

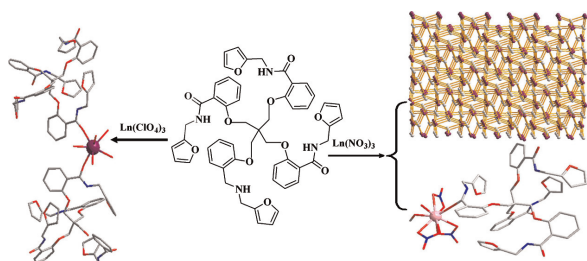
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Regular Articles

Synthesis, structure and luminescence properties of lanthanide complex with a new tetrapodal ligand featuring salicylamide arms

Xue-Qin Song, Xiao-Guang Wen, Wei-Sheng Liu and Da-Qi Wang

Page 1



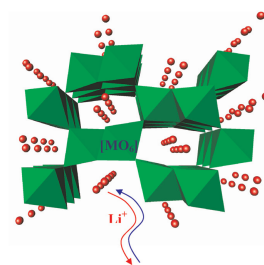
We present here a series of zero- to three-dimensional lanthanide coordination structures and luminescence properties of Eu(III) complex of a new tetrapodal ligand.

Regular Articles—Continued

New ramsdellites $\text{LiTi}_{2-y}\text{V}_y\text{O}_4$ ($0 \leq y \leq 1$): Synthesis, structure, magnetic properties and electrochemical performances as electrode materials for lithium batteries

Alois Kuhn, María Martín and Flaviano García-Alvarado

Page 20

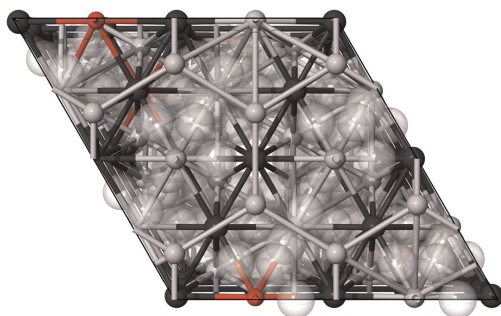


Ti-based ramsdellite compounds can make up cathode and anode materials for lithium batteries by introducing vanadium. Lithium deinsertion experiments on $\text{LiTi}_{2-y}\text{V}_y\text{O}_4$ materials develop a high operating voltage (3V) useful as the cathode, while lithium insertion experiments yield a low operating voltage, 1.5V, useful as the anode. Vanadium-rich compounds show specific theoretical capacity values in the high voltage range that are even comparable to those reported for LiFePO_4 which is presently one of the preferred cathode materials for lithium batteries.

Neutron powder diffraction and first-principles computational studies of $\text{CuLi}_x\text{Mg}_{2-x}$ ($x \cong 0.08$), CuMg_2 , and Cu_2Mg

M.H. Braga, J.J.A. Ferreira, J. Siewenie, Th. Proffen, S.C. Vogel and L.L. Daemen

Page 10

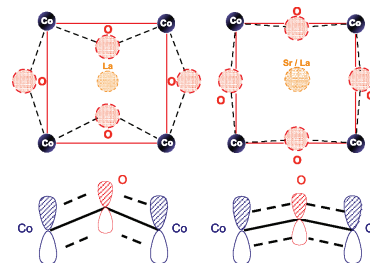


$\text{CuLi}_x\text{Mg}_{2-x}$ with $x=0.08$ crystallizes in a $P6_22$ hexagonal structure in which Li (red) will substitute Mg1 ($1/2, 0, z$) sites (Mg-grey). Cu atoms are represented by black spheres and empty spaces by transparent ones.

Chemical and electronic characterization of cobalt in a lanthanum perovskite. Effects of strontium substitution

Jose L. Hueso, Juan P. Holgado, Rosa Pereñíguez, Simon Mun, Miquel Salmeron and Alfonso Caballero

Page 27

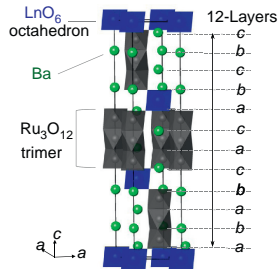


Change in spin multiplicity induced by the bigger size of Sr(II) cations, aligning the Co–O–Co atoms, and favoring the overlapping of π -symmetry cobalt and oxygen orbitals.

Magnetic properties of quadruple perovskites $Ba_4LnRu_3O_{12}$ ($Ln = La, Nd, Sm-Gd, Dy-Lu$)

Yuki Shimoda, Yoshihiro Doi, Makoto Wakeshima and Yukio Hinatsu

Page 33

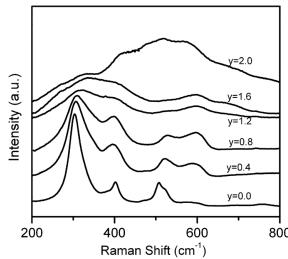


Quadruple perovskites $Ba_4LnRu_3O_{12}$ ($Ln = La, Nd, Sm-Gd, Dy-Lu$) were prepared. They adopt the 12L-perovskite-type structure consisting of Ru_3O_{12} trimers and LnO_6 octahedra. All of these compounds show an antiferromagnetic transition at 2.5–30 K. For $Ba_4NdRu_3O_{12}$, ferrimagnetic ordering has been observed at 11.5 K. The observed magnetic transition is due to the magnetic behavior of the $Ru_3^{4.33+}O_{12}$ trimer with $S = \frac{1}{2}$. Magnetic properties of $Ba_4LnRu_3O_{12}$ were compared with those of triple perovskites $Ba_3LnRu_2O_9$ and double perovskites Ba_2LnRuO_6 .

Order-disorder transition in the $Nd_{2-y}Y_yZr_2O_7$ system: Probed by X-ray diffraction and Raman spectroscopy

B.P. Mandal, P.S.R. Krishna and A.K. Tyagi

Page 41

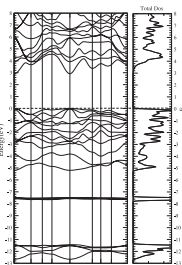


In $Nd_{2-y}Y_yZr_2O_7$ series, the structure changes from pyrochlore to defect fluorite with increase in Y content in the series. The Raman spectra explicitly shows how the structural changes take place in the system.

Ab-initio study of the structural, linear and nonlinear optical properties of $CdAl_2Se_4$ defect-chalcopyrite

T. Ouahrani, Ali H. Reshak, R. Khenata, B. Amrani, M. Mebrouki, A. Otero-de-la-Roza and V. Luaña

Page 46

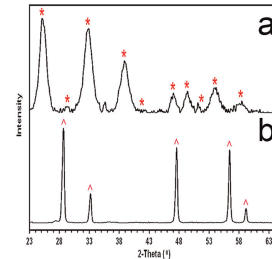


Calculated band structure and total density of $CdAl_2Se_4$.

Thermolysis of lanthanide dithiocarbamate complexes

William L. Boncher, Michelle D. Regulacio and Sarah L. Stoll

Page 52

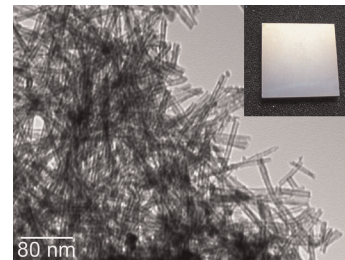


Polycrystalline lanthanide sulfide materials were formed at low temperatures using a single-source precursor based on the lanthanide dithiocarbamate complex.

TiO₂ nanotube, nanowire, and rhomboid-shaped particle thin films fixed on a titanium metal plate

Yuko Inoue, Iwao Noda, Toshio Torikai, Takanori Watari, Takao Hotokebuchi and Mitsunori Yada

Page 57

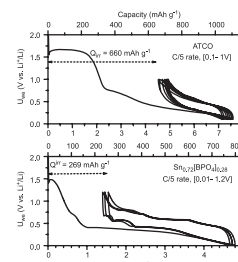


Titanium dioxide nanotube, nanowire, and rhombic particle thin films could be formed by various treatments on a sodium titanate nanotube thin film fixed on a titanium metal plate.

$Sn_x[BPO_4]_{1-x}$ composites as negative electrodes for lithium ion cells: Comparison with amorphous $SnB_{0.6}P_{0.4}O_{2.9}$ and effect of composition

Donato Ercole Conte, Abdelmaula Aboulaich, Florent Robert, Josette Olivier-Fourcade, Jean-Claude Jumas, Christian Jordy and Patrick Willmann

Page 65

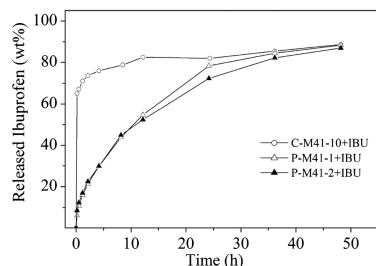


Galvanostatic discharge-charge curves of ATCO and $Sn_{0.72}[BPO_4]_{0.28}$ composite materials at C/5 rate, respectively.

Drug delivery from hydrophobic-modified mesoporous silicas: Control via modification level and site-selective modification

Qunli Tang, Yuxi Chen, Jianghua Chen, Jin Li, Yao Xu, Dong Wu and Yuhan Sun

Page 76

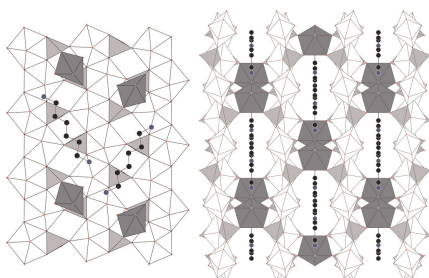


The distribution of DMS groups on the pore surfaces of the mesostructures strongly affects the drug release rate. The P-M41-1 and the P-M41-2 possess the close DMS modification levels as the C-M41-10, but the ibuprofen release rates from the P-M41-1 and P-M41-2 are much slower than that from the C-M41-10.

A new series of pillared uranyl-vanadates based on uranophane-type sheets in the uranium-vanadium-linear alkyl diamine systems

Laurent Jouffret, Murielle Rivenet and Francis Abraham

Page 84

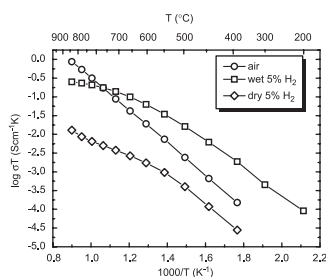


The $(C_6N_2H_{20})\{[(UO_2)(H_2O)][(UO_2)(VO_4)]_4\}$ compound: projection in the (100) and in the (001) planes showing the amine position.

Proton conductivity of potassium doped barium zirconates

Xiaoxiang Xu, Shanwen Tao and John T.S. Irvine

Page 93

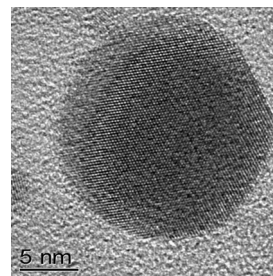


Potassium doped barium zirconates have been synthesized by solid state reactions. It was found that the solubility limit of potassium on A-sites is between 5% and 10 %. The sintering conditions and conductivity can be improved significantly by adding 1 wt% ZnO during material synthesis. Five percent doping of potassium at A-site can double the total conductivity.

Magnetite and magnetite/silver core/shell nanoparticles with diluted magnet-like behavior

Marco Garza-Navarro, Alejandro Torres-Castro, Virgilio González, Ubaldo Ortiz and Elder De la Rosa

Page 99

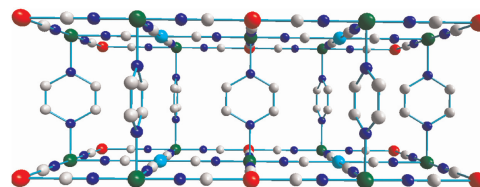


Biopolymer chitosan was used as stabilization media to synthesize both magnetite and magnetite/silver core/shell nanoparticles. Results of HRTEM and NBD patterns confirm core/shell morphology of the obtained nanoparticles. It was found that the composites show diluted magnet-like behavior.

Low temperature structural transformation in $T[Ni(CN)_4] \cdot xpyz$ with $x = 1, 2$; $T = Mn, Co, Ni, Zn, Cd$; $pyz = pyrazine$

J. Rodríguez-Hernández, A.A. Lemus-Santana, J. Ortiz-López, S. Jiménez-Sandoval and E. Reguera

Page 105

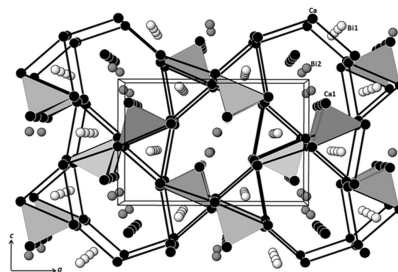


Low temperature ordered structure for pyrazine in $T[Ni(CN)_4] \cdot pyz$.

Hydrogen in polar intermetallics: Syntheses and structures of the ternary $Ca_5Bi_3D_{0.93}$, $Yb_5Bi_3H_x$, and $Sm_5Bi_3H_{\sim 1}$ by powder neutron or single crystal X-ray diffraction

E. Alejandro Leon-Escamilla, Panagiotis Dervenagas, Constantine Stassis and John D. Corbett

Page 114

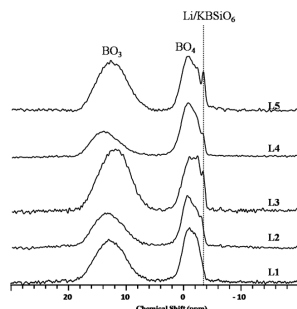


The structure of $Ca_5Bi_3H_{0.93}$ occurs in the novel Ca_5Sb_3F structure type with D centered in the shaded calcium tetrahedra.

Continued

MAS-NMR studies of lithium aluminum silicate (LAS) glasses and glass–ceramics having different $\text{Li}_2\text{O}/\text{Al}_2\text{O}_3$ ratio

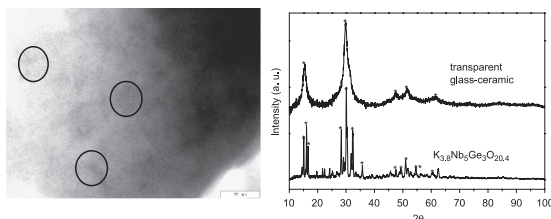
A. Ananthanarayanan, G.P. Kothiyal, L. Montagne and B. Revel
 Page 120



The ^{11}B MAS-NMR spectra of lithium aluminum silicate (LAS) glass–ceramics indicating the formation of Li/KBSiO_6 phase. This phase is isostructural with virgilite and cannot be distinguished in X-ray diffractograms.

Crystallization of niobium germanosilicate glasses

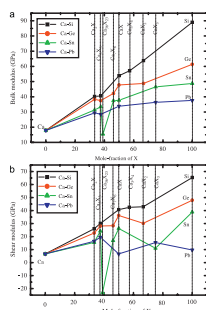
Rodrigo Santos, Luís F. Santos, Rui M. Almeida, Joachim Deubener and Lothar Wondraczek
 Page 128



TEM image and XRD pattern of the glass ceramic produced (circles indicate nanocrystals).

First-principle studies of $\text{Ca}-\text{X}$ ($\text{X} = \text{Si}, \text{Ge}, \text{Sn}, \text{Pb}$) intermetallic compounds

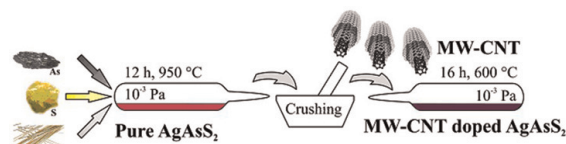
Zhiwen Yang, Dongmin Shi, Bin Wen, Roderick Melnik, Shan Yao and Tingju Li
 Page 136



Calculated (a) bulk moduli and (b) shear moduli of $\text{Ca}-\text{X}$ system intermetallic compounds.

Carbon nanotube—chalcogenide glass composite

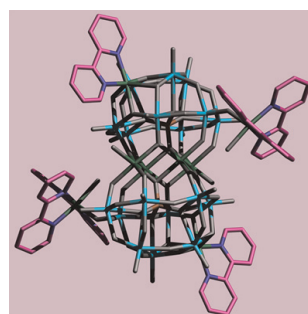
Stepan Stehlik, Jiri Orava, Tomas Kohoutek, Tomas Wagner, Miloslav Frumar, Vitezslav Zima, Toru Hara, Yoshio Matsui, Kazuyuki Ueda and Martin Pumera
 Page 144



Preparation of multi-walled carbon nanotube-doped chalcogenide glasses by direct synthesis and the melt-quenching method

Sandwich-type polyoxotungstate hybrids decorated by nickel-aromatic amine complexes

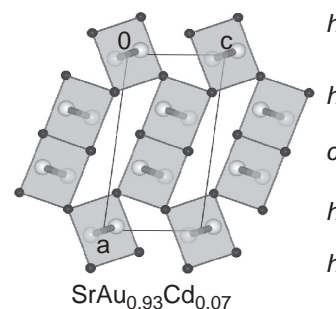
Peng-Tao Ma, Jun-Wei Zhao, Jing-Ping Wang, Yue Shen and Jing-Yang Niu
 Page 150



Three new sandwich-type polyoxotungstates (POTs) decorated by nickel-2,2'-bpy complexes were successfully synthesized under hydrothermal conditions and structurally characterized.

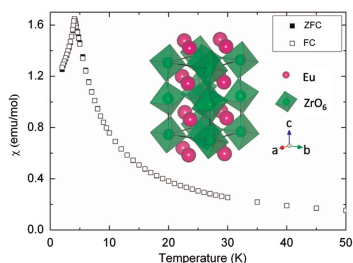
$(\text{Ca}/\text{Sr})\text{Au}_x\text{Cd}_{1-x}$: Stacking variants of the $\text{CrB}-\text{FeB}$ series

Wiebke Harms, Ines Dürr, Michael Daub and Caroline Röhr
 Page 157



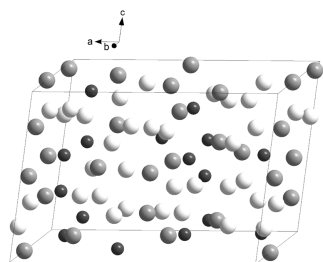
$\text{SrAu}_{0.93}\text{Cd}_{0.07}$, one of the stacking sequences of the CrB/FeB structure type series found in the quasibinary section $\text{SrAu}-\text{SrCd}$.

Antiferromagnetism of perovskite EuZrO_3
 Yanhua Zong, Koji Fujita, Hirofumi Akamatsu,
 Shunsuke Murai and Katsuhisa Tanaka
 Page 168



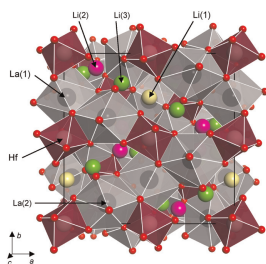
Perovskite EuZrO_3 with almost all Eu ions present as Eu^{2+} has been synthesized and its structure and magnetic properties have been studied. An antiferromagnetic transition was observed around 4.1 K for the first time. The mechanism of the magnetic transition has been discussed.

Crystal structures of three intermetallic phases in the Mo–Pt–Si system
 J.-M. Joubert, Ya. Tokaychuk and R. Černý
 Page 173



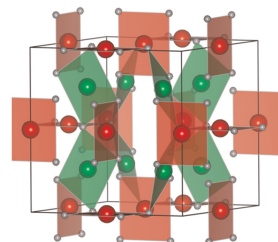
The crystal structures of three ternary Mo–Pt–Si intermetallic compounds have been determined *ab initio* from powder X-ray diffraction data. The three structures represent new structure types.

Neutron powder diffraction study of tetragonal $\text{Li}_7\text{La}_3\text{Hf}_2\text{O}_{12}$ with the garnet-related type structure
 Junji Awaka, Norihito Kijima, Kunimitsu Kataoka,
 Hiroshi Hayakawa, Ken-ichi Ohshima and Junji Akimoto
 Page 180



The crystal structure of tetragonal $\text{Li}_7\text{La}_3\text{Hf}_2\text{O}_{12}$ had the garnet-related type structure with a space group of $I4_1/acd$ (no. 142) with the lattice constants of $a = 13.106(2) \text{ \AA}$ and $c = 12.630(2) \text{ \AA}$. The tetragonal $\text{Li}_7\text{La}_3\text{Hf}_2\text{O}_{12}$ had the fully ordered Li arrangement.

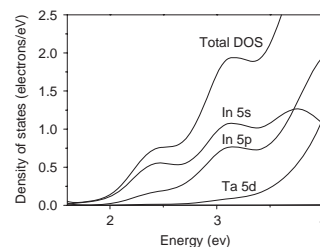
Crystal structure of the monoclinic and cubic polymorphs of $\text{BiMn}_7\text{O}_{12}$
 H. Okamoto, N. Imamura, M. Karppinen, H. Yamauchi
 and H. Fjellvåg
 Page 186



The complex perovskite $\text{BiMn}_7\text{O}_{12}$ occurs with polymorphic structures, cubic and monoclinic. Structural analysis reveals unusual behavior for oxygen and bismuth in the monoclinic and cubic phases, respectively. Unusually large (and anisotropic) displacement parameters for some of the oxygen ions in the monoclinic phase indicated competition between non-equivalent Mn–O bonds for the corner-sharing d -type JT Mn_BO_6 and square-planar Mn_AO_4 polyhedra.

Photocatalytic splitting of water under visible-light irradiation over the NiOx-loaded $\text{Sm}_2\text{InTaO}_7$ with $4f-d^{10}-d^0$ configuration

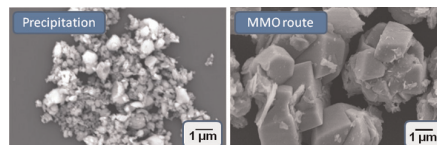
Xinde Tang, Hongqi Ye, Hui Liu, Chenxia Ma and Zhi Zhao
 Page 192



A new visible-light-response photocatalyst $\text{Sm}_2\text{InTaO}_7$ with $4f-d^{10}-d^0$ configuration was developed. DFT calculation indicated that strong dispersion from the hybridized In $5s$ $5p$ orbitals was responsible for the high photocatalytic activity.

Comparative study of the synthesis of layered transition metal molybdates

S. Mitchell, A. Gómez-Avilés, C. Gardner and W. Jones
 Page 198

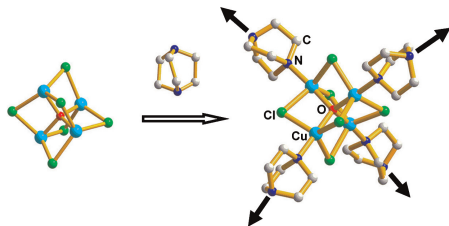


Mixed metal oxides (MMOs) derived from layered double hydroxide precursors differ in their reactivity on exposure to aqueous molybdate containing solutions. We investigate the influence of the molybdate source, the rehydration pH and the ratio of T/Mo on the reactivity of some T -Al containing MMOs ($T = \text{Co}, \text{Ni}, \text{Cu}$ or Zn) towards the formation of layered transition metal molybdates of general formula $A\text{T}_2(\text{OH})(\text{MoO}_4)_2 \cdot \text{H}_2\text{O}$ (where $A^+ = \text{NH}_4^+, \text{K}^+$ or Na^+).

Continued

[Cu₄OCl₆(DABCO)₂] · 0.5DABCO · 4CH₃OH (“MFU-5”): Modular synthesis of a zeolite-like metal-organic framework constructed from tetrahedral {Cu₄OCl₆} secondary building units and linear organic linkers

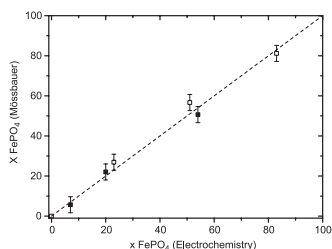
Ying-Ya Liu, Maciej Grzywa, Matthias Weil and Dirk Volkmer
 Page 208



The metal-organic framework [Cu₄OCl₆(DABCO)₂] · 0.5DABCO · 4CH₃OH (MFU-5) is constructed from a molecular precursor containing {Cu₄OCl₆} secondary building units which become cross-linked into a 3D zeolite-type network with hexagonal symmetry by linear DABCO ligands (DABCO = 1,4-diazabicyclo[2.2.2]octane).

Determination of the Lamb-Mössbauer factors of LiFePO₄ and FePO₄ for electrochemical *in situ* and *operando* measurements in Li-ion batteries

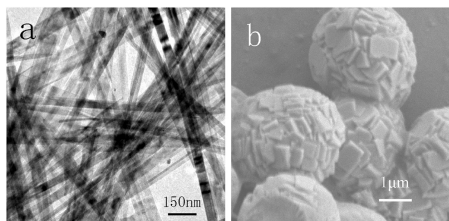
L. Aldon, A. Perea, M. Womes, C.M. Ionica-Bousquet and J.-C. Jumas
 Page 218



Relative amount of FePO₄ obtained by Mössbauer and electrochemical data. We have corrected Mössbauer spectral intensities with our *f* factor of both LiFePO₄ and FePO₄. Open (filled) squares correspond to values obtained during charging (discharging) process. The dashed line, given as a guideline for the eye, corresponds to the ideal case where amounts deduced from different experimental measurements are equal.

Hydrothermal synthesis of NiS nanobelts and NiS₂ microspheres constructed of cuboids architectures

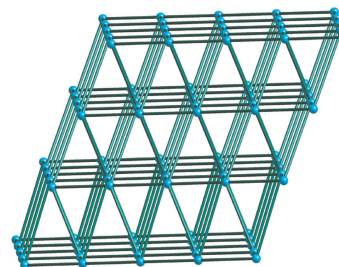
Lili Wang, Yongchun Zhu, Haibo Li, Qianwen Li and Yitai Qian
 Page 223



Hexagonal NiS nanobelts and cubic NiS₂ microspheres were hydrothermally synthesized in the reaction of Ni(CH₃COO)₂ · 4H₂O and Na₂S₂O₃ · 5H₂O.

Polyoxometalate-based eight-connected self-catenated network and fivefold interpenetrating framework

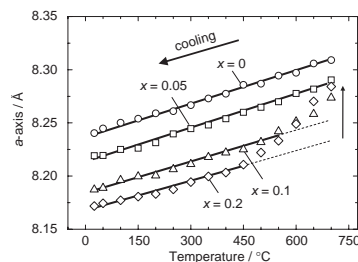
Zhiming Zhang, Jia Liu, Yangguang Li, Shuang Yao, Enbo Wang and Xinlong Wang
 Page 228



Compound **1** is the POM-based unprecedented eight-connected self-penetrating organic-inorganic hybrid network constructed from the cuprous chloride clusters [Cu₆Cl₃], Lindquist-type polyoxoanions [Mo^VW₅O₁₉], and the 4,4'-bipyridine ligands.

High-temperature X-ray diffraction study of crystallization and phase segregation on spinel-type lithium manganese oxides

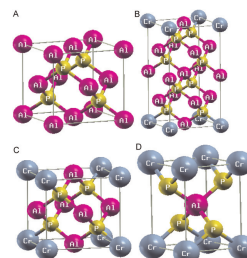
Shinichi Komaba, Naoaki Yabuuchi and Sachi Ikemoto
 Page 234



Non-linear variation of lattice parameters of the Li excess LiMn₂O₄ spinels was observed during cooling process from 700 to 25 °C.

First principles calculations of electronic structure and magnetic properties of Cr-based magnetic semiconductors Al_{1-x}Cr_xX (X=N, P, As, Sb)

Y. Saeed, A. Shaikat, S. Nazir, N. Ikram and Ali Hussain Reshak
 Page 242

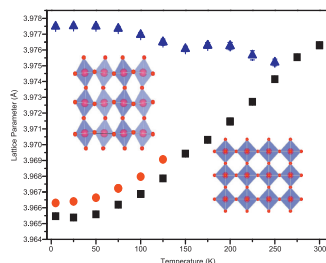


The prototype structures of Cr doped AlX (X=N, P, As, Sb) compounds: (A) zinc blende AlP for x=0, (B) Cr₁Al₇P₈ for x=0.125, (C) Cr₁Al₃P₄ for x=0.25, (D) Cr₁Al₁P₂ for x=0.5.

Neutron diffraction study of phase transitions in perovskite-type strontium molybdate SrMoO₃

René B. Macquart, Brendan J. Kennedy and Maxim Avdeev

Page 250

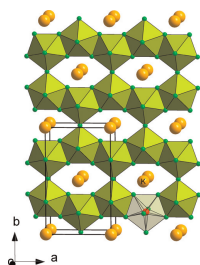


Variable temperature neutron diffraction measurements of SrMoO₃ from 5 K to room temperature show the presence of two phase transitions associated with tilting of the octahedra. On cooling, the structure transforms from cubic (*Pm* $\bar{3}$ *m*) to tetragonal (*I4/mcm*) and ultimately orthorhombic (*Imma*).

High pressure synthesis and properties of ternary titanium (III) fluorides in the system KF–TiF₃ containing regular pentagonal bipyramids [TiF₇]

Shoji Yamanaka, Akira Yasuda and Hajime Miyata

Page 256

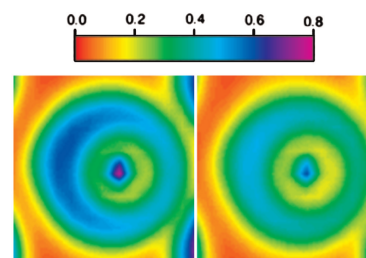


A new ternary fluoride KTi₂F₇ has been developed under high-pressure and high-temperature conditions, which contains pentagonal bipyramid polyhedra [TiF₇].

The influence of sulfur substitution on the atomic displacement in Bi₂Ti₂O₇

Beverly Brooks Hinojosa, Paul M. Lang and Aravind Asthagiri

Page 262

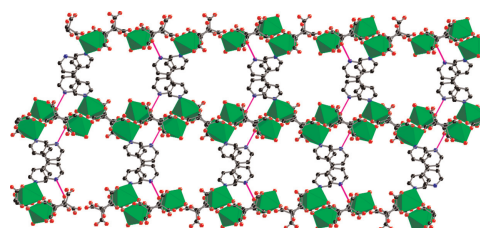


The electron localization function for Bi₂Ti₂O₆O' and Bi₂Ti₂O₆S' respectively show that sulfur substitution on the O' site will suppress lone pair formation.

Homochiral frameworks derived from magnesium, zinc and copper salts of L-tartaric acid

Jeffrey A. Rood, Bruce C. Noll and Kenneth W. Henderson

Page 270



Five metal-organic frameworks derived from L-tartarate and the divalent metal ions magnesium, zinc or copper have been prepared and structurally characterized. Significant structural diversity is displayed within this set of complexes.

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