

CONTENTS

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Regular Articles

The first quaternary lanthanide(III) nitride iodides: Na $M_4N_2I_7$ (M = La-Nd) Christian M. Schurz and Thomas Schleid Page 2253



View at the main structural features of the Na M_4 N₂I₇ series (M = La-Nd): The ${}^{1}_{4} \{ [\text{NM}^{e}_{4/2}]^{3+} \}$ chains, consisting of *trans*-edge connected $[\text{NM}_4]^{9+}$ tetrahedra, and the special kind of iodide anions, namely (17)⁻, form cages, in which isolated $[\text{NaI}_6]^{5-}$ octahedra are embedded.

Predicted energies and structures of β-Ca₃(PO₄)₂ E.E. Jay, E.M. Michie, D. Parfitt, M.J.D. Rushton, S.K. Fong, P.M. Mallinson, B.L. Metcalfe and R.W. Grimes *Page 2261*

One of the 6*a* cation sites of the β - Ca₃(PO₄)₂ structure has previously been described as half occupied. Here, classical static lattice techniques are used to model the different configurations that the Ca ions can exhibit over these Ca(4) 6*a* sites. All possible configurations in the single primitive unit cell and a hexagonal supercell (3_h × 1 × 1) have been generated, along with configurationally averaged structures, that exhibits experimentally reported *R* 3*c* symmetry. The lowest energy configuration of the primitive cell exhibits *R* 3 symmetry. Conversely, the lowest energy configurations derived from the hexagonal supercell cell, which are considerably more stable, exhibit *P* 3₁ and *P* 3₂ symmetries, which are isomorphic supergroups of *R* 3*c*. The implication of these simulations are discussed in terms of refined structural models of the material.

Regular Articles—Continued

Thermal annealing synthesis of titanium-dioxide nanowire-nanoparticle hetero-structures Choongho Yu and Jongbok Park *Page 2268*



Schematic of proposed reaction mechanisms for synthesizing the hetero-structures: (a) TiO_2 nanowires were grown as base structures for capturing $TiCl_4$ gas. (b) $TiCl_4$ gas was oxidized, precipitating crystalline TiO_2 nanoparticles. (c) Repeated particle-incorporation process created tree-like hetero-structures.

Structural investigation of the Cu₂Se–In₂Se₃–Ga₂Se₃ phase diagram, X-ray photoemission and optical properties of the Cu_{1-z}(In_{0.5}Ga_{0.5})_{1 + z/3Se₂ compounds}

M. Souilah, A. Lafond, C. Guillot-Deudon, S. Harel and M. Evain

Page 2274



Pseudo-ternary diagram in the Cu₂Se–In₂Se₃–Ga₂Se₃ system showing the composition of all the synthesized compounds. The crystal structure of the compounds corresponding to red circles are presented in this study.

Single crystal studies on boron-rich τ -borides Ni_{23-x} M_x B₆ (M = Zn, Ga, In, Sn, Ir)—The surprising occurrence of B₄-tetraheda as a normal case?

Dominik Kotzott, Martin Ade and Harald Hillebrecht Page 2281



Crystal structure of τ -Borides $M_{23}B_6$; M1: M_8 -cubes, M2: M_{12} cuboctahedra centred by M3, isolated M-atoms: M4; grey circles: boron, black circles: metal atoms.

New three-dimensional inorganic frameworks based on the uranophane-type sheet in monoamine templated uranylvanadates

Laurent Jouffret, Zhenmian Shao, Murielle Rivenet and Francis Abraham

Page 2290



The various type of PBP pillars P2, P3, P4, and P4' in the threedimensional inorganic frameworks based on the uranophane-type sheet in monoamine templated uranyl-vanadates.

Two 3D network complexes of Y(III) and Ce(III) with 2-fold interpenetration and reversible desorption–adsorption behavior of lattice water

Wenjuan Chu, Yong He, Qinghuan Zhao, Yaoting Fan and Hongwei Hou

Page 2298



Two inorganic–organic 3D network, namely $\{[Ln(L)_{1.5}(H_2O)_2] \cdot 5H_2O\}n [Ln = Y (1), Ce (2)]$, have been prepared under hydrothermal condition and structurally characterized by single-crystal X-ray diffractions. Both 1 and 2 exhibit 3D network structures with 2-fold interpenetration. Interestingly, the reversible desorption–adsorption behavior of lattice water is significantly observed in the two compounds. The result shows their potential application as late-model water absorbent in the field of adsorption material.

Anisotropic compression of a synthetic potassium aluminogermanate zeolite with gismondine topology

Young-Nam Jang, Chi-Chang Kao, Thomas Vogt and Yongjae Lee

Page 2305



High pressure study of a synthetic gismondine zeolite reveals channel-dependent anisotropic compression, i.e., the *b*-axis, normal to the 8-ring channels, is three times more compressible than the *a*- and *c*-axes.

Nano/micro-scaled La(1,3,5-BTC)(H₂O)₆ coordination polymer: Facile morphology-controlled fabrication and color-tunable photoluminescence properties by co-doping Eu^{3+} , Tb^{3+}

Kai Liu, Yuhua Zheng, Guang Jia, Mei Yang, Yanhua Song, Ning Guo and Hongpeng You *Page 2309*



 $La(1,3,5-BTC)(H_2O)_6$ with 3D flowerlike, wheatearlike, spherical, sheaflike, taillike, bundlelike architectures, and 1D nanorods were selectively prepared; color-tunable photoluminescence from red to green was also realized by co-doping Eu³⁺ and Tb³⁺.

Novel correlation of Schottky constants with lattice energies for II–VI and I–VII compounds

Heribert Wiedemeier

Page 2317



For the Zn-chalcogenides, the quantities *n* and *I*_e are 2.007 and 650.3 kcal (2722 kJ), respectively. For the other groups of compounds, they are approximately equal to the formal valences and ionization energies of the metals: $\text{Log } K_{\text{S}} \approx -(2.303nRT)^{-1}$ (0.99 $\Delta H^{\circ}_{\text{T,L}}$ -*I*_e).

Reversible intercalation of ammonia molecules into a layered double hydroxide structure without exchanging nitrate counter-ions

Gregorio Guadalupe Carbajal Arizaga, Fernando Wypych, Felipe Castillón Barraza and Oscar Edel Contreras Lopez *Page 2324*



LDH-nitrate precipitated with ammonia expands the interlayer space if ammonia is bubbled up to pH 10. The basal distance decreased when the compound was heated at 150 °C or stirred in acetone. Nitrate ions are not exchanged.

Crystal structure and physical properties of quaternary clathrates $Ba_8Zn_xGe_{46-x-y}Si_y$, $Ba_8(Zn,Cu)_xGe_{46-x}$ and $Ba_8(Zn,Pd)_xGe_{46-x}$

Navida Nasir, Andriy Grytsiv, Nataliya Melnychenko-Koblyuk, Peter Rogl, Ingeborg Bednar and Ernst Bauer *Page 2329*



Quaternary phase diagram of Ba-Pd-Zn-Ge system at 800 °C.

New ternary rare-earth metal boride carbides $R_{15}B_4C_{14}$ (R = Y, Gd-Lu) containing BC₂ units: Crystal and electronic structures, magnetic properties

Volodymyr Babizhetskyy, Arndt Simon, Hansjürgen Mattausch, Kurt Hiebl and Chong Zheng Page 2343



The ternary rare earth boride carbides $R_{15}B_4C_{14}$ (R=Y, Gd–Lu) were prepared from the elements by arc-melting followed by annealing in silica tubes at 1270 K for 1 month. Tb₁₅B₄C₁₄ is a new member of the rare-earth metal boride carbide series in which the finite quasi-molecular CBC entities as well as isolated C atoms are embedded in the voids of the metal atom matrix. The structure of Tb₁₅B₄C₁₄ contains two types of slabs: one slab contains finite bent CBC units and isolated carbon atoms whereas another is formed only from octahedral coordinated single carbon atoms. The electronic structure for the idealized composition corresponds to an electron partitioning according to (Tb³⁺)₁₅(C⁴⁻)₆(CBC⁵⁻)₄•e⁻ giving rise to a single electron per formula for Tb–Tb framework bonding. The magnetism of the ternary rare earth boride carbides $R_{15}B_4C_{14}$ (R=Tb, Dy, Er) is characterized by the onset of ferromagnetic order below T < 150 K.

Synthesis, crystal structure and thermal behavior of Sr₃B₂SiO₈ borosilicate

M.G. Krzhizhanovskaya, R.S. Bubnova, S.V. Krivovichev, O.L. Belousova and S.K. Filatov *Page 2352*



A fragment of $Sr_3B_2SiO_8$ structure showing isolated B,Si–O pseudo-chain and Sr atom ellipsoids, comparing with pole figure of thermal expansion coefficients.

Cetyltrimethylammonium bromide assisted self-assembly of NiTe₂ nanoflakes: Nanoflake arrays and their photoluminescence properties

Ling Jiang, Ying-Jie Zhu and Jing-Biao Cui Page 2358



 $NiTe_2$ nanoflakes and their self-assembled nanoflake arrays have been prepared by a single-step hydrothermal method using $Ni(CH_3COO)_2 \cdot 4H_2O$, Na_2TeO_3 , glucose, and cetyltrimethylammonium bromide (CTAB).

Thermoluminescence and synchrotron radiation studies on the persistent luminescence of $BaAl_2O_4$: Eu^{2+} , Dy^{3+}

L.C.V. Rodrigues, R. Stefani, H.F. Brito,

M.C.F.C. Felinto, J. Hölsä, M. Lastusaari, T. Laamanen and M. Malkamäki

Page 2365



BaAl₂O₄:Eu²⁺,Dy³⁺ phosphors: Thermoluminescence glow curve and synchrotron radiation spectra. Persistent luminescence photographs obtained after ceased UV irradiation.

Structure alterations in microporous (Mg,Fe)₂Al₄Si₅O₁₈ crystals induced by energetic heavy-ion irradiation

Ronald Miletich, G. Diego Gatta, Günther J. Redhammer, Michael Burchard, Hans-Peter Meyer, Christian Weikusat, Nicola Rotiroti, Ulrich A. Glasmacher,

Christina Trautmann and Reinhard Neumann Page 2372



Cordierite single-crystal specimen showing the color change from pale blue (unirradiated) to a yellowish brown layer (irradiated) after exposure to relativistic ¹²⁴Xe ions at a fluence of 1×10^{12} ions per cm².

Simple synthesis of ultra-long Ag₂Te nanowires through solvothermal co-reduction method

Feng Xiao, Gang Chen, Qun Wang, Lin Wang, Jian Pei and Nan Zhou

Page 2382



Ultra-long single crystal β -Ag₂Te nanowires with the diameter of about 300 nm were fabricated by the solvothermal route in ethylene glycol (EG) system without any template. The diagram displays the variation of the phases and morphologies of products with different reaction time.

Role of surface hydroxyl groups in promoting room temperature CO sensing by Pd-modified nanocrystalline SnO₂

Artem V. Marikutsa, Marina N. Rumyantseva, Lada V. Yashina and Alexander M. Gaskov *Page 2389*



Nanocrystalline SnO_2 modified by PdO/Pd clusters exhibit high CO sensitivity at room temperature. An extensive study revealed surface OH-groups participation in CO oxidation on SnO_2 leading to enhanced sensitivity at low operating temperature (25–150 °C). PdO/Pd clusters supposedly initiate a chain of CO reactions with surface hydroxyls.

A primitive tetragonal intermediate in the orthorhombic–cubic phase transition of perovskite-type strontium niobate $Sr_{0.92}NbO_3$

René B. Macquart, Brendan J. Kennedy and Maxim Avdeev *Page 2400*



Variable temperature powder neutron diffraction measurements reveal that $Sr_{0.92}NbO3$ undergoes a sequence of phase transitions $Pnma \rightarrow P4/mbm \rightarrow Pm3m$ with unanticipated softening of the *M* point rather than *R* point resulting in the formation of the primitive tetragonal intermediate.

In[NC₅H₃(CO₂)₂](OH₂)F: A new layered indium-organic framework material (NC₅H₃(CO₂)₂ = 2,6pyridinedicarboxylate)

Min Kyung Kim, Dong Woo Lee and Kang Min Ok *Page 2406*



Wire representation exhibiting 2,6-pyridinedicarboxylate groups that are packed parallel.

Solid-state syntheses, crystal structures and properties of two novel metal sulfur chlorides—Zn₆S₅Cl₂ and Hg₃ZnS₂Cl₄ Wen-Tong Chen, Han-Mao Kuang and Hua-Long Chen *Page 2411*



Two novel compounds were synthesized via solid-state reactions. One is the first example of ternary zinc–Q–X chalcogenides and the other is the first example of quaternary IIB–Q–X metal chalcogenides.

Ion-beam irradiation of lanthanum compounds in the systems La_2O_3 -Al_2O_3 and La_2O_3 -TiO₂

Karl R. Whittle, Gregory R. Lumpkin, Mark G. Blackford, Robert D. Aughterson, Katherine L. Smith and Nestor J. Zaluzec *Page 2416*



 $La_2 TiO_5$ with atypical co-ordination for Ti, TiO_5 is found to be different in radiation resistance to $La_2 Ti_2 O_7$ and $La_{2/3} TiO_3$. Irradiation of La–Ti–O, and La–Al–O based systems has found that radiation damage resistance is related to the ability of the system to disorder.

A one-pot synthetic approach to prepare palladium nanoparticles embedded hierarchically porous TiO₂ hollow spheres for hydrogen peroxide sensing

Lirong Kong, Xiaofeng Lu, Xiujie Bian, Wanjin Zhang and Ce Wang

Page 2421



A new one-step solvothermal method was developed to prepare Pd nanoparticles embedded hierarchically porous TiO₂ hollow spheres. Due to its unique nanostructure, the prepared TiO₂/Pd modified GC electrode exhibit a high sensitivity (226.72 μ A mM⁻¹ cm⁻²), a relatively low reduction potential (-0.2 V), a fast response time (<3 s) and a relatively low detection limit of 3.81 μ M (*S*/*N*=3) towards H₂O₂.

Oxygen-permeable membranes based on partially *B*-site substituted $BaFe_{1-y}M_yO_{3-\delta}$ (*M* = Cu or Ni) Tetsuya Kida, Atsunori Yamasaki, Ken Watanabe, Noboru Yamazoe and Kengo Shimanoe *Page 2426*



Partially Cu-substituted $BaFe_{1-y}Cu_yO_{3-\delta}$ (y=0.1-0.15) membranes exhibit high oxygen permeation fluxes at intermediate high temperatures (700–930 °C) under an air/He gradient, due to the stabilization of the cubic perovskite phase by the substitution.

Eu doping effects on structural and magnetic properties of $(Sr_{2-x}Eu_x)FeMoO_6$ compounds

Q. Zhang, Y.G. Xiao, Z.F. Xu, G.Y. Liu, J.B. Li and G.H. Rao

Page 2432



Temperature dependence of saturation magnetization of $(Sr_{1.8}Eu_{0.2})FeMoO_6$ (filled circle) and $(Sr_{1.8}Nd_{0.2})FeMoO_6$ (open circle).

Preparation of nanodispersed titania using stabilized ammonium nitrate melts

Monica Raciulete, Anna Kachina, Eric Puzenat and Pavel Afanasiev

Page 2438



Ammonium nitrate melts stabilized by nitrogen-containing organic molecules can be applied for expedite one-step preparation of highly dispersed oxides, as exemplified by synthesis of titania photocatalysts.

Annealing effects on the structure, photoluminescence, and magnetic properties of GaN/Mn₃O₄ core–shell nanowires Hyo Sung Kim, Han Gil Na, Ju Chan Yang,

Jong Hoon Jung, Yong Sung Koo, Nam Jung Hur and Hyoun Woo Kim

Page 2445



Novel GaN/Mn_3O_4 core-shell nanowires were synthesized and the effects of thermal annealing on the structure, photoluminescence, and magnetic properties were investigated.

Micro-Raman analysis of titanium oxide/carbon nanotubesbased nanocomposites for hydrogen sensing applications

S. Santangelo, G. Messina, G. Faggio, A. Donato, L. De Luca, N. Donato, A. Bonavita and G. Neri *Page 2451*



Micro-Raman analysis of TiO₂/CNTs and Pt/TiO₂/CNTs hybrids for H₂ sensing applications evidences that regardless of C/Ti molar ratio titania crystallizes in the anatase phase. The very small size of TiO₂ crystallites (4.3–5.0 nm) is responsible for the observed phonon confinement effects.

Microstructure and electrical-optical properties of cesium tungsten oxides synthesized by solvothermal reaction followed by ammonia annealing

Jing-Xiao Liu, Yoshihiko Ando, Xiao-Li Dong, Fei Shi, Shu Yin, Kenji Adachi, Takeshi Chonan, Akikazu Tanaka and Tsugio Sato

Page 2456



Cesium tungsten oxides (Cs_xWO_3) with different morphology were synthesized by solvothermal reaction, and the effects of post-ammonia annealing on the microstructure and electrical–optical properties were investigated.

The anti-perovskite type hydride InPd₃H_{0.89}

H. Kohlmann, A.V. Skripov, A.V. Soloninin and T.J. Udovic

Page 2461



Hydrogen induces a rearrangement in $InPd_3$ from a ZrAl₃ type structure to a cubic AuCu₃ type structure, thus forming an antiperovskite type hydride $InPd_3H_{0.89}$

Microwave hydrothermal synthesis and photocatalytic activity of AgIn₅S₈ for the degradation of dye

Wenjuan Zhang, Danzhen Li, Meng Sun, Yu Shao, Zhixin Chen, Guangcan Xiao and Xianzhi Fu *Page 2466*



Compared with $TiO_{2-x}N_x$, $AgIn_5S_8$ has exhibited a superior activity under the same condition.

Synthesis, structure, solid-state thermolysis, and thermodynamic properties of new heterometallic complex Li₂Co₂(Piv)₆(NEt₃)₂

Zn.V. Dobrohotova, A.A. Sidorov, M.A. Kiskin, G.G. Aleksandrov, K.S. Gavrichev, A.V. Tyurin, A.L. Emelina, M.A. Bykov, A.S. Bogomyakov, I.P. Malkerova, A.S. Alihanian, V.M. Novotortsev and I.L. Eremenko *Page 2475*



The solid-state thermolysis, study of the vaporization process, and temperature dependence of C_p for the new heterometallic complex $Co_2Li_2(Piv)_6(NEt_3)_2$ were performed. Decomposition of Co_2Li_2 (Piv)₆(NEt₃)₂ results in the formation of LiCoO₂.

Structural characterization of the FeTiO₃-MnTiO₃ solid solution

Xiang Wu, Shan Qin and Leonid Dubrovinsky *Page 2483*



Raman spectra of the $(Mn_{1-x}Fe_x)TiO_3$ $(0.0 \le x \le 1.0)$ system. Inset: the enlarged view from 310 to 390 cm⁻¹. $E_{g(3)}$ shifts to high frequency and the remaining shifts to low frequency as $xFeTiO_3$ content increases.

One-step fabrication and characterization of silica-sheathed ITO nanowires

Hyoun Woo Kim, Hyo Sung Kim, Han Gil Na, Ju Chan Yang, Rino Choi, Jae Kyeong Jeong, Chongmu Lee and Doo Young Kim *Page 2490*



Novel ITO/amorphous SiO_x core-shell structures were synthesized by thermal evaporation. A Au-catalyzed VLS process is the dominant mechanism for the ITO nanowires, whereas SiO_x was grown in a tubular structure.

Rapid Communications

A new $BaB_2Si_2O_8:Eu^{2+}/Eu^{3+}$, Tb^{3+} phosphor – Synthesis and photoluminescence properties

M.P. Saradhi, S. Boudin, U.V. Varadaraju and B. Raveau Page 2496



The figure shows structure refinement of both $MB_2Si_2O_8$ [M = Sr, Ba]. The structure refinement of newly synthesized phase BaB₂. Si₂O₈ was carried out by taking SrB₂Si₂O₈ as starting structure model. Inset in the figure shows the structure projection of BaB₂Si₂O₈. The Sr²⁺/Ba²⁺ are embedded in polyanionic network formed by corner sharing BO₄⁵⁻ and SiO₄⁴⁻ tetrahedral that intern form interconnected layers of 4 and 8 membered rings perpendicular to *b*-axis.

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Transport properties, specific heat and thermal conductivity of GaN nanocrystalline ceramic

Czesław Sułkowski, Andrzej Chuchmała, Andrzej J. Zaleski, Marcin Matusiak, Jan Mucha, Paweł Głuchowski and Wiesław Stręk *Page 2501*



Thermal resistivity and thermopower measurements indicates the high phonon scattering and lack of phonon-drag contribution to thermopower in GaN nanoceramics pressed under 4 GPa at 800 °C.

Geometric parameterization of the *YBa*Co₄O₇ structure type: Implications for stability of the hexagonal form and oxygen uptake

M. Avdeev, V.V. Kharton and E.V. Tsipis *Page 2506*



Global Instability Index (GII) for an M^{3+} BaCo₄^{2.25+}O₇.