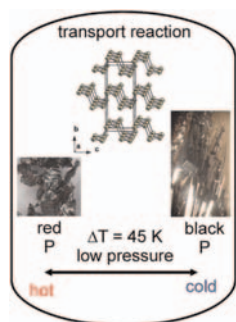


Abstracted/indexed in BioEngineering Abstracts, Chemical Abstracts, Coal Abstracts, Current Contents/Physics, Chemical, & Earth Sciences, Engineering Index, Research Alert, SCISEARCH, Science Abstracts, and Science Citation Index. Also covered in the abstract and citation database SCOPUS[®]. Full text available on ScienceDirect[®].

Regular Articles

A fast low-pressure transport route to large black phosphorus single crystals

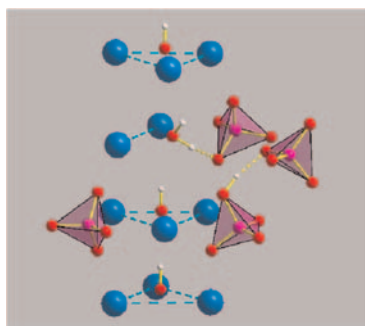
Tom Nilges, Marcel Kersting and Thorben Pfeifer
Page 1707



A low-pressure transport reaction route representing the first effective and scalable access to black phosphorus.

On the composition and atomic arrangement of calcium-deficient hydroxyapatite: An ab-initio analysis

Dirk Zahn and Oliver Hochrein
Page 1712

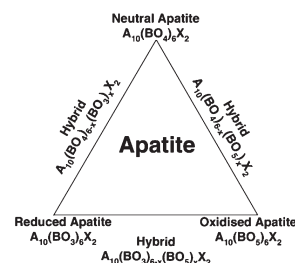


Preferred constellation of a Ca vacancy in hydroxyapatite, accompanied by a H₂O defect and a HPO₄²⁻ defect adjacent to the deficient Ca site. The preferential defect arrangement reflects a compromise of local charge compensation, different proton affinities of the anions and hydrogen bonding.

Regular Articles—Continued

A taxonomy of apatite frameworks for the crystal chemical design of fuel cell electrolytes

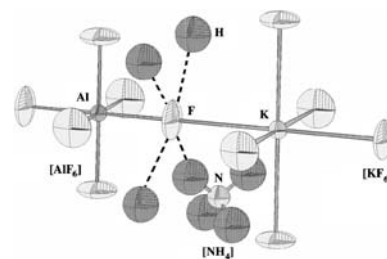
Stevin S. Pramana, Wim T. Klooster and Timothy J. White
Page 1717



Apatite framework taxonomy succinctly rationalises the crystallographic modifications of this structural family as a function of chemical composition. Neutron diffraction identified that the excess oxygen in La₉SrGe₆O_{26.5} is tenanted in the framework as [La₉Sr][(GeO₄)_{5.5}(GeO₅)_{0.5}]O₂. The implication of this approach is that in addition to the three known apatite genera—A₁₀(BO₃)₆X₂, A₁₀(BO₄)₆X₂, A₁₀(BO₅)₆X₂—hybrid electrolytes of the types A₁₀(BO₃/BO₄/BO₅)₆X₂ can be designed.

Syntheses and characterization of elpasolite-type ammonium alkali metal hexafluorometallates(III)

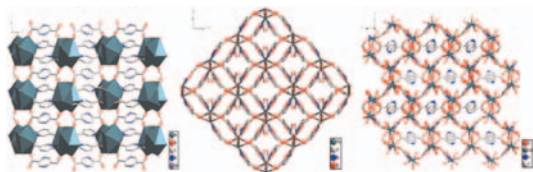
Jin-Xiao Mi, Shu-Ming Luo, Hua-Yu Sun, Xiao-Xuan Liu and Zan-bin Wei
Page 1723



Abnormal anisotropic thermal parameters of fluorine atoms have been observed in the compound [(NH₄)_{1-x}K_x]₂KAlF₆ (x ≈ 0.17), and interpreted to arise from four strong hydrogen bonds (F...H-N) that are distributed in a square form around each fluorine atom. The endmembers' phase transitions at low temperature are believed to be caused by them.

Syntheses, structures, and photoluminescence of three-dimensional lanthanide coordination polymers with 2,5-pyridinedicarboxylic acid

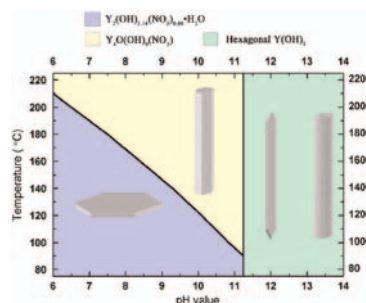
Yan Huang, Yi-Shan Song, Bing Yan and Min Shao
Page 1731



Four new lanthanide coordination polymers have been hydrothermally synthesized by the reaction of 2,5-pyridinedicarboxylic acid with the corresponding lanthanide nitrates, and they show three types of 3D open-framework architecture. Complexes **2** and **5** show strong characteristic green (or red) luminescence and long lifetimes.

Controlling the morphology of yttrium oxide through different precursors synthesized by hydrothermal method

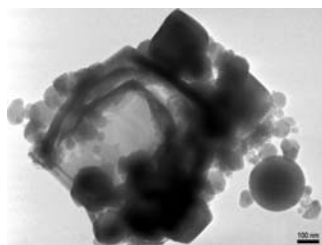
Nan Li and Kazumichi Yanagisawa
Page 1738



Y_2O_3 particles in the shape of sheet, rod, needle and tube with controlled size were synthesized from three precursors, $Y_2(OH)_{5.14}(NO_3)_{0.86} \cdot H_2O$, $Y_4O(OH)_9(NO_3)$ and hexagonal $Y(OH)_3$, obtained by hydrothermal reactions with controlled pH value and reaction temperature.

Solid-state ^{27}Al and ^{29}Si NMR characterization of hydrates formed in calcium aluminate–silica fume mixtures

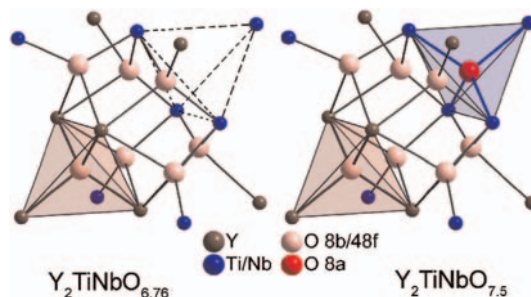
P. Pena, J.M. Rivas Mercury, A.H. de Aza, X. Turrillas, I. Sobrados and J. Sanz
Page 1744



Transmission electron micrograph of $CaAl_2O_4$ -microsilica mixture hydrated at 90 °C for 31 days showing a cubic $Ca_3Al_{2.0 \pm 0.2}(SiO_4)_{0.9 \pm 0.2}(OH)_{1.8}$ crystal surrounded by unreacted amorphous silica spheres.

Structural and magnetic properties of pyrochlore solid solutions $(Y,Lu)_2Ti_{2-x}(Nb,Ta)_xO_{7 \pm y}$

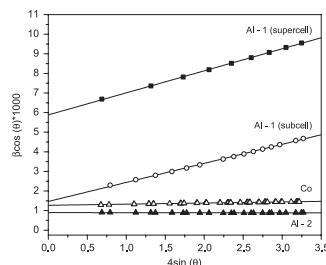
D.V. West, T.M. McQueen, Q. Huang and R.J. Cava
Page 1753



Synthesis of pyrochlore solid solutions $(Y,Lu)_2Ti_{2-x}(Nb,Ta)_xO_{7 \pm y}$ under high vacuum at 1600 °C results in oxygen deficient, paramagnetic compounds with reduced B-site cations. Studies indicate Ti^{3+} as the source of the localized moments, with no evidence for localized Nb^{4+} moments. Annealing under O_2 results in fully oxidized, oxygen excess pyrochlores as white powders. Powder neutron diffraction studies show the excess oxygen on the normally vacant 8a site.

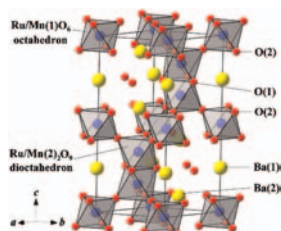
Crystal structures and cation ordering of Sr_2AlSbO_6 and Sr_2CoSbO_6

A. Faik, M. Gateshki, J.M. Igartua, J.L. Pizarro, M. Insausti, R. Kaindl and A. Grzechnik
Page 1759



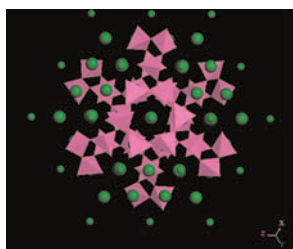
Williamson–Hall plot of the diffraction peaks in Sr_2AlSbO_6 , samples 1 and 2, and in Sr_2CoSbO_6 . β denotes the integral breadth corrected for instrumental effects, θ is the diffraction angle. It can be seen that in the case of sample 1, β of the superstructure reflections (solid squares) are clearly larger than those of the rest of the peaks. It was found that depending on the preparation conditions, the Al^{3+} and Sb^{3+} cations can be either entirely or partially ordered. In the case of the partially ordered Sr_2AlSbO_6 sample, the extension of cation ordering was estimated from the hkl -dependent broadening of the diffraction peaks and the results were interpreted as evidence of the formation of anti-phase domains in the material. In the case of Sr_2CoSbO_6 , despite the high synthesis temperature (1770 K), the degree of ordering is relatively low. This can be explained by the small difference between the radii of the B-site cations. Another interesting fact is that the sample-related broadening of the diffraction peaks of Sr_2CoSbO_6 does not show any significant hkl -dependence. This suggests that no extended anti-phase boundaries are formed within the crystallites and the observed low degree of ordering is caused by randomly distributed anti-site defects. In the case of trigonal perovskites the effect of the cation ordering on the peak widths cannot be visualized easily as in the case of cubic perovskites due to the overlapping of the order-related reflections with sub-cell reflections.

Structural and physical properties evolution in the 6H BaRu_{1-x}Mn_xO₃ synthesized under high pressure
 J.G. Zhao, L.X. Yang, Y. Yu, F.Y. Li, R.C. Yu and C.Q. Jin
 Page 1767



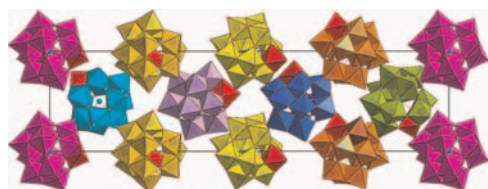
The 6H BaRu_{1-x}Mn_xO₃ was synthesized using high-pressure sintering. The substitution of Mn for Ru cations gives rise to the short-range magnetic ordering, with the maximal Curie temperature T_c 175.2 K at $x=0.10$. The compounds are of spin-class magnetism at lower temperature at $x \geq 0.05$. Mn doping results in the transition from the primal metal to semiconductor at $x=0.30$.

Preparation and photoluminescence property of a loose powder, Ca₃Al₂O₆:Eu³⁺ by calcination of a layered double hydroxide precursor
 Xiaorui Gao, Lixu Lei, Changgui Lv, Yueming Sun, Hegen Zheng and Yiping Cui
 Page 1776



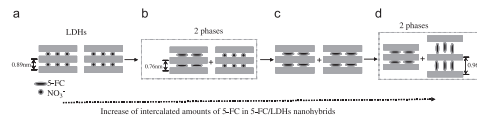
Calcination of a layered double hydroxide precursor produces Ca₃Al₂O₆:Eu³⁺, which is very easy to be pulverized. It is proposed that Eu³⁺ takes the place of one Ca²⁺ (green spheres in the picture, pink pyramids are [AlO₄] tetrahedrons) in the cell of Ca₃Al₂O₆. The Ca²⁺ could be any one of the bigger green spheres without inversion symmetry, and emits red light under a UV radiation of $\lambda=250$ nm.

Structural study of ammonium metatungstate
 Joel B. Christian and M. Stanley Whittingham
 Page 1782



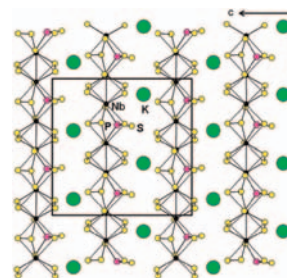
The structure of ammonium metatungstate powders are highly dependent on hydration and POM molecule rotation, with cation and hydrogen bonding forces directing a mixture of structures that have been studied with bulk and single-crystal methods. The illustration shows Monte Carlo simulated anion structural disorder for the fully dehydrated form of the title compound.

Synthesis and characterization of 5-fluorocytosine intercalated Zn-Al layered double hydroxide
 Chunxia Liu, Wanguo Hou, Lifang Li, Yan Li and Shaojie Liu
 Page 1792



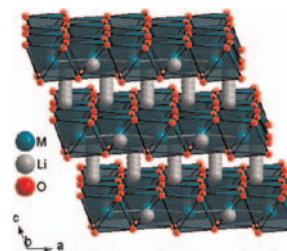
The 5-fluorocytosine (5-FC) has been intercalated into layered double hydroxide using coprecipitation method. The morphology of 5-FC molecules in obtained nanohybrids was dependent on the intercalated amount of 5-FC. The in vitro drug release from the nanohybrids was remarkably lower than that from the corresponding physical mixture, which shows these drug-inorganic nanohybrids can be used as a potential drug delivery system.

Dimensional reductions from 2-D Nb₄P₂S₂₁ to 1-D ANb₂PS₁₀ (A=Na, K, Rb, Cs, Tl) and to 0-D Tl₅[Nb₂S₄C₁₈]Cl using halide molten salts
 Hyunjin Bang, Youngmee Kim, Seri Kim and Sung-Jin Kim
 Page 1798



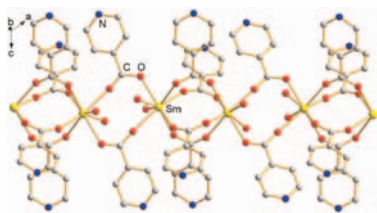
We developed new synthetic routes to obtain 1-D quaternary thiophosphate compounds and a molecular complex containing a Nb₂S₄ core from a 2-D ternary thiophosphate, Nb₄P₂S₂₁. When Nb₄P₂S₂₁ was reacted with alkali metal halides or TlCl, the -S-S-S- bridges in 2-D Nb₂PS₁₀-S-S₁₀PNb₂ were excised to form a 1-D chain, and cations were inserted between the chains.

Structure and properties of ordered Li₂IrO₃ and Li₂PtO₃
 Matthew J. O'Malley, Henk Verweij and Patrick M. Woodward
 Page 1803



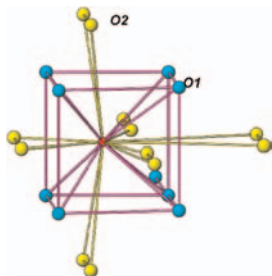
The Li₂IrO₃ and Li₂PtO₃ were synthesized. Refinements are presented along with thermal and electrical properties, which are compared and contrasted with Li₂RuO₃ when appropriate.

Synthesis, structure, and physical properties of $[\text{Sm}(\text{C}_6\text{NO}_2\text{H}_5)_3(\text{H}_2\text{O})_2]_{2n} \cdot (\text{H}_5\text{O}_2)_n(\text{ZnCl}_5)_n(\text{ZnCl}_4)_{2n} \cdot (\text{H}_2\text{O})_{2n}$ with unprecedented ZnCl_5^{3-} species
Yi-Ming Xie, Wen-Tong Chen and Ji-Huai Wu
Page 1853



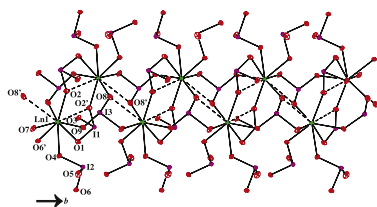
A novel bimetallic 4f-3d metal-isonicotinic acid inorganic-organic hybrid complex was synthesized. It is characteristic of a one-dimensional polycationic chain-like structure. Photoluminescent investigation reveals that the title complex displays interesting emissions in a wide region. Optical absorption spectra of **1** reveal the presence of a wide optical bandgap.

Oxidation/reduction studies on $\text{Zr}_y\text{U}_{1-y}\text{O}_{2+x}$ and delineation of a new orthorhombic phase in U-Zr-O system
S.K. Sali, N.K. Kulkarni, K. Krishnan, S.N. Achary and A.K. Tyagi
Page 1859



Local surrounding of M ions in $\text{Zr}_{0.33}\text{U}_{0.67}\text{O}_{2.33}$.

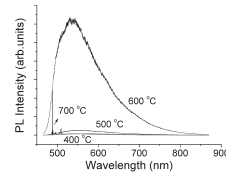
Magnetism and Raman spectroscopy of the dimeric lanthanide iodates $\text{Ln}(\text{IO}_3)_3$ ($\text{Ln} = \text{Gd}, \text{Er}$) and magnetism of $\text{Yb}(\text{IO}_3)_3$
Richard E. Sykora, Peter Khalifah, Zerihun Assefa, Thomas E. Albrecht-Schmitt and Richard G. Haire
Page 1867



Three *f*-element iodates $\text{Ln}(\text{IO}_3)_3$ ($\text{Ln} = \text{Gd}, \text{Er}, \text{Yb}$), all containing the $\text{Bi}(\text{IO}_3)_3$ structure type, were characterized by Raman spectroscopy and magnetic property measurements. The results of the Raman studies indicated that the vibrational profiles are adequately sensitive to distinguish between the structures of the iodates reported here and other lanthanide iodate systems. The magnetic measurements indicate that only in $\text{Gd}(\text{IO}_3)_3$ did the $3+$ lanthanide ion exhibit its full $7.9 \mu_B$ Hund's rule moment; Er^{3+} and Yb^{3+} exhibited ground state moments and gap energy scales of $8.3 \mu_B/70 \text{ K}$ and $3.8 \mu_B/160 \text{ K}$, respectively. $\text{Er}(\text{IO}_3)_3$ exhibited extremely weak ferromagnetic correlations ($+0.4 \text{ K}$), while the magnetic ions in $\text{Gd}(\text{IO}_3)_3$ and $\text{Yb}(\text{IO}_3)_3$ were fully non-interacting within the resolution of our measurements ($\sim 0.2 \text{ K}$).

Photoluminescence in the $\text{Ca}_x\text{Sr}_{1-x}\text{WO}_4$ system at room temperature

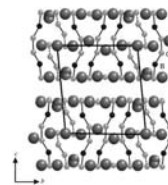
S.L. Pôrto, E. Longo, P.S. Pizani, T.M. Boschi, L.G.P. Simões, S.J.G. Lima, J.M. Ferreira, L.E.B. Soledade, J.W.M. Espinoza, M.R. Cássia-Santos, M.A.M.A. Maurera, C.A. Paskocimas, I.M.G. Santos and A.G. Souza
Page 1876



The structural and room temperature photoluminescence of $\text{Ca}_x\text{Sr}_{1-x}\text{WO}_4$ synthesized by a soft chemical method was studied. The most intense PL emission was obtained for the sample calcined at $600 \text{ }^\circ\text{C}$, that is neither highly disordered ($400\text{--}500 \text{ }^\circ\text{C}$), nor completely ordered ($700 \text{ }^\circ\text{C}$). Corroborating the role of disorder in the PL phenomenon, the most intense PL response was not observed for pure CaWO_4 or SrWO_4 , but for $\text{Ca}_{0.6}\text{Sr}_{0.4}\text{WO}_4$.

New examples of ternary rare-earth metal boride carbides containing finite boron-carbon chains: The crystal and electronic structure of $\text{RE}_{15}\text{B}_6\text{C}_{20}$ ($\text{RE} = \text{Pr}, \text{Nd}$)

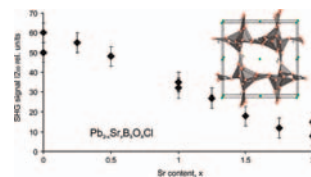
Volodymyr Babizhetskyy, Hansjürgen Mattausch, Arndt Simon, Kurt Hiebl, Mouna Ben Yahia, Régis Gautier and Jean-François Halet
Page 1882



The ternary rare-earth metal boride carbides $\text{RE}_{15}\text{B}_6\text{C}_{20}$ ($\text{RE} = \text{Pr}, \text{Nd}$) were synthesized by co-melting the elements. They exist above 1270 K . Their structure consists of a three-dimensional framework of rare-earth metal atoms resulting from the stacking of slightly corrugated and distorted square nets, leading to cavities filled with unprecedented B_2C_4 finite chains, disordered C_3 entities and isolated carbon atoms, respectively. Structural and theoretical analyses suggest the ionic formulation $(\text{RE}^{3+})_{15}[(\text{B}_2\text{C}_4)^{6-}]_3[(\text{C}_3)^{4-}]_2(\text{C}^{4-})_2$ 11 \bar{e} . $\text{Pr}_{15}\text{B}_6\text{C}_{18}$ exhibits antiferromagnetic order at $T_N = 7.9 \text{ K}$, followed by a meta-magnetic transition above a critical external field $B > 0.03 \text{ T}$. On the other hand, $\text{Nd}_{15}\text{B}_6\text{C}_{18}$ is ferromagnetic below $T_C \approx 40 \text{ K}$.

Lead-strontium borate halides with hilgardite-type structure and their SHG properties

B.V. Egorova, A.V. Olenev, P.S. Berdonosov, A.N. Kuznetsov, S.Yu. Stefanovich, V.A. Dolgikh, T. Mahenthirarajah and P. Lightfoot
Page 1891

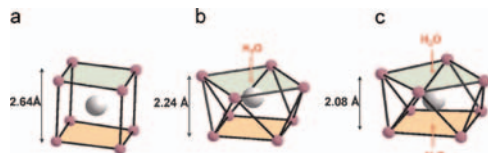


$\text{Sr}_2\text{B}_5\text{O}_9\text{Cl}$, $\text{Pb}_2\text{B}_5\text{O}_9\text{Cl}$ and the solid solution range $\text{Pb}_{2-x}\text{Sr}_x\text{B}_5\text{O}_9\text{Cl}$ has been prepared, and studied by powder neutron and X-ray diffraction and SHG measurements.

Continued

Adaptable coordination of U(IV) in the 2D-(4,4) uranium oxalate network: From 8 to 10 coordinations in the uranium (IV) oxalate hydrates

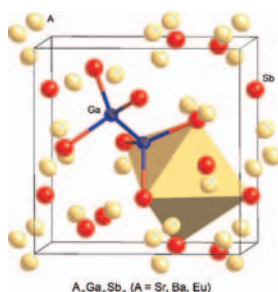
L. Duviébourg-Garela, N. Vigier, F. Abraham and S. Grandjean
 Page 1899



The adaptable environment of U(IV) in U(IV) oxalates: from eight cubic coordination in $U(C_2O_4)_2 \cdot 6H_2O$ (a) completed by water oxygens to nine in $[U(C_2O_4)_2 \cdot H_2O](C_2NH_3)$ (b) and ten coordination in $U(C_2O_4)_2 \cdot 2H_2O$ (c).

Gallium substitutions as a means to stabilize alkaline-earth and rare-earth metal pnictides with the cubic Th_3P_4 type: Synthesis and structure of $A_7Ga_2Sb_6$ ($A = Sr, Ba, Eu$)

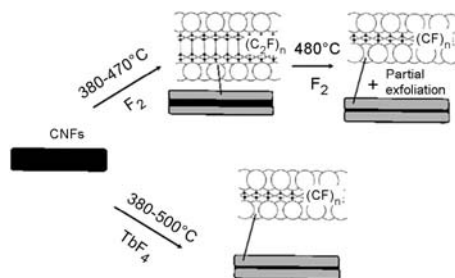
Sheng-Qing Xia, Jonathan Hullmann and Svilen Bobev
 Page 1909



Three new antimonides have been structurally characterized by single-crystal X-ray diffraction. Their structures are best described as derivatives of the body-centered cubic, anti- Th_3P_4 type. Unlike the one-electron-deficient A_4Sb_3 phases ($A = Sr, Ba, Eu$), the new, $A_7Ga_2Sb_6$ compounds are Zintl phases with closed-shell configurations for both the cations and anions.

Solid-state NMR and EPR study of fluorinated carbon nanofibers

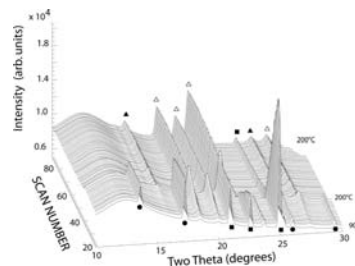
Wei Zhang, Marc Dubois, Katia Guérin, André Hamwi, Jérôme Giraudet and Francis Masin
 Page 1915



Scheme of the fluorination process using F_2 and TbF_4 as fluorinating agent.

Hydrothermal synthesis of nanocrystalline ZnSe: An *in situ* synchrotron radiation X-ray powder diffraction study

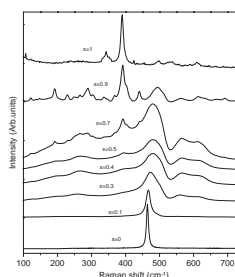
J.-E. Jørgensen, T.R. Jensen and J.C. Hanson
 Page 1925



Stack of powder diagrams showing the formation of nanocrystalline ZnSe under hydrothermal conditions.

Raman, XRD and microscopic investigations on $CeO_2-Lu_2O_3$ and $CeO_2-Sc_2O_3$ systems: A sub-solidus phase evolution study

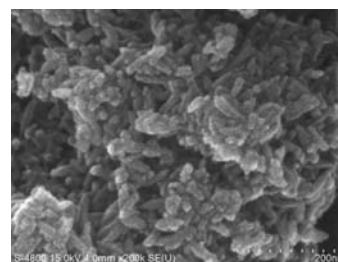
V. Grover, Ankita Banerji, P. Sengupta and A.K. Tyagi
 Page 1930



Powder XRD and Raman spectroscopy were used in conjunction to delineate the phases present in $CeO_2-Lu_2O_3$ and $CeO_2-Sc_2O_3$ systems. $LuO_{1.5}$ has 30 mol% miscibility, whereas Sc_2O_3 has no discernible solubility in CeO_2 . Raman spectroscopy clearly showed the evolution of second phase with change in concentration of the reactants thus supporting XRD data. Back scattered images obtained on representative compositions verify the results.

CTAB-assisted synthesis of mesoporous F-N-codoped TiO_2 powders with high visible-light-driven catalytic activity and adsorption capacity

Yi Xie, Xiujian Zhao, Yuanzhi Li, Qingnan Zhao, Xuedong Zhou and Qihua Yuan
 Page 1936

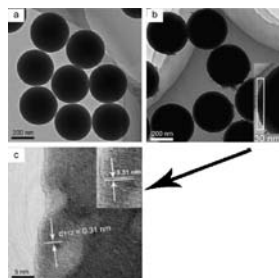


The introduction of surfactant CTAB not only extended the visible light absorption of mesoporous F-N-codoped TiO_2 up to 600 nm but also significantly enhanced the adsorption capacity and visible-light-induced degradation for methyl orange. Mesoporous rod-like F-N-codoped TiO_2 powder photocatalysts were synthesized via a sol-gel route at low temperature of 373 K.

Fabrication and luminescent properties of the core-shell structured $\text{YNbO}_4:\text{Eu}^{3+}/\text{Tb}^{3+}@\text{SiO}_2$ spherical particles

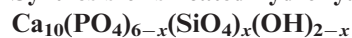
Piaoping Yang, Zewei Quan, Chunxia Li, Jun Yang, Huang Wang, Xiaoming Liu and Jun Lin

Page 1943



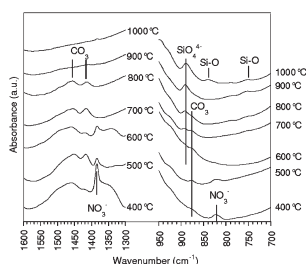
$\text{YNbO}_4:\text{Eu}^{3+}/\text{Tb}^{3+}$ layers were deposited on spherical SiO_2 particles via a sol-gel process, resulting in the formation of core-shell structured $\text{YNbO}_4:\text{Eu}^{3+}/\text{Tb}^{3+}@\text{SiO}_2$ phosphors. The luminescence properties of phosphors in the core-shell particles can be tuned by altering the annealing temperature and the coating layers of the phosphors.

Synthesis of silicated hydroxyapatite



Mickaël Palard, Eric Champion and Sylvie Foucaud

Page 1950

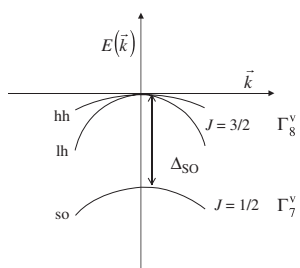


The preparation of pure silicated hydroxyapatite $\text{Ca}_{10}(\text{PO}_4)_{6-x}(\text{SiO}_4)_x(\text{OH})_{2-x}$ powders with controlled silicon content was investigated. The synthesis route included a precipitation in aqueous media. It required an additional high temperature solid-state reaction to fully incorporate the silicon into the apatite crystals.

The higher excited electronic states and spin-orbit splitting of the valence band in three-dimensional assemblies of close-packed ZnSe and CdSe quantum dots in thin film form

Biljana Pejova

Page 1961

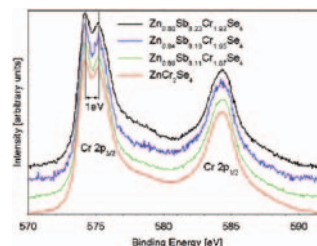


Accounting for S - D mixing of hole states, the observed optical transitions in very small sphalerite-type ZnSe and CdSe nanoclusters are attributed to the ground state— $(1S_{3/2}, 1S_c)$ and the ground state— $(1S_{1/2}, 1S_c)$. The “splittings” do not correspond to SO splitting energy, but are complex functions of it.

Structural and magnetic properties of $\text{Zn}_{1-x}\text{Sb}_x\text{Cr}_{2-x/3}\text{Se}_4$ ($x = 0.11, 0.16$ and 0.20) single crystals

E. Malicka, A. Waśkowska, J. Heimann, T. Mydlarz, R. Sitko and D. Kaczorowski

Page 1970

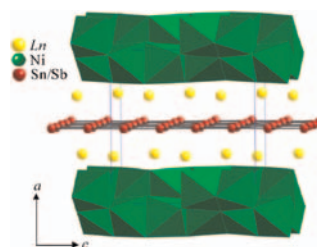


XPS spectrum of $\text{Cr}2p$ core-levels in the $(\text{Zn}_{1-x}\text{Sb}_x)[\text{Cr}_{2-x/3}]\text{Se}_4$ system ($x = 0.11, 0.16$ and 0.20).

Synthesis, structure and physical properties of $\text{LnNi}(\text{Sn},\text{Sb})_3$ ($\text{Ln} = \text{Pr}, \text{Nd}, \text{Sm}, \text{Gd}, \text{Tb}$)

Dixie P. Gautreaux, Cigdem Capan, John F. DiTusa, David P. Young and Julia Y. Chan

Page 1977

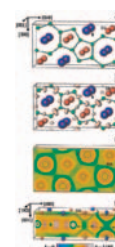


Five new single crystalline analogues of the $\beta\text{-LnNiSb}_3$ family ($\text{Ln} = \text{Pr}, \text{Nd}, \text{Sm}, \text{Gd}, \text{or Tb}$) have been synthesized and determined to be $\text{LnNi}(\text{Sn},\text{Sb})_3$. The structures are compared to the previously reported $\beta\text{-CeNiSb}_3$. Magnetic and transport behavior are reported and discussed.

Synthesis, chemical bonding and physical properties of RErRhB_4 ($\text{RE} = \text{Y}, \text{Dy-Lu}$)

I. Veremchuk, T. Mori, Yu. Prots, W. Schnelle, A. Leithe-Jasper, M. Kohout and Yu. Grin

Page 1983



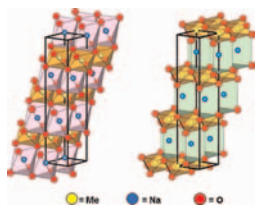
The compounds of rare-earth metals with rhodium and boron RErRhB_4 ($\text{RE} = \text{Y}, \text{Dy-Lu}$) crystallize with the orthorhombic structure type YCrB_4 . Analysis of chemical bonding for YrRhB_4 and YbRhB_4 was performed by electron localizability indicator and by calculation of quantum chemical charges (quantum theory of atoms in molecules). Boron and rhodium form the 3-D polyanion containing planar nets of three-bonded boron atoms interconnected by rhodium along $[001]$. The interaction of the RE species with the rhodium-boron polyanion is predominantly ionic.

Continued

Chemical equilibria involved in the oxygen-releasing step of manganese ferrite water-splitting thermochemical cycle

L. Seralessandri, M. Bellusci, C. Alvani, A. La Barbera, F. Padella and F. Varsano

Page 1992

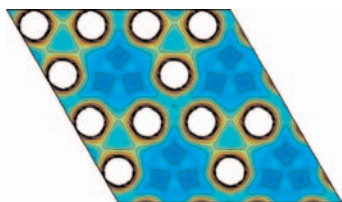


$\text{Na}(\text{Mn}_{1/3}\text{Fe}_{2/3})\text{O}_2$ disproportionation reaction in the presence of CO_2 was studied. Chemical equilibria among $\text{Na}_{1-x}(\text{Mn}_{1/3}\text{Fe}_{2/3})\text{O}_2$, MnFe_2O_4 and Na_2CO_3 compounds were evidenced and studied by means of Rietveld analysis performed on XRD patterns. Two different sodium-depleted lamellar structures were identified. The role of sodium carbonate formation/dissociation equilibrium in the oxygen-releasing step of the manganese ferrite thermochemical cycle has been highlighted.

Electron charge distribution of $\text{CaAl}_{2-x}\text{Zn}_x$: Maximum entropy method combined with Rietveld analysis of high-resolution-synchrotron X-ray powder diffraction data

Karin Söderberg, Yoshiki Kubota, Norihiro Muroyama, Daniel Grüner, Arisa Yoshimura and Osamu Terasaki

Page 1998

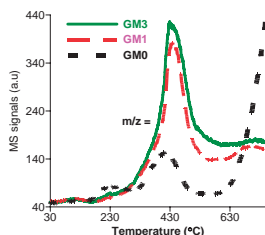


Using short wavelength X-rays from synchrotron radiation (SPRING-8), high-resolution powder diffraction patterns of the Laves (MgCu_2 and MgNi_2 type) and KHg_2 -type phases in the $\text{CaAl}_{2-x}\text{Zn}_x$ system were collected. The charge density distribution in the Laves phases as a function of x was obtained from the diffraction data by Rietveld analysis combined with the maximum entropy method (MEM).

Characterization and reactivity of nanoscale $\text{La}(\text{Co,Cu})\text{O}_3$ perovskite catalyst precursors for CO hydrogenation

Nguyen Tien-Thao, Houshang Alamdari and Serge Kaliaguine

Page 2006

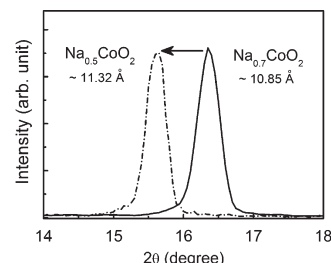


The ground $\text{La}(\text{Co,Cu})\text{O}_3$ perovskite precursors were reduced as catalysts for CO hydrogenation. The TPSR results show that the presence of a neighboring copper along with remnant sodium ions on the catalyst surface of these solids has remarkably affected the reactivity of cobalt for CO hydrogenation. The addition of copper into the perovskite framework leads to a change in the product distribution of CO hydrogenation and a decrease in reaction temperature. An increased copper content leads to a substantial decline in the rate of methanation and an increase in the formation of higher alcohols.

Fabrication and optical conductivities of strained epitaxial Na_xCoO_2 thin films: $x = 0.5, 0.7$

J.Y. Son, Y.H. Shin and C.S. Park

Page 2020

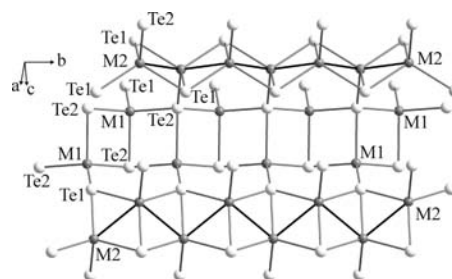


From the spectroscopic ellipsometry analysis, we obtained optical constants as well as optical conductivities for $\text{Na}_{0.5}\text{CoO}_2$ and $\text{Na}_{0.7}\text{CoO}_2$ thin films. The energy splitting between e_g and a_{1g} increased as a result of the structural strain of the $\text{Na}_{0.7}\text{CoO}_2$ thin film.

Structure and physical properties of the new telluride BaAg_2Te_2 and its quaternary variants $\text{BaCu}_\delta\text{Ag}_{2-\delta}\text{Te}_2$

Abdeljalil Assoud, Yanjie Cui, Stephanie Thomas, Brodie Sutherland and Holger Kleinke

Page 2024

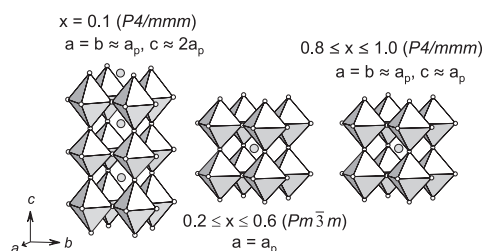


The tellurides $\text{BaCu}_\delta\text{Ag}_{2-\delta}\text{Te}_2$ all crystallize in the α - BaCu_2S_2 type. The Ag atoms prefer the M2 sites with short $M-M$ bonds (solid lines). The materials are (degenerate) p-type semiconductors. Higher Ag content reflects itself in higher Seebeck coefficient and lower electrical conductivity.

Influence of iron addition on the oxygen-deficient $\text{Sr}_{0.85}\text{Bi}_{0.15}\text{Co}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$ ($0.0 \leq x \leq 1.0$) perovskites

Annika K. Eriksson, Fredrik Lindberg, Gunnar Svensson, Peter Svedlindh, Paul F. Henry, Sten-G. Eriksson and Christopher S. Kneé

Page 2031

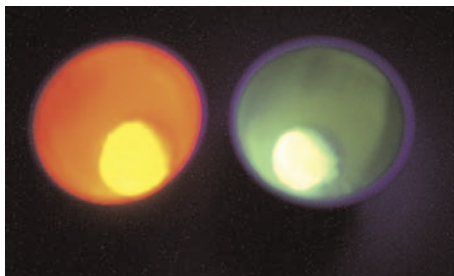


Evolving crystal structures of the as-prepared $\text{Sr}_{0.85}\text{Bi}_{0.15}\text{Co}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$ perovskites as a function of iron content for the compositional range $0.1 \leq x \leq 1.0$.

Alpha-particle-induced luminescence of rare-earth-doped Y_2O_3 nanophosphors

Cory D. Cress, Christopher S. Redino, Brian J. Landi and Ryne P. Raffaele

Page 2041

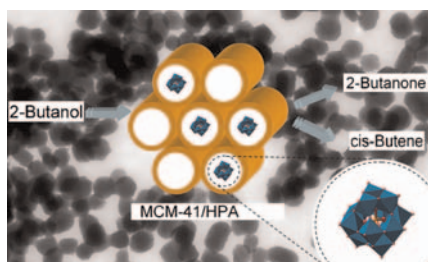


The photoluminescence and radioluminescence emission from rare-earth doped Y_2O_3 nanophosphors are being investigated. Below is a representative image of the photoluminescence from $Y_2O_3:Eu^{3+}$ (left) and $Y_2O_3:Tb^{3+}$ (right) under UV-light excitation.

PMo or PW heteropoly acids supported on MCM-41 silica nanoparticles: Characterisation and FT-IR study of the adsorption of 2-butanol

Daniel Carriazo, Concepción Domingo, Cristina Martín and Vicente Rives

Page 2046

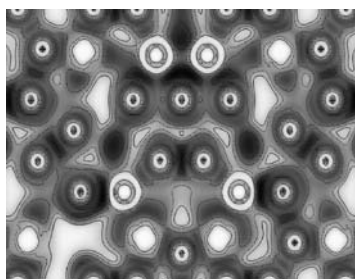


Samples based in MCM-41 nanoparticles loaded with tungstophosphoric and molybdophosphoric acids have been synthesised. The uncalcined solids and that derived upon their calcination in the temperature range 250–550 °C have been characterised and evaluated in the decomposition of 2-butanol monitored by FT-IR spectroscopy.

High pressure study and bonding analysis of $Mg_2Co_3Sn_{10+x}$

G. Krauss and Q.F. Gu

Page 2058

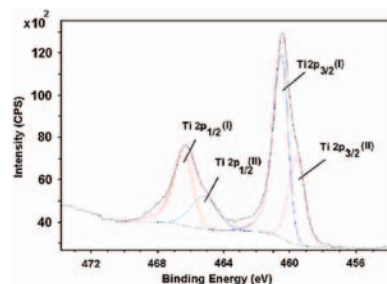


$Mg_2Co_3Sn_{10+x}$ belongs to the fascinating group of compounds combining localized and delocalized chemical bonding of the same element type in their structure. The structural stability up to 9.69 GPa and chemical bonding of this complex metallic alloy (120 atoms per unit cell) is reported.

A porous open-framework titanium oxophenylphosphate

Krishanu Sarkar, Subhash Chandra Laha, Nawal Kishor Mal and Asim Bhaumik

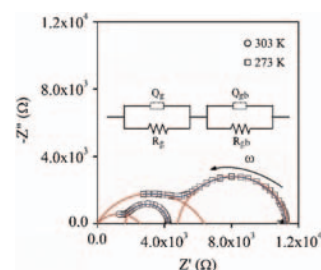
Page 2065



Low-temperature impedance and dielectric relaxation of NiO nanocrystals

Lijuan Chen, Liping Li and Guangshe Li

Page 2073

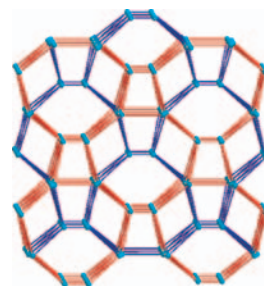


NiO nanocrystals showed distinct low-temperature bulk and grain boundary conduction that are highly dependent on the particle sizes.

Four Zn(II)/Cd(II)-3-amino-1,2,4-triazolate frameworks constructed by in situ metal/ligand reactions: Structures and fluorescent properties

Zilu Chen, Xiaoling Li and Fupei Liang

Page 2078

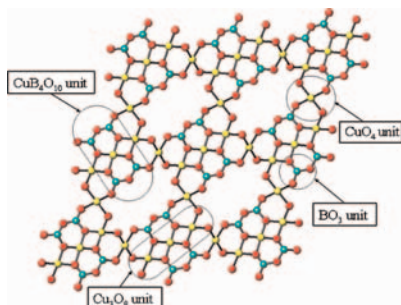


The solvothermal reactions of Cd(II) and Zn(II) salts bearing different anions with 5-amino-1H-1,2,4-triazole-3-carboxylic acid (AmTAZAc) produced four Cd(II) and Zn(II) MOFs with the in situ-generated 3-amino-1,2,4-triazolate ($AmTAZ^-$) ion as ligand, which display different structural topologies and fluorescent properties.

Continued

Synthesis, crystal structure, and nonlinear optical properties of $\text{Bi}_2\text{Cu}_5\text{B}_4\text{O}_{14}$

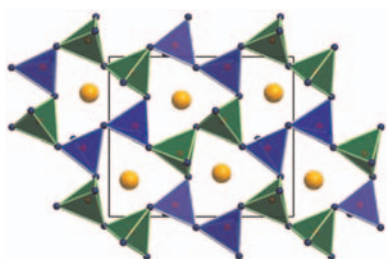
Shilie Pan, Jared P. Smit, Michael R. Marvel, Evan S. Stampler, Jacob M. Haag, Jaewook Baek, P. Shiv Halasyamani and Kenneth R. Poeppelmeier
Page 2087



The figure shows a layered structure that is built up from sheets of distorted rectangular CuO_4 and trigonal BO_3 groups. The sheets are connected by infinite chains of edge shared BiO_6 polyhedra that intersect the bc plane. These distortions lead to the second-harmonic generation efficiency of $\text{Bi}_2\text{Cu}_5\text{B}_4\text{O}_{14}$ about one half times that of KH_2PO_4 .

Synthesis and crystal structure of the high-pressure iron borate $\alpha\text{-FeB}_2\text{O}_4$

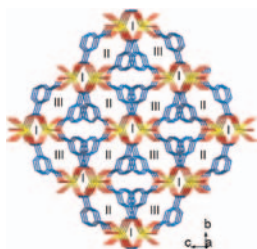
Johanna S. Knyrim and Hubert Huppertz
Page 2092



High-pressure/high-temperature synthesis (multianvil technique) led to the new phase $\alpha\text{-FeB}_2\text{O}_4$, which is exclusively built up from corner-sharing BO_4 -tetrahedra, isotypic to the monoclinic phases $\beta\text{-SrGa}_2\text{O}_4$, $\text{CaAl}_2\text{O}_4\text{-II}$, and CaGa_2O_4 .

Syntheses, structures and luminescence properties of lanthanide coordination polymers with helical character

Rui-Sha Zhou, Xiao-Bing Cui, Jiang-Feng Song, Xiao-Yu Xu, Ji-Qing Xu and Tie-Gang Wang
Page 2099

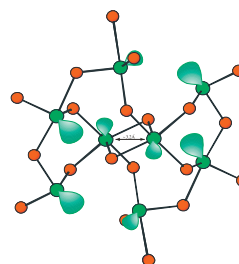


A series of lanthanide coordination polymers, $(\text{Him})_n[\text{Ln}(\text{ip})_2(\text{H}_2\text{O})]_n$ [$\text{Ln} = \text{La}(1)$, $\text{Pr}(2)$, $\text{Nd}(3)$ and $\text{Dy}(4)$] and $[\text{Y}_2(\text{ip})_3(\text{H}_2\text{O})_2]_n \cdot n\text{H}_2\text{O}$ (**5**), have been reported. The isostructural compounds **1–4** possess 3-D structures with three different kinds of channels. Compound **5** displays a 2-D network making of two kinds of quadruple-helical chains.

Rapid Communications

A rare multi-coordinate tellurite, $\text{NH}_4\text{ATe}_4\text{O}_9 \cdot 2\text{H}_2\text{O}$ ($A = \text{Rb}$ or Cs): The occurrence of TeO_3 , TeO_4 , and TeO_5 Polyhedra in the same material

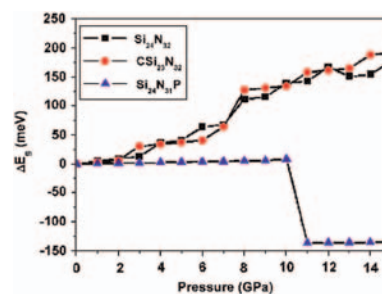
Jun-Ho Kim and P. Shiv Halasyamani
Page 2108



Two unprecedented tellurites, $\text{NH}_4\text{ATE}_4\text{O}_9 \cdot 2\text{H}_2\text{O}$ ($A = \text{Rb}$ or Cs) have been synthesized and characterized. The materials represent rare examples of tellurites that contain TeO_3 , TeO_4 , and TeO_5 polyhedra in the same compound. All of the polyhedra are in asymmetric polar coordination environments attributable to their stereo-active lone-pair.

Density functional study on electronic properties of P-doped spinel silicon carbon nitride

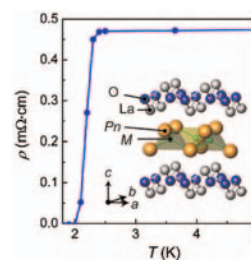
Yufen Zhang, Xian Zhao, Xiufeng Cheng and Yuguang Mu
Page 2113



We performed density functional calculations to predict the insulator-to-metal transition by replacing Si by C at the tetrahedral sites of P-doped $\text{c-Si}_3\text{N}_4$.

Nickel-based layered superconductor, LaNiOAs

Takumi Watanabe, Hiroshi Yanagi, Yoichi Kamihara, Toshio Kamiya, Masahiro Hirano and Hideo Hosono
Page 2117



A new layered oxyarsenide, LaNiOAs , which exhibits a superconducting transition at 2.4 K, was synthesized by solid-state reactions. This compound had a tetragonal ZrCuSiAs -type structure similar to recently discovered superconductors, LaFeOP , LaFeOAs , and LaNiOP . Superconductivity was observed for doped LaNiOAs , which differs from the case of LaFeOAs .

Corrigenda

Corrigendum to “Characterization of $\text{Bi}_5\text{Nb}_3\text{O}_{15}$ by refinement of neutron diffraction pattern, acid treatment and reaction of the acid-treated product with *n*-alkylamines”

[*J. Solid State Chem.* **180** (2007) 2517–2524]

Seiichi Tahara, Akira Shimada, Nobuhiro Kumada and Yoshiyuki Sugahara

Page 2121

Author inquiries

Submissions

For detailed instructions on the preparation of electronic artwork, consult the journal home page at <http://authors.elsevier.com>.

Other inquiries

Visit the journal home page (<http://authors.elsevier.com>) for the facility to track accepted articles and set up e-mail alerts to inform you of when an article's status has changed. The journal home page also provides detailed artwork guidelines, copyright information, frequently asked questions and more.

Contact details for questions arising after acceptance of an article, especially those relating to proofs, are provided after registration of an article for publication.

Language Polishing

Authors who require information about language editing and copyediting services pre- and post-submission should visit <http://www.elsevier.com/wps/find/authorhome.authors/languagepolishing> or contact authorsupport@elsevier.com for more information. Please note Elsevier neither endorses nor takes responsibility for any products, goods, or services offered by outside vendors through our services or in any advertising. For more information please refer to our Terms & Conditions at http://www.elsevier.com/wps/find/termsconditions.cws_home/termsconditions.

For a full and complete Guide for Authors, please refer to *J. Solid State Chem.*, Vol. 180, Issue 1, pp. *bmi–bmw*. The instructions can also be found at http://www.elsevier.com/wps/find/journaldescription.cws_home/622898/authorinstructions.

Journal of Solid State Chemistry has no page charges.