

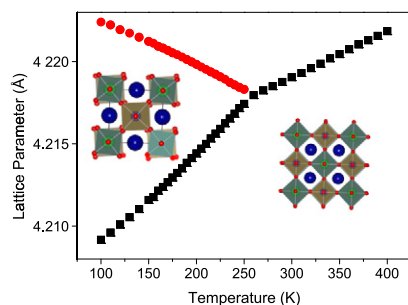
CONTENTS

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Regular Articles

The effect of disorder in Ba_2YTao_6 on the tetragonal to cubic phase transition

Qingdi Zhou, Brendan J. Kennedy and Justin A. Kimpton
page 729

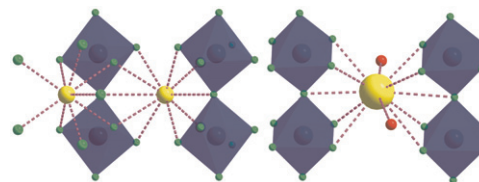


The tetragonal–cubic phase transition observed in the cation ordered double perovskite Ba_2YTao_6 is inhibited when these are disordered.

Regular Articles—Continued

$\text{A}_2\text{TiF}_5 \cdot n\text{H}_2\text{O}$ ($\text{A} = \text{K}, \text{Rb}, \text{or Cs}; n = 0 \text{ or } 1$): Synthesis, structure, characterization, and calculations of three new uni-dimensional titanium fluorides

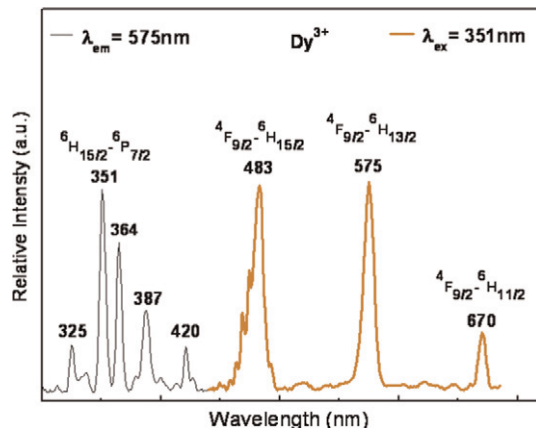
Vinna Jo, Dong Woo Lee, Hyun-Joo Koo and Kang Min Ok
page 741



Ball-and-stick and polyhedral representations for (a) $\beta\text{-K}_2\text{TiF}_5$ and (b) $\text{Rb}_2\text{TiF}_5 \cdot \text{H}_2\text{O}$ or $\text{Cs}_2\text{TiF}_5 \cdot \text{H}_2\text{O}$ with the K^+ and Rb^+ (or Cs^+) coordination environment emphasized.

Syntheses, structure and rare earth metal photoluminescence of new and known isostructural $\text{A}_2\text{Mo}_4\text{Sb}_2\text{O}_{18}$ ($\text{A} = \text{Ce}, \text{Pr}, \text{Sm}, \text{Eu}, \text{Gd}, \text{Tb}, \text{Dy}, \text{Ho}, \text{Er}, \text{Tm}, \text{Yb}, \text{Lu}$) compounds

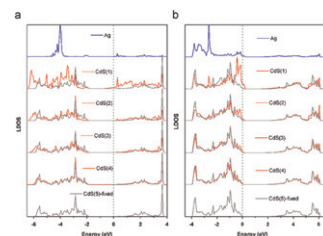
Shrikant A. Mohitkar, G. Kalpana and K. Vidyasagar
page 735



Among the fifteen isostructural $\text{A}_2\text{Mo}_4\text{Sb}_2\text{O}_{18}$ ($\text{A} = \text{rare earth metal}$) molybdoantimonites, eight ($\text{A} = \text{Pr}, \text{Sm}, \text{Eu}, \text{Tb}, \text{Dy}, \text{Ho}, \text{Er}, \text{Tm}$) compounds exhibit neat characteristic lanthanide photoluminescence in the 200–800 nm range at room temperature.

Ag adsorption on Cd-terminated CdS (0 0 0 1) and S-terminated CdS (0 0 0 $\bar{1}$) surfaces: First-principles investigations

Yandong Ma, Ying Dai, Wei Wei, Xianghong Liu and Baibiao Huang
page 747



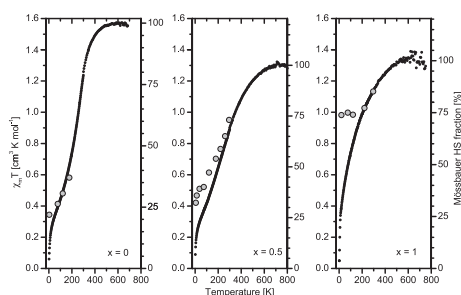
The Ag-induced changes in electronic structures mainly concentrate on surface region and decay quickly with the increase of site depth from surface.

We studied the adsorption of Ag at Cd-terminated CdS (0 0 0 1) and S-terminated CdS (0 0 0 $\bar{1}$) surfaces as a function of Ag coverage by means of the first-principles calculations. In addition, related properties of Ag cluster adsorption at Cd-terminated (0 0 0 1) surface are also discussed. Our *ab initio* calculations are useful complement to the intense experimental studies for Ag@CdS interface.

Continued

Thermal low spin–high spin equilibrium of Fe(II) in thiospinels $\text{CuFe}_{0.5}(\text{Sn}_{1-x}\text{Ti}_x)_{1.5}\text{S}_4$ ($0 \leq x \leq 1$)

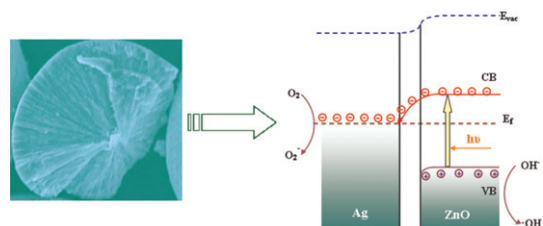
M. Womes, C. Reibel, A. Mari and D. Zitoun
page 753



Comparison of fractions of high spin Fe(II) from Mössbauer spectra (circles) with plots of $\chi_m T$ (dots) versus T . Discrepancies between both methods indicate anti-ferromagnetic spin coupling.

Hierarchical Ag/ZnO micro/nanostructure: Green synthesis and enhanced photocatalytic performance

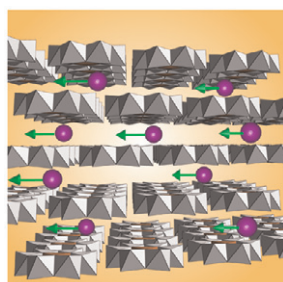
Shuyan Gao, Xiaoxia Jia, Shuxia Yang, Zhengdao Li and Kai Jiang
page 764



A green strategy is report to construct Ag/ZnO metal–semiconductor nanocomposites with hierarchical micro/nanostructure and enhanced photocatalytic activity.

Insertion-release of guest species and ionic conduction in polyoxometalate solids with a layer-like Anderson structure

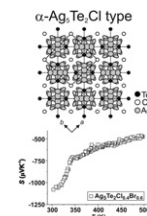
Haruo Naruke, Naoyuki Kajitani and Takayuki Konya
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Two compounds $\text{Na}_{2.5}\text{K}_{5.3}[\text{SbW}_6\text{O}_{24}](\text{NO}_3)_{0.8} \cdot 12\text{H}_2\text{O}$ (**1**) and $\text{Na}_2\text{K}_{5.35}[\text{SbW}_6\text{O}_{24}]\text{Cl}_{0.35} \cdot 12\text{H}_2\text{O}$ (**2**) possessing a layer-like Anderson (LLA) structure exhibited pseudo intercalation-deintercalation behavior. The dehydrated form of **1** is a high alkaline cation conductor with a conductivity of $1.2 \times 10^{-2} \Omega^{-1} \text{cm}^{-1}$ at 400°C .

Effects of partial anion substitution on the thermoelectric properties of silver(I) chalcogenide halides in the system $\text{Ag}_5\text{Q}_2\text{X}$ with $\text{Q} = \text{Te, Se and S}$ and $\text{X} = \text{Br and Cl}$

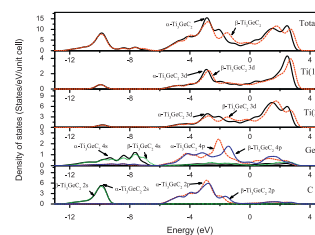
Nadine Eckstein, Tom Nilges, Rodolphe Decourt, Jean-Louis Bobet and Bernard Chevalier
page 778



A structure section of the $\alpha\text{-Ag}_5\text{Te}_2\text{Cl}$ structure type and the thermopower evolution of $\text{Ag}_5\text{Te}_2\text{Cl}_{0.4}\text{Br}_{0.6}$ undergoing a silver ion order/disorder phase transition.

Effect of high hydrostatic pressure on structural stability of Ti_3GeC_2 : A first-principles investigation

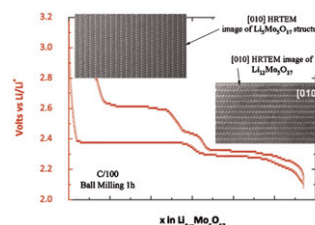
Shouxin Cui, Wenxia Feng, Haiquan Hu, Guiqing Zhang, Zengtao Lv and Zizheng Gong
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The less phase stability of $\beta\text{-Ti}_3\text{SiC}_2$ compared to that of $\alpha\text{-Ti}_3\text{SiC}_2$ can be interpreted by the states between -6.0 and 3.6 eV shift toward the higher energy region for $\beta\text{-Ti}_3\text{SiC}_2$.

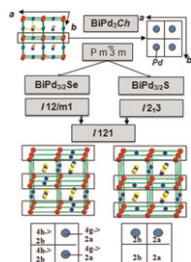
HRTEM and neutron diffraction study of $\text{Li}_x\text{Mo}_5\text{O}_{17}$: From the ribbon ($x = 5$) structure to the rock salt ($x = 12$) structure

O.I. Lebedev, V. Caignaert, B. Raveau, N. Pop, F. Gozzo, G. Van Tendeloo and V. Pralong
page 790



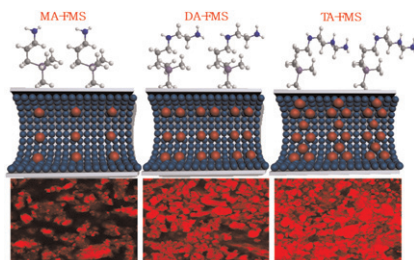
Structure determination of the fully intercalated phase $\text{Li}_{12}\text{Mo}_5\text{O}_{17}$ and of the deintercalated oxide $\text{Li}_5\text{Mo}_5\text{O}_{17}$ has been carried out by electron microscopy and neutron powder diffraction. The reversible topotactic transformation between the ordered rock salt structure of the former and the ribbon structure of the latter is explained on the following basis: both structures can be described as strips built up as an assembly of infinite ribbons of MoO_6 octahedra that are five octahedra thick, and that differ by slight displacements of the octahedral ribbons. We show that the electrochemical behavior of the $\text{Li}_x\text{Mo}_5\text{O}_{17}$ system is based on two sorts of Li^+ sites; those that are located within the strips between the ribbons, and those that are located at the border of the strips. The high rate of Li intercalation in this oxide and its reversibility are discussed in terms of its peculiar structure.

Palladium site ordering and the occurrence of superconductivity in $\text{Bi}_2\text{Pd}_3\text{Se}_{2-x}\text{S}_x$
 R. Weihrich, S.F. Matar, I. Anusca, F. Pielhofer, P. Peter, F. Bachhuber and V. Eyert
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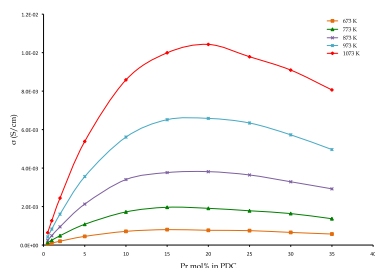
Structure relations for perovskite type BiPd_3C , $\text{BiPd}_{3/2}\text{Se}$ and $\text{BiPd}_{3/2}\text{S}$.

Electrostatic interaction effect for human DNA separation with functionalized mesoporous silicas
 Hong Kyung Choi, Jeong Ho Chang, Il Hwan Ko, Jin Hyung Lee, Bong Yong Jeong, Jong Hee Kim and Jung Bae Kim
 page 805



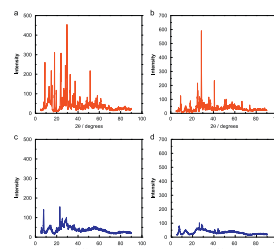
Control of electrostatic interaction for DNA binding by amino-functionalized modification: mono-amine (MA), di-amine (DA), and tri-amine (TA). The red-ball means the amine groups of FMS.

Kinetic lattice Monte Carlo model for oxygen vacancy diffusion in praseodymium doped ceria: Applications to materials design
 Pratik P. Dholabhai, Shahriar Anwar, James B. Adams, Peter Crozier and Renu Sharma
 page 811



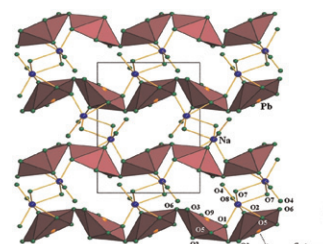
Ionic conductivity in praseodymium doped ceria as a function of dopant concentration calculated using the kinetic lattice Monte Carlo vacancy-repelling model, which predicts the optimal composition for achieving maximum conductivity.

Synthesis and characterization of hybrid materials based on 1-butyl-3-methylimidazolium tetrafluoroborate ionic liquid and Dawson-type tungstophosphate $\text{K}_7[\text{H}_4\text{PW}_{18}\text{O}_{62}] \cdot 18\text{H}_2\text{O}$ and $\text{K}_6[\text{P}_2\text{W}_{18}\text{O}_{62}] \cdot 13\text{H}_2\text{O}$
 Malika Ammam and Jan Fransaer
 page 818



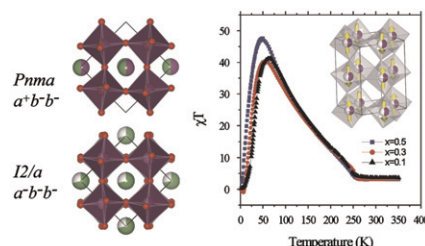
Powder XRD patterns of (a) PW_{18} , (b) $\text{K}[\text{BMIM}]_6\text{H}_4\text{PW}_{18}\text{O}_{62}$, (c) P_2W_{18} , and (d) $\text{K}_2[\text{BMIM}]_4\text{P}_2\text{W}_{18}\text{O}_{62}$.

Synthesis, crystal structure and optical properties of a novel sodium lead pentaborate, NaPbB_5O_9
 Min Zhang, Shilie Pan, Jian Han and Zhongxiang Zhou
 page 825



A new phase, NaPbB_5O_9 , has been discovered in the ternary $\text{M}_2\text{O}-\text{PbO}-\text{B}_2\text{O}_3$ (M = alkali-metal) system. The crystal structure consists of a novel infinite $\infty[\text{PbO}_6]$ chains.

Structure and magnetic order in the series $\text{Bi}_x\text{RE}_{1-x}\text{Fe}_{0.5}\text{Mn}_{0.5}\text{O}_3$ ($\text{RE} = \text{La}, \text{Nd}$)
 C.A. Bridges, A.S. Sefat, E.A. Payzant, L. Cranswick and M.P. Paranthaman
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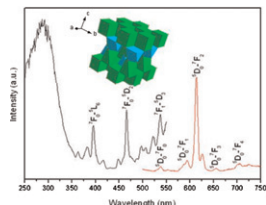


The influence of Bi^{3+} on the structural and magnetic properties of the rare-earth-containing perovskites $\text{REFe}_{0.5}\text{Mn}_{0.5}\text{O}_3$ ($\text{RE} = \text{La}, \text{Nd}$) was studied. Crystal structures in both La and Nd series were determined using X-ray and neutron diffraction to be GdFeO_3 -type Pnma with the exception of the $\text{Bi}_{0.3}\text{La}_{0.7}\text{Fe}_{0.5}\text{Mn}_{0.5}\text{O}_3$ sample, which is monoclinic $\text{I}2/a$ in the $a^-b^-b^-$ tilt scheme. The samples undergo a transition to G-type antiferromagnetic order along with a weak ferromagnetic component, mixed with the cluster-glass type behavior.

Continued

Determining the structure of tetragonal Y_2WO_6 and the site occupation of Eu^{3+} dopant

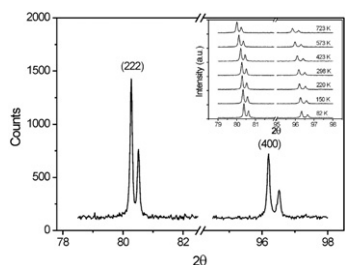
Jinping Huang, Jun Xu, Hexing Li, Hongshan Luo, Xibin Yu and Yikang Li
page 843



The excitation and emission spectra of $\text{Y}_2\text{WO}_6:\text{Eu}^{3+}$ indicates the effect of long wavelength-excited property, which is ascribed to the cube coordination environment of Eu^{3+} ions with the uniform Eu–O bond length.

Crystal structure of $\text{Ba}_2\text{InTaO}_6$ as determined by the Rietveld refinement

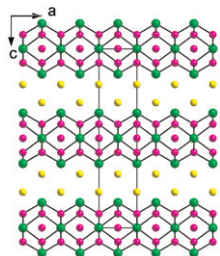
T.S. Hammink, W.T. Fu and D.J.W. IJdo
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Enlarged sections of the X-ray diffraction pattern of $\text{Ba}_2\text{InTaO}_6$ showing the basic (222) and (400) reflections. Insert shows the evolution of these reflections as function of temperature. No peak splitting is observed in the temperature range between 82 and 723 K.

$\text{K}_2\text{Mg}_{5-x}\text{Sn}_3$ and $\text{K}_3\text{Mg}_{18}\text{Tl}_{11}$ ($\text{Tl} = \text{Sn, pb}$) with two types of Mg–Sn/Pb frameworks

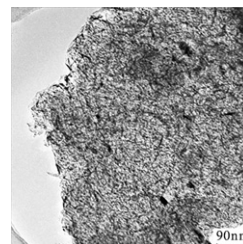
Xiao-Wu Lei
page 852



Two new K–Mg–Tl phases, $\text{K}_2\text{Mg}_{5-x}\text{Sn}_3$ ($x=0.28$) and $\text{K}_3\text{Mg}_{18}\text{Tl}_{11}$ ($\text{Tl} = \text{Sn, Pb}$), have been synthesized and structurally characterized. $\text{K}_2\text{Mg}_{5-x}\text{Sn}_3$ is isostructural with $\text{Ni}_{7-x}\text{SbQ}_2$ ($Q = \text{Se, Te}$) and features a 2D corrugated $[\text{Mg}_5\text{Sn}_3]$ layer that is separated by K^+ cations, and $\text{K}_3\text{Mg}_{18}\text{Tl}_{11}$ ($\text{Tl} = \text{Sn, Pb}$) is closely related to the $\text{Ho}_2\text{Rh}_{12}\text{As}_7$ structure type and features a 3D $[\text{Mg}_{18}\text{Tl}_{11}]$ network with 1D hexagonal tunnels along the c -axis occupied by K^+ cations.

Simple synthesis of mesoporous boron nitride with strong cathodoluminescence emission

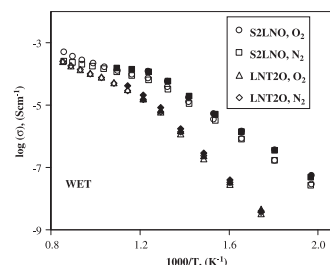
Xiang-Lin Meng, Ning Lun, Yong-Xin Qi, Hui-Ling Zhu, Fu-Dong Han, Long-Wei Yin, Run-Hua Fan, Yu-Jun Bai and Jian-Qiang Bi
page 859



The mesoporous BN with a high specific surface area of $219 \text{ m}^2 \text{ g}^{-1}$ exhibits a strong luminescence emission around 3.41 eV in the CL spectra, high thermal stability in both morphology and structure, and good oxidation resistance up to 800°C .

B-site substitutions in $\text{LaNb}_{1-x}\text{M}_x\text{O}_{4-\delta}$ materials in the search for potential proton conductors ($M = \text{Ga, Ge, Si, B, Ti, Zr, P, Al}$)

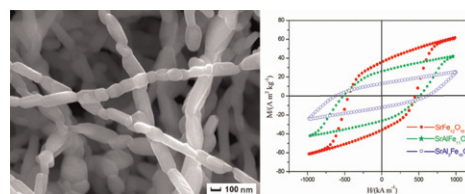
A.D. Brandão, J. Gracio, G.C. Mather, V.V. Kharton and D.P. Fagg
page 863



Comparison of total (open symbols) and bulk (closed symbols) conductivities measured in wet ($p(\text{H}_2\text{O}) \approx 0.026 \text{ atm.}$) nitrogen and oxygen atmospheres for $\text{LaNb}_{0.98}\text{Ti}_{0.02}\text{O}_{4-\delta}$ (LNT2O) and $\text{Sr}_{0.02}\text{La}_{0.98}\text{NbO}_{4-\delta}$ (S2LNO) materials.

Microstructure and magnetic properties of electrospun one-dimensional Al^{3+} -substituted $\text{SrFe}_{12}\text{O}_{19}$ nanofibers

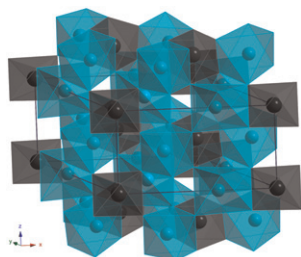
Mingquan Liu, Xiangqian Shen, Fuzhan Song, Jun Xiang and Xianfeng Meng
page 871



Al^{3+} ions substituted strontium ferrite nanofibers have been prepared by the electrospinning with a diameter of about 100 nm and the Al^{3+} ion substitution has a great effect on the microstructure and magnetic property of $\text{SrAl}_x\text{Fe}_{12-x}\text{O}_{19}$ nanofibers.

Compositionally controlled metal–insulator transition in $\text{Ti}_{2-x}\text{In}_x\text{TeO}_6$

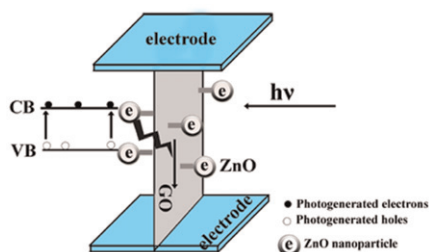
Theeranun Siritanon, A.W. Sleight and M.A. Subramanian
page 877



A complete solid solution between Ti_2TeO_6 and In_2TeO_6 is formed. A compositionally controlled metal–insulator transition occurs in $\text{Ti}_{2-x}\text{In}_x\text{TeO}_6$ at an x value of about 1.5. No superconductivity could be detected down to 5 K.

Photovoltaic properties of graphene oxide sheets beaded with ZnO nanoparticles

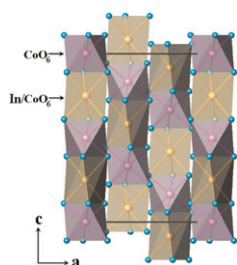
Huan Wang, Li Wang, Chaoqun Qu, Yadong Su, Shansheng Yu, Weitao Zheng and Yichun Liu
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Upon irradiating the GO–ZnO sample with a light having an energy equalizing the band gap energy, the photogenerated charge–hole pairs are produced, and have been separated effectively.

Phase diagram of $\text{SrO–InO}_{1.5}\text{–CoO}_x$ and a new compound $\text{Sr}_3\text{In}_{0.9}\text{Co}_{1.1}\text{O}_6$

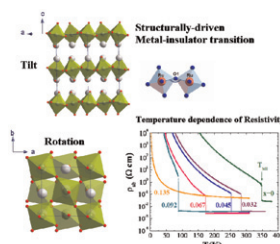
Kuo Li, Denis Sheptyakov, Yingxia Wang, Chun-Keung Loong and Jianhua Lin
page 888



$\text{Sr}_3\text{In}_{0.9}\text{Co}_{1.1}\text{O}_6$ possesses 1D chains constructed by alternating face-sharing CoO_6 octahedra and $(\text{In}_{0.9}\text{Co}_{0.1})\text{O}_6$ trigonal prisms. The high spin Co^{3+} ($S=2$) in trigonal prism shows a g factor of 2.0.

Structurally-driven metal–insulator transition in $\text{Ca}_2\text{Ru}_{1-x}\text{Cr}_x\text{O}_4$ ($0 \leq x < 0.14$): A single crystal X-ray diffraction study

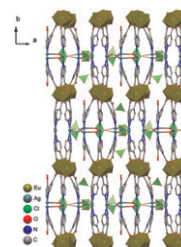
T.F. Qi, M. Ge, O.B. Korneta, S. Parkin, L.E. De Long and G. Cao
page 893



The metal–insulator transition temperature (T_{MI}) was drastically reduced by Cr doping, and is closely related to the distortion of structure.

Synthesis, crystal structures and luminescent properties of two 4d–4f Ln–Ag heterometallic coordination polymers based on anion template

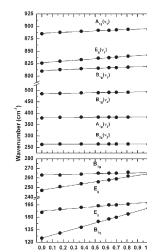
Le-Qing Fan, Yuan Chen, Ji-Huai Wu and Yun-Fang Huang
page 899



Two new anion-templated 2D 4d–4f Ln–Ag heterometallic coordination polymers based on novel lanthanide–carboxylate chains and pillared $\text{Ag}(\text{IN})_2$ units, $\{[\text{Ln}_3\text{Ag}_5(\text{IN})_{10}(\text{H}_2\text{O})_7] \cdot 4(\text{ClO}_4) \cdot 4(\text{H}_2\text{O})\}_n$ ($\text{Ln} = \text{Eu}$ (**1**) and Sm (**2**), HIN = isonicotinic acid), have been hydrothermally synthesized and structurally characterized. **1** and **2** exhibit good luminescent properties.

Phonons in isostructural $(\text{Nd}, \text{Yb})\text{:Y}_x\text{Gd}_{1-x}(\text{VO}_4)$ laser crystals: A Raman scattering study

Nana Zhang, Jiyang Wang, Xiaobo Hu, Huaijin Zhang, C.C. Santos, A.P. Ayala and I. Guedes
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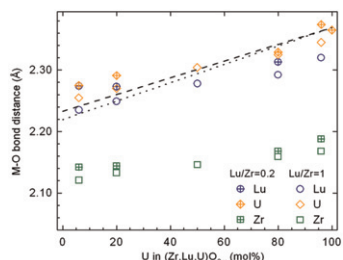
Plot of the observed wavenumbers of $\text{Nd:Y}_x\text{Gd}_{1-x}(\text{VO}_4)$ versus Y content (x). The linear trend indicates that most of the observed wavenumbers exhibit a one-phonon-like behavior.

Continued

Local structure in solid solutions of stabilised zirconia with actinide dioxides (UO₂, NpO₂)

Marcus Walter, Joseph Somers, Daniel Bouëxière and Jörg Rothe

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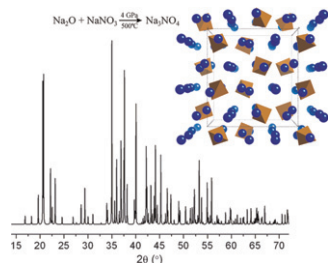


Metal-oxygen bond distances in (Zr,Lu,U)O_{2-x} solid solutions with different oxygen vacancy concentrations (Lu/Zr=1 and Lu/Zr=0.5).

High-pressure synthesis and structural behavior of sodium orthonitrate Na₃NO₄

R. Quesada Cabrera, A. Sella, E. Bailey, O. Leynaud and P.F. McMillan

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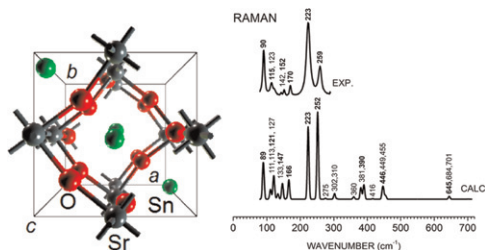


We studied Na₃NO₄ at high pressure using Raman spectroscopy and X-ray diffraction and determined $V(P)$ to 64 GPa. We investigated synthesis and phase behavior of the orthonitrate at high- P,T conditions.

Structural, optoelectronic, infrared and Raman spectra of orthorhombic SrSnO₃ from DFT calculations

E. Moreira, J.M. Henriques, D.L. Azevedo, E.W.S. Caetano, V.N. Freire and E.L. Albuquerque

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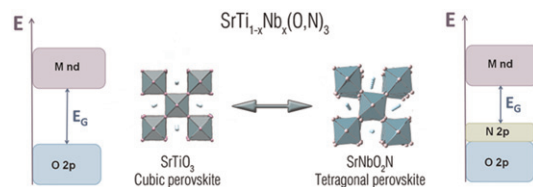


Orthorhombic SrSnO₃: a view of the unit cell (left) and plots showing the calculated and experimental Raman spectra (right).

Perovskite-type SrTi_{1-x}Nb_x(O,N)₃ compounds: Synthesis, crystal structure and optical properties

Alexandra Maegli, Songhak Yoon, Eugenio Otal, Lassi Karvonen, Peter Mandaliev and Anke Weidenkaff

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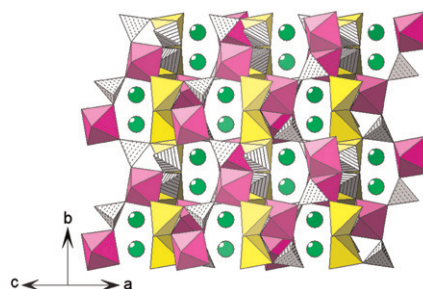


The system SrTi_{1-x}Nb_x(O,N)₃ is described and the changes in crystal structure, nitrogen content and width of the band gap are discussed.

Structural study and physical properties of a new phosphate KCuFe(PO₄)₂

Abdesslem Badri, Mourad Hidouri, María Luisa López, Carlos Pico, Alain Wattiaux and Mongi Ben Amara

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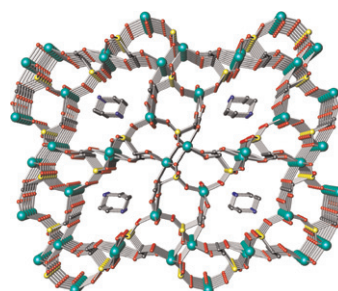


A projection along the [010] direction of the structure showing the six-edged tunnels, occupied by the K⁺ ions.

Syntheses, crystal structures, thermal stabilities and luminescence of six M(II)-hydroxyphosphonoacetate materials

Ruibiao Fu, Shengmin Hu and Xintao Wu

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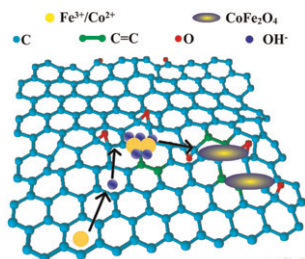
Six new metal phosphonates exhibit layered or 3D frameworks based on 2-hydroxyphosphonoacetate with five new coordination modes.

Rapid Communication

Preparation of magnetic CoFe_2O_4 -functionalized graphene sheets via a facile hydrothermal method and their adsorption properties

Nianwu Li, Mingbo Zheng, Xiaofeng Chang, Guangbin Ji, Hongling Lu, Luping Xue, Lijia Pan and Jieming Cao

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OH^- was recognized as a tie to integrate the inorganic salts with the graphene sheets, which made reaction started and developed on the surface of graphene sheets and formed cobalt ferrite nanoparticles on graphene sheets.

Author inquiries

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