversion fluorescence of rare earth $(Er^{3\,+} \mbox{ or } Yb^{3\,+}/Er^{3\,+})\mbox{-doped TiO}_2$ nanobelts

Tianhao Ji, Yang Liu, Hui Zhao, Haiyan Du, Jiayue Sun and Guanglu Ge

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Anatase TiO₂ nanobelts doped with Er^{3+} or $\mathrm{Yb}^{3+}/\mathrm{Er}^{3+}$ cations were simply synthesized using two-step preparation proceedings of ion-exchange and hydrothermal treatment, and their upconversion emissions were also investigated. SEM images of TiO₂ nanobelts (NBs) doped with Er^{3+} (the left) and codoped with $\mathrm{Yb}^{3+}/\mathrm{Er}^{3+}$ (the right).

One-dimensional organic photoconductive nanoribbons built on Zn-Schiff base complex

Li Liu, Ming-Wang Shao and Xiu-Hua Wang Page 590



The Schiff base zinc nanoribbons nanowires exhibited good photoresponse under an incandescent lamp, which indicated their potential application as organic semiconductive or photoconductive nanodevices in the future.

A facile processing way of silica needle arrays with tunable orientation by tube arrays fabrication and etching method Mingwei Zhu, Haigen Gao, Hongwei Li, Jiao Xu and Yanfeng Chen Page 595

Silica needle arrays are fabricated by tube arrays fabrication and etching method. They show super hydrophobic property after being treated with PDMS.

A Facile synthesis of flower-like Co_3O_4 porous spheres for the lithium-ion battery electrode

Jun Zheng, Jing Liu, Dongping Lv, Qin Kuang, Zhiyuan Jiang, Zhaoxiong Xie, Rongbin Huang and Lansun Zheng

Page 600



The flower-like Co_3O_4 porous spheres with hierarchical structure have been successfully prepared via a simple calcination process using cobalt hydroxide as precursor.

Synthesis, crystal structure, and properties of the rhombohedral modification of the thiospinel $CuZr_{1.86(1)}S_4$ Yongkwan Dong, Michael A. McGuire, Hoseop Yun and Francis J. DiSalvo *Page 606*



The projected view of the rhombohedral modification, $CuZr_{1.86(1)}S_4$, down the [100] direction. Large letters denote the packing sequence of the S atoms (yellow circles) along the *c* axis. Zr (black circles) and Cu (red circles) atoms occupy the octahedral and tetrahedral holes, respectively, between close packed S layers.

The effect of low levels of dopants upon the formation and properties of beta-phase molybdenum nitride

A.G. Cairns, J.G. Gallagher, J.S.J. Hargreaves, D. Mckay, J.L. Rico and K. Wilson *Page 613*





Low levels of Pd, Au, Ni and Cu dopant have significant effects upon the morphology, formation and dentitridation characteristics of beta-phase molybdenum nitride.

Luminescence enhancement of Eu^{2+} , Ce^{3+} co-doped $Ba_3Si_5O_{13-\delta}N_{\delta}$ phosphors

Ruili Zhang, Tomonori Maeda, Ryosuke Maruta, Sho Kusaka, Bingjun Ding, Kei-ichiro Murai and Toshihiro Moriga *Page 620*



Emission spectra for $Ba_{3(1-x-y)}Si_5O_{13-\delta}N_{\delta}/xEu^{2+}$, yCe^{3+} ($0 \le x \le 2\%$, $0 \le y \le 2\%$) under the excitation wavelength of 365 nm.

New high permittivity tetragonal tungsten bronze dielectrics $Ba_2LaMNb_4O_{15}$: M = Mn, Fe

Emma E. McCabe and Anthony R. West *Page 624*



Tetragonal tungsten bronze structure of $Ba_2La(Mn, Fe)Nb_4O_{15}$ from two different viewpoints.

Solution precursor synthesis and magnetic properties of $Eu_{1-x}Ca_xTiO_3$

Nathaniel L. Henderson, Xianglin Ke, Peter Schiffer and Raymond E. Schaak

Page 631



Twelve members of the $\text{Eu}_{1-x}\text{Ca}_x\text{TiO}_3$ solid solution $(0 \le x \le 1)$ were synthesized by first forming a homogeneously mixed precursor using a modified sol-gel process, followed by reductive annealing. Samples with $x \le 0.60$ are antiferromagnetic, with T_N decreasing as the level of calcium substitution increases.

Synthesis and structural characterization of Al_4SiC_4 homeotypic aluminum silicon oxycarbide, $[Al_{4.4}Si_{0.6}]$ $[O_{1.0}C_{2.0}]C$

Motoaki Kaga, Tomoyuki Iwata, Hiromi Nakano and Koichiro Fukuda

Page 636



A new oxycarbide discovered in the Al–Si–O–C system, Al_4SiC_4 homeotypic [$Al_{4.4}Si_{0.6}$][$O_{1.0}C_{2.0}$]C. 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.

Enhancement of magnetic ordering temperature in iron substituted ytterbium manganate (YbMn_{1-x}Fe_xO₃) S.L. Samal, T. Magdaleno, K.V. Ramanujachary,

S.E. Lofland and A.K. Ganguli Page 643



Hexagonal manganites of the type YbMn_{1-x}Fe_xO₃; $x \le 0.3$ have been synthesized by the solid state route. The distortion of the MnO₅ polyhedra (tbp) decreases and the Mn–O–Mn bonds in the *a*-*b* plane become shorter with Fe-substitution. The compounds were found to be antiferromagnetic and the ordering temperature T_N increased from 82 K for pure YbMnO₃ to 95 K for YbMn_{0.7} Fe_{0.3}O₃. The increase in the ordering temperature in YbMn_{1-x} Fe_xO₃ is explained on the basis of increase in covalence of Mn/Fe–O–Mn/Fe bonds with iron substitution. Low temperature dielectric measurements show a unique correlation between the magnetic and electric fields for all compositions.

Interactions of $Ba_2YCu_3O_{6+y}$ with the Gd_3NbO_7 buffer layer in coated conductors

W. Wong-Ng, Z. Yang, J.A. Kaduk, L.P. Cook and M. Paranthaman *Page 649*



Crystal structure for $(Gd_xY_{3-x})NbO_7$ showing the partial layered feature. The alternate stacking of distorted NbO₆ octahedra and $(Gd,Y)O_7$ polyhedra are illustrated. The $(Gd,Y)O_8$ polyhedra are omitted for clarity.

$Sr_{10}[(PO_4)_{5.5}(BO_4)_{0.5}](BO_2)$: Growth and crystal structure of a strontium phosphate orthoborate metaborate closely related to the apatite-type crystal structure

Shuang Chen, Stefan Hoffmann, Wilder Carrillo-Cabrera, Lev G. Akselrud, Yurii Prots, Ulrich Schwarz, Jing-Tai Zhao and Rüdiger Kniep *Page 658*



Single crystals of the strontium phosphate orthoborate metaborate, $Sr_{10}[(PO_4)_{5.5}(BO_4)_{0.5}](BO_2)$, were grown from the melt and structurally characterized. The crystal structure is closely related to apatite and contains uncommon linear $[BO_2]^-$ metaborate groups taking positions within the channels running along the three-fold inversion axis.

Kirkendall-effect-based growth of dendrite-shaped CuO hollow micro/nanostructures for lithium-ion battery anodes Yingying Hu, Xintang Huang, Kai Wang, Jinping Liu, Jian Jiang, Ruimin Ding, Xiaoxu Ji and Xin Li Page 662



SEM images of 3D dendrite-shaped CuO hollow micro/nanostructures prepared *via* a Kirkendall-effect-based approach have been shown. The as-prepared CuO electrode exhibited significantly improved cyclability for Li-ion batteries.

Synthesis and crystal structure of CuZrTiO₅—A new crystal structure type

Ulrike Troitzsch, Andrew G. Christy, Anthony C. Willis and David J. Ellis

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The new compound CuZrTiO₅ is orthorhombic ($P2_12_12_1$), with a=3.5871(3) Å, b=6.6968(4) Å, c=14.6679(9) Å. The structure, determined with single crystal XRD, represents a new crystal structure type that is a slight distortion of that of In₂TiO₅ but differs in space group and cation coordination.

Synthesis, structures and magnetic properties of n=3Ruddlesden–Popper compounds $Ca_4Mn_{3-x}Ta_xO_{10}$ $(0 \le x \le 0.3)$

Ping Chai, Xiaojuan Liu, Yao Liu, Minfeng Lv and Jian Meng

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The magnetic structures of $Ca_4Mn_{3-x}Ta_xO_{10}$ transit from G-type AFM to cluster glass state with the intermediate state of FM clusters exhibited in AFM matrix as Ta increasing.

Mixed oxides of sodium, antimony (5+) and divalent metals (Ni, Co, Zn or Mg)

V.V. Politaev, V.B. Nalbandyan, A.A. Petrenko, I.L. Shukaev, V.A. Volotchaev and B.S. Medvedev *Page 684*



It is shown that the powder patterns for Na₃ M_2 SbO₆ (M=Ni and Co) may be equally well described by a trigonal $P3_112$ cell and a monoclinic C2/m cell. In addition, the Ni compound exhibits a series of extremely weak reflections (I<0.3%) that need doubling of the monoclinic c axis, and the final cell is C2/c.

Stability and oxygen-storage characteristics of Al-substituted $YBaCo_4O_{7+\delta}$

Samuli Räsänen, Teruki Motohashi, Hisao Yamauchi and Maarit Karppinen

Page 692



A small amount of aluminum replacing cobalt in YBaCo₄O_{7+ δ} works efficiently for boosting up the phase-decomposition temperature ($T_{\rm D}$), but yet retains the unique low-temperature oxygenstorage characteristics of the phase.

Triple assembly of ZnO, large-scale hollow spherical shells with flower-like species consisting of rods grown on the outer surfaces of shells

Yazhuo Shang, Jun Hu, Honglai Liu and Ying Hu Page 696



A proposed growth mechanism of large scale hollow ZnO. Bubbles provide the aggregation center for ionic liquids that leads to the formation of hollow Zn particle-dotted shells, buoyancy promotes shells to go upward, the breach occurs when shells are subjected to overpressure.

Synthesis and crystal structure of the isotypic rare earth thioborates Ce[BS₃], Pr[BS₃], and Nd[BS₃]

Jens Hunger, Marija Borna and Rüdiger Kniep Page 702



The isotypic orthothioborates Ce[BS₃], Pr[BS₃] and Nd[BS₃] were prepared using different preparation routes. The crystal structure of the title compounds was determined from X-ray powder diffraction data. The crystal structures contain isolated [BS₃]³⁻ groups with boron in trigonal-planar coordination. The sulfur atoms form the vertices of corrugated kagome nets (sketched with blue dotted lines), which are stacked along [100] according to the sequence ABAB. Within these nets every second triangle is occupied by boron and the large hexagons are centered by rare earth ions, which are surrounded by overall nine sulfur species.

Magnetic order and heavy fermion behavior in $CePd_{1+x}Al_{6-x}$: Synthesis, structure, and physical properties Paul H. Tobash, Filip Ronning, J.D. Thompson, Svilen Bobev and Eric D. Bauer *Page 707*



The compound $\text{CePd}_{1+x}\text{Al}_{6-x}$ (x=0.5) has been synthesized and structurally characterized by single-crystal X-ray diffraction. The measured physical properties of temperature and field dependent magnetic susceptibility, specific heat, and electrical resistivity suggests that the compound undergoes ferromagnetic order at *ca*. 2.8 K and further exhibits relatively heavy fermion behavior with a Sommerfeld coefficient of 500 mJ/mol-K2.

Phase formation features in the systems M_2 MoO₄– Fe₂(MoO₄)₃ (M=Rb, Cs) and crystal structures of new double polymolybdates M_3 FeMo₄O₁₅

Klara M. Khal'baeva, Sergey F. Solodovnikov, Elena G. Khaikina, Yuliya M. Kadyrova, Zoya A. Solodovnikova and Olga M. Basovich *Page 712*



Systems M_2 MoO₄-Fe₂(MoO₄)₃ (M = Rb, Cs) are non-quasibinary joins of the systems M_2 O-Fe₂O₃-MoO₃ where new compounds M_3 FeMo₄O₁₅ were revealed. Their structures have diverse mutual arrangements of the adjacent chains of Fe³⁺O₆, MoO₆ and MoO₄ polyhedra.

Structural and physical properties evolution of $BaIr_{1-x}$ Mn_xO₃ solid solutions synthesized by high-pressure sintering J.G. Zhao, L.X. Yang, Y. Yu, F.Y. Li, R.C. Yu and C.Q. Jin

Page 720



The BaRu_{1-x}Mn_xO₃ solid solutions were synthesized by using the solid-state chemical method and high-pressure sintering, and the pressure–composition "phase diagram" at 1000 °C was obtained.

Synthesis, structures, and phase transitions of barium bismuth iridium oxide perovskites Ba₂BiIrO₆ and Ba₃BiIr₂O₉

Chris D. Ling, Brendan J. Kennedy, Qingdi Zhou, Jarrah R. Spencer and Maxim Avdeev *Page 727*



Structure of $Ba_3BiIr_2O_9$ at 300 K. BiO_6 octahedra are purple, IrO_6 octahedra are gold, and Ba atoms are green. Thermal ellipsoids at 90% probability.

In situ generated dense shell-engaged Ostwald ripening: A facile controlled-preparation for $BaFe_{12}O_{19}$ hierarchical hollow fiber arrays

Fang-zhi Mou, Jian-guo Guan, Zhi-gang Sun, Xi-an Fan and Guo-xiu Tong

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This paper described a simple and convenient approach that allows for the facile fabrication of $BaFe_{12}O_{19}$ hierarchical nanotubes or nanotube arrays by a deliberately devised two-step heat-treatment process, in which the dense shells generated in situ during the short-time pre-treatment procedure direct Ostwald ripening of flake-shaped $BaFe_{12}O_{19}$ nanocrystals in the elevated temperature heat-treatment procedure.

Mn₃O₄ nanoplates and nanoparticles: Synthesis, characterization, electrochemical and catalytic properties Khalid Abdelazez Mohamed Ahmed, Qiumei Zeng, Kangbing Wu and Kaixun Huang *Page 744*



 Mn_3O_4 hexagonal nanoplates and nanoparticles were synthesized via a solvent-assisted hydrothermal oxidation process at low temperature and a solvothermal oxidation method, respectively. Their capability of catalytic oxidation of aldehyde at room temperature and atmospheric pressure and electrochemical properties by cyclic voltammogram were compared.

The $A \text{FeO}_2$ (A = K, Rb and Cs) family: A comparative study of structures and structural phase transitions

Naveed Zafar Ali, Jürgen Nuss, Denis Sheptyakov and Martin Jansen

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Reciprocal layer hk0 for the orthorhombic room temperature phase, with pseudo cubic symmetry due to twinning, and the cubic high temperature phase of CsFeO₂. Upon heating the major structural changes are driven by the enhancement of librational motion of the [FeO_{4/2}]⁻ corner-sharing tetrahedra, a phenomenon related to the high/low phase transition of cristobalite.

Continued

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