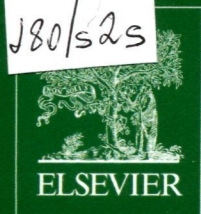


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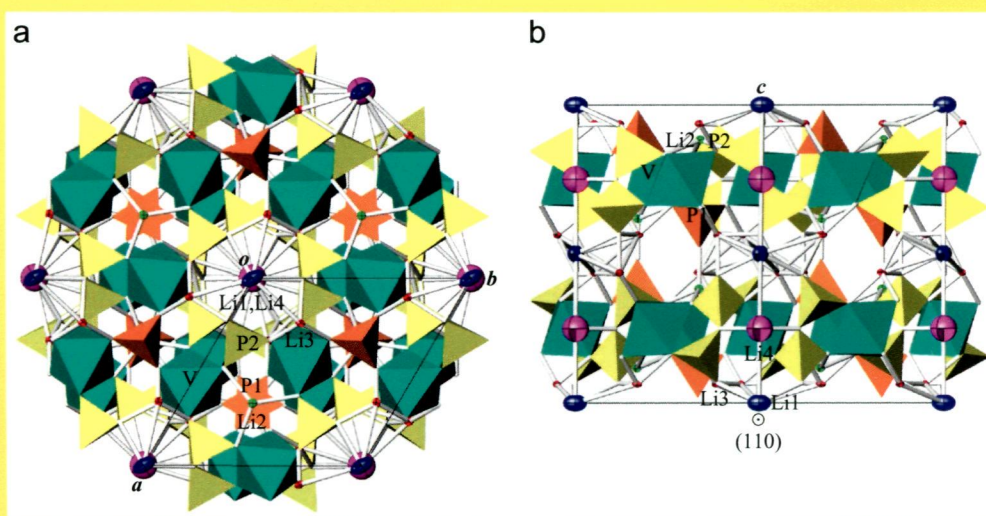
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IN THIS ISSUE:

**Crystal structures and electronic properties for the over-lithiated
and Li-Ag substituted phases of $\text{Li}_9\text{V}_3(\text{P}_2\text{O}_7)_3(\text{PO}_4)_2$
insertion electrode system**



Masashige Onoda, Makoto Inagaki and Hiroaki Saito

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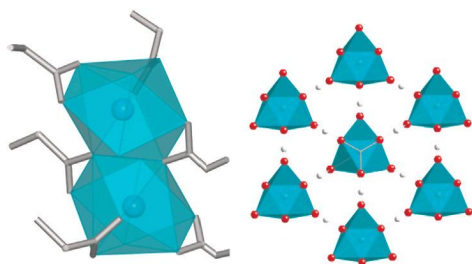
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Regular Articles

Dysprosium complexes with mono-/di-carboxylate ligands— From simple dimers to 2D and 3D frameworks

Yingjie Zhang, Mohan Bhadbhade, Nicholas Scales,
Inna Karatchevtseva, Jason R. Price, Kim Lu and
Gregory R. Lumpkin
page 1

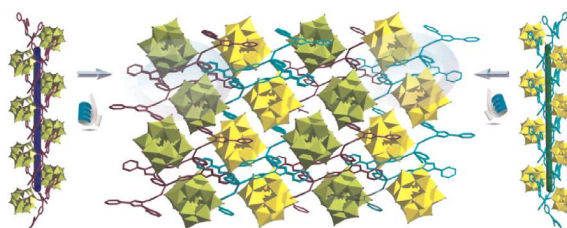


Four dysprosium (Dy) complexes with formate, propionate, butyrate and oxalate ligands have been synthesized and characterized. The Dy formate complex has a 3D pillared metal organic framework and the structure is stable up to 360 °C whilst the complexes with longer alkyl chained mono-carboxylates possess similar di-nuclear structures. The Dy oxalato complex has a 2D hexagonal (honeycomb-type) structure. Their Raman vibration modes have been investigated.

Regular Articles—Continued

Two new helical compounds based on Keggin clusters and N-donor multidentate ligand: Syntheses, structures and properties

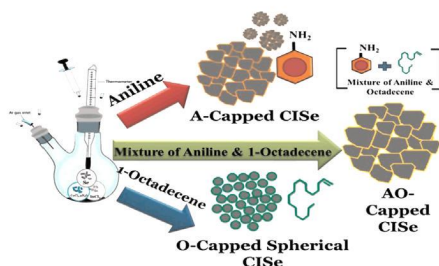
Shi Zhou, Bo Liu, Xiao-Min Li, Tian Shi and Ya-Guang Chen
page 15



Two new compounds, $[\text{CuH}_3\text{L}_2(\text{GeMo}_{12}\text{O}_{40})]\cdot 2\text{H}_2\text{O}$ (1) and $[\text{CuH}_3\text{L}_2(\text{SiMo}_{12}\text{O}_{40})]\cdot 2\text{H}_2\text{O}$ (2) have been synthesized under hydrothermal conditions. The two compounds possess the left- and right-handed helical chains.

Low-cost fabrication of ternary CuInSe_2 nanocrystals by colloidal route using a novel combination of volatile and non-volatile capping agents

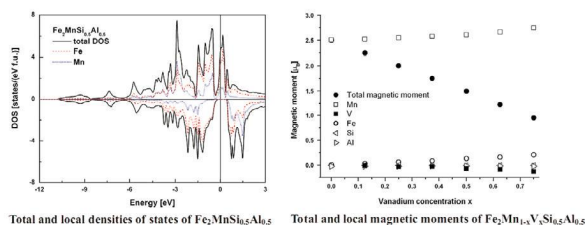
Parul Chawla, Shailesh Narain Sharma and Son Singh
page 9



Without resorting to any post-selenization process and using the colligative properties of the mixture comprising of volatile aniline and non-volatile 1-octadecene to manoeuvre the growth conditions to promote Ostwald ripening, a single phase, monodisperse and nearly stoichiometric ternary CISE nanocrystals are formed by wet-synthesis route.

Ab-initio study of electronic structure and magnetic properties of half-metallic $\text{Fe}_2\text{Mn}_{1-x}\text{V}_x\text{Si}_{10.5}\text{Al}_{0.5}$ alloys

Anna Go
page 21

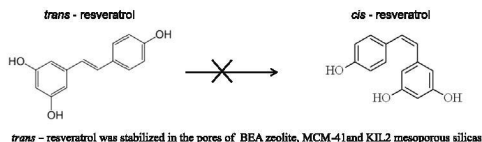


Densities of states of $\text{Fe}_2\text{MnSi}_{10.5}\text{Al}_{0.5}$ and magnetic moments of $\text{Fe}_2\text{Mn}_{1-x}\text{V}_x\text{Si}_{10.5}\text{Al}_{0.5}$.

Preparation of resveratrol-loaded nanoporous silica materials with different structures

Margarita Popova, Agnes Szegedi, Vesselina Mavrodinova, Natasa Novak Tušar, Judith Mihály, Szilvia Klébert, Niko Benbassat and Krassimira Yoncheva

page 37



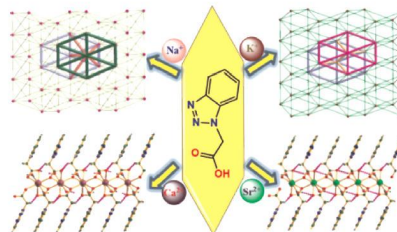
trans-resveratrol was stabilized in the pores of BEA zeolite, MCM-41 and KIL2 mesoporous silicas

trans-Resveratrol was stabilized in the pores of BEA zeolite, MCM-41 and KIL2 mesoporous silicas.

A set of alkali and alkaline-earth coordination polymers based on the ligand 2-(1*H*-benzotriazol-1-yl)acetic acid: Effects the radius of metal ions on structures and properties

Jin-Hua Wang, Gui-Mei Tang, Ting-Xiao Qin, Shi-Chen Yan, Yong-Tao Wang, Yue-Zhi Cui and Seik Weng Ng

page 55

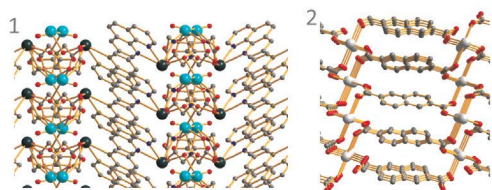


A set of alkali and alkaline-earth metal coordination polymers were hydrothermally synthesized by 2-(1*H*-benzotriazol-1-yl)acetic acid, displaying interesting topologic motifs from two-dimension to one-dimension and specific physical properties.

Two three-dimensional coordination polymers of lead(II) with iminodiacetate and naphthalene-dicarboxylate anions: Synthesis, characterization and luminescence behavior

Debdoot Hazari, Swapan Kumar Jana, Michel Fleck, Ennio Zangrando and Sudipta Dalai

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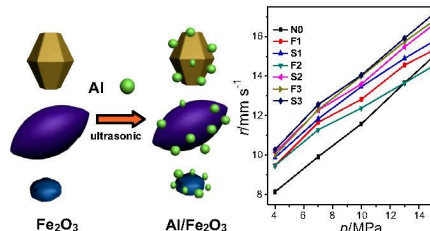


Two new topologically different 1D coordination polymers formed by Pb_4 clusters have been synthesized and characterized by x-ray analysis. The luminescence and thermal properties have been studied.

Dependence of catalytic properties of Al/Fe₂O₃ thermites on morphology of Fe₂O₃ particles in combustion reactions

Ningning Zhao, Cuicui He, Jianbing Liu, Hujun Gong, Ting An, Huixiang Xu, Fengqi Zhao, Rongzu Hu, Haixia Ma and Jinzhong Zhang

page 67

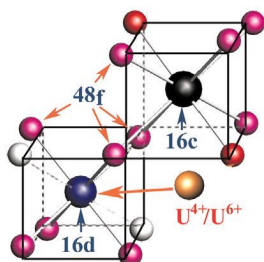


Effects of Fe_2O_3 and Al/Fe_2O_3 have been compared for the first time by analyzing combustion properties of formulations containing them, suggesting their potential application in AP/HTPB composite propellant systems.

Incorporation of uranium in pyrochlore oxides and pressure-induced phase transitions

F.X. Zhang, M. Lang, C. Tracy, R.C. Ewing, D.J. Gregg and G.R. Lumpkin

page 49

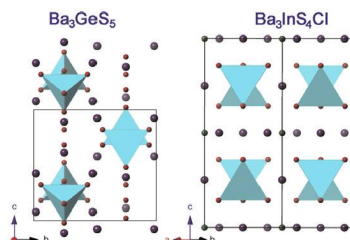


In U-bearing pyrochlore, U ions mainly occupy the 16*d* site and replace the smaller Zr^{4+} , part of the oxygen will occupy the 8*b* site, which is empty to most pyrochlores. At pressure of 22 GPa, the pyrochlore lattice is not stable and transforms to a cotunnite-type structure. The high-pressure structure is not stable and transform to a fluorite or back to the pyrochlore structure when pressure is released.

Ba₃GeS₅ and Ba₃InS₄Cl: Interesting size effects originated from the tetrahedral anions

Ming-Yan Pan, Sheng-Qing Xia, Xiao-Cun Liu and Xu-Tang Tao

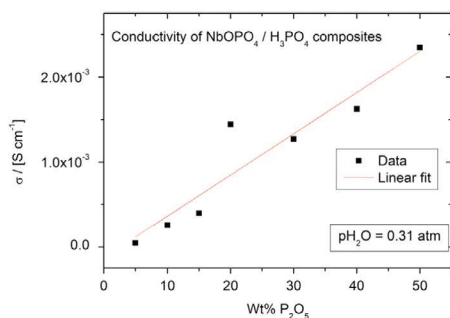
page 74



The polyhedral structure view for Ba_3GeS_5 and Ba_3InS_4Cl in which Ba, S and Cl atoms are plotted in purple, red and green spheres.

Solid state ^{31}P MAS NMR spectroscopy and conductivity measurements on NbOPO_4 and H_3PO_4 composite materials

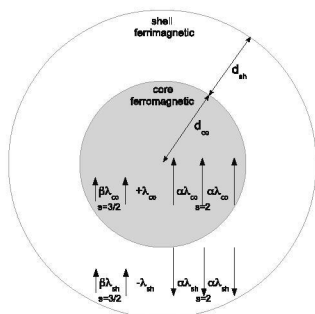
Daniel Risskov Sørensen, Ulla Gro Nielsen and Eivind M. Skou
page 80



Conductivity of $\text{NbOPO}_4/\text{H}_3\text{PO}_4$ composites as a function of equivalent P_2O_5 content. The conductivity is insignificant for pure NbOPO_4 .

Magnetic and structural investigations on $\text{La}_{0.6}\text{Sr}_{0.4}\text{MnO}_3$ nanostructured manganite: Evidence of a ferrimagnetic shell

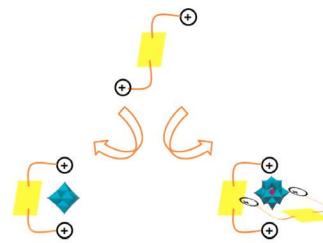
V.M. Andrade, R.J. Carballo-Vivas, T. Costas-Soares, S.S. Pedro, D.L. Rocco, M.S. Reis, A.P.C. Campos and A.A. Coelho
page 87



Core-shell model: The core has a ferromagnetic character, while the shell is ferrimagnetic. Each one has two sub-lattices (Mn^{3+} and Mn^{4+}) that interact through a mean-field (see Eq. (6)). Interactions strength and signals are also represented in this figure. In this figure the arrows (or vectors) represent the magnetic moment of ions Mn^{3+} ($s=2$) and Mn^{4+} ($s=3/2$). $\beta\lambda$'s describe the ferromagnetic interaction between Mn^{4+} ions into the core ($\beta\lambda_{co}$) and into the shell ($\beta\lambda_{sh}$), while $\alpha\lambda$'s represent ferromagnetic interaction between Mn^{3+} ions into the core ($\alpha\lambda_{co}$) and into the shell ($\alpha\lambda_{sh}$). The $-\lambda_{sh}$ and $+\lambda_{co}$ are associated to the mean field parameter of interaction between Mn^{3+} and Mn^{4+} sub-lattices in the shell (ferrimagnetic, negative sign) and core (ferromagnetic, positive sign), respectively.

Synthesis and energy band characterization of hybrid molecular materials based on organic-polyoxometalate charge-transfer salts

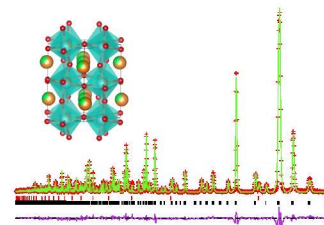
Chunxia Tan and Weifeng Bu
page 93



Hybrid molecular materials with charge-transfer characters formed by a positively charged donor L and acceptors of the Lindqvist-type and Keggin-type POMs have lamellar and cubic structures in their solid state.

Lattice constant prediction of defective rare earth titanate perovskites

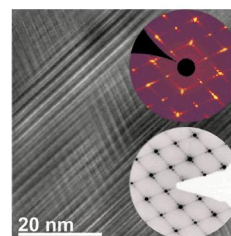
Steven Letourneau, Zhen Zhen, Josh Owens, Kevin Tolman, Rick Uvic and Waltraud M. Kriven
page 99



Atomistic model of $\text{Sr}_{0.3}\text{Nd}_{0.7}\text{Mg}_{0.35}\text{Ti}_{0.65}\text{O}_3$ and Rietveld refinement of neutron diffraction data.

Novel superstructure of the rocksalt type and element distribution in germanium tin antimony tellurides

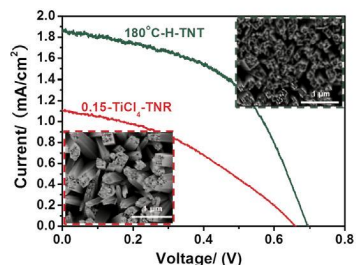
Tobias Rosenthal, Simon Welzmilller, Lukas Neudert, Philipp Urban, Andy Fitch and Oliver Oeckler
page 108



High-resolution transmission electron micrograph, SAED pattern and reciprocal lattice section of X-ray single crystal data of $\text{Ge}_{3.25}\text{Sn}_{1.1}\text{Sb}_{1.1}\text{Te}_6$ with an 11P-type superstructure of the rocksalt type.

Controllable hydrothermal synthesis of rutile TiO₂ hollow nanorod arrays on TiCl₄ pretreated Ti foil for DSSC application

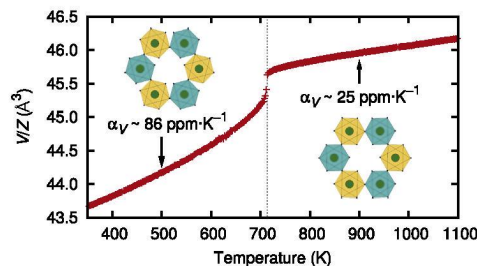
Min Xi, Yulan Zhang, Lizhen Long and Xinjun Li
page 118



Rutile hollow TiO₂ nanorod array photoanode obtained from original TiO₂ nanorod array photoanode by hydrothermal etching demonstrates enhanced photoelectric efficiency of DSSC.

Thermal expansion and phase transitions of α -AlF₃

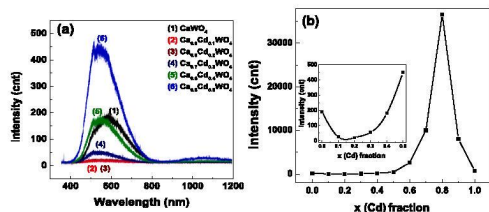
Cody R. Morelock, Justin C. Hancock and Angus P. Wilkinson
page 143



α -AlF₃ has a rhombohedrally distorted ReO₃-type structure at ambient conditions and displays strongly positive volume thermal expansion that is highly anisotropic; the material becomes cubic on heating above ~713 K and continues to show positive thermal expansion.

Structural, vibrational and luminescence properties of the (1-x)CaWO₄-xCdWO₄ system

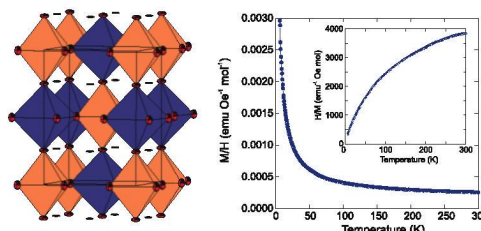
A. Taoufyq, F. Guinneton, J-C. Valmalette, M. Arab, A. Benlhachemi, B. Bakiz, S. Villain, A. Lyoussi, G. Nolibe and J-R. Gavarrri
page 127



Luminescence on UV excitation (364.5 nm) of (1-x)CaWO₄-xCdWO₄ system, elaborated from coprecipitation technique at 1000 °C, with 0 < x < 1. (a) Experimental emission bands of the Ca_{1-x}Cd_xWO₄ polycrystalline phases with 0 ≤ x ≤ 0.5. (b) Maximum of luminescence intensity for the composition x=0.8.

Structural and magnetic characterisation of the novel spin frustrated double perovskite Sr₂ScMoO₆

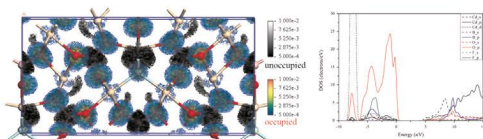
Thomas K. Wallace and Abbie C. McLaughlin
page 148



A novel double perovskite Sr₂ScMoO₆ has been synthesised which has corner sharing MoO₆ and ScO₆ octahedra. The Sr²⁺ cations reside in the cavities and exhibit anisotropic thermal motion. There is no evidence of magnetic order down to 6 K.

The interaction between cations and anionic groups inducing SHG enhancement in a series of apatite-like crystals: A first-principles study

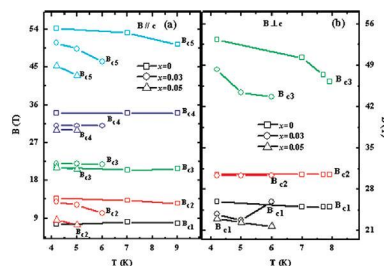
Qun Jing, Xiaoyu Dong, Zhihua Yang, Shilie Pan, Bingbing Zhang, Xuchu Huang and Mingwei Chen
page 138



Combined with the first-principles method, SHG-density method and real-space atom-cutting method, the enhancement of SHG response are attributed to the interaction between cadmium and BO₃ groups.

High magnetic field induced spin flip/flop behavior and magnetic phase diagram of CuFe_{1-x}Ga_xO₂

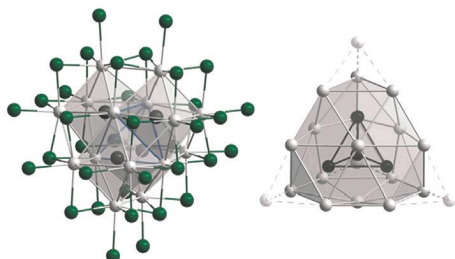
L.R. Shi, Z.C. Xia, Z. Jin, M. Wei, J.W. Huang, B.R. Chen, L.X. Xiao, H.K. Zuo and Z.W. Ouyang
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Temperature dependence of the critical fields for CuFe_{1-x}Ga_xO₂ (x=0, 0.03, 0.05). (a) and (b) The magnetic field's parallel and perpendicular cases respectively. In which, the square, circle and triangular represent x=0, 0.03 and 0.05 respectively.

Oligomeric rare-earth metal cluster complexes with endohedral transition metal atoms

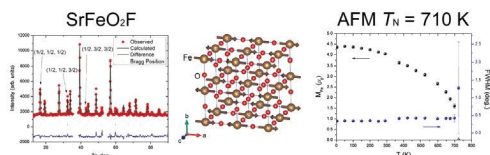
Simon Steinberg, Sina Zimmermann, Matthias Brühmann, Eva Meyer, Christian Rustige, Marike Wolberg, Kathrin Daub, Thomas Bell and Gerd Meyer
page 159



Rare earth-metal cluster complexes with endohedral transition metal atoms $\{TR_6\}$ may connect via common edges or faces to form dimers, trimers, tetramers and pentamers of which the tetramers are the most prolific. Packing effects and electron counts play an important role.

Structural and magnetic behavior of the cubic oxyfluoride $SrFeO_2F$ studied by neutron diffraction

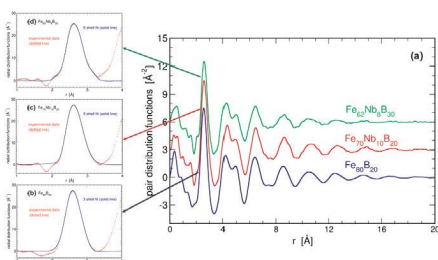
Corey M. Thompson, Colin K. Blakely, Roxana Flacau, John E. Greedan and Viktor V. Poltavets
page 173



Variable temperature powder neutron diffraction was employed to follow the evolution of the long range antiferromagnetic state in $SrFeO_2F$.

Short-range order in Fe-based metallic glasses: Wide-angle X-ray scattering studies

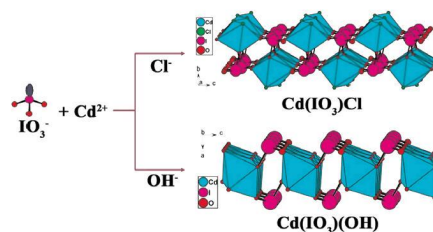
Rafał Babilas, Łukasz Hawełek and Andrzej Burian
page 179



Pair distribution functions (a) and best-fit model and experimental radial distribution functions for $Fe_{80}B_{20}$ (b), $Fe_{70}Nb_{10}B_{20}$ (c) and $Fe_{62}Nb_8B_{30}$ (d) metallic glasses.

Synthesis, crystal structure and optical properties of two new layered cadmium iodates: $Cd(IO_3)X$ ($X=Cl, OH$)

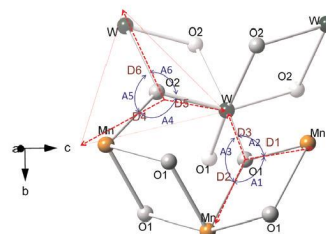
Bing-Ping Yang and Jiang-Gao Mao
page 185



Two new layered cadmium iodates $Cd(IO_3)X$ ($X=Cl, OH$) are reported. $Cd(IO_3)Cl$ features a unique double layered structure whereas $Cd(IO_3)(OH)$ displays an ordinary layered structure.

Synthesis and characterisation of In-doped $MnWO_4$ -type solid-solutions: $Mn_{1-3x}In_{2x}□_xWO_4$ ($x=0-0.11$)

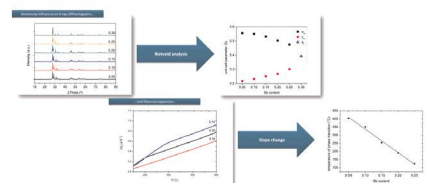
U. Gattermann, S.-H. Park and M. Kaliwoda
page 191



Despite of substitution of smaller In^{3+} for larger Mn^{2+} , the In-rich solid solution $Mn_{0.71(2)}In_{0.19(1)}□_{0.10}WO_4$ undergoes a volume expansion of 0.4% with respect to $MnWO_4$. This could be explained by a local space expansion of 0.13% around bridging oxygen at O2 sites, as illustrated by dashed lines for clarity.

Effect of isovalent substitution on microstructure and phase transition of $LaNb_{1-x}M_xO_4$ ($M=Sb, V$ or Ta ; $x=0.05-0.3$)

S. Wachowski, A. Mielewczyk-Gryn and M. Gazda
page 201

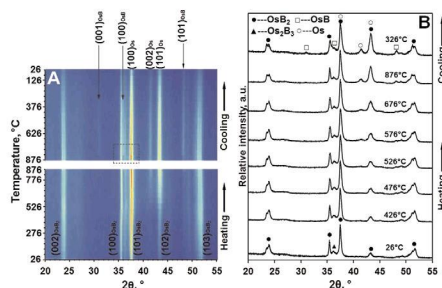


Substitution of niobium by other pentavalent elements in $LaNbO_4$ leads to change in phase transition temperature. In case of Sb substituent a shift of phase transition into the lower temperature region is observed. $LaNb_{0.7}Sb_{0.3}O_4$ substitution allows to achieve material with tetragonal crystal structure at room temperature and no phase transition up to 1000 °C.

Continued

Thermal stability of hexagonal OsB₂

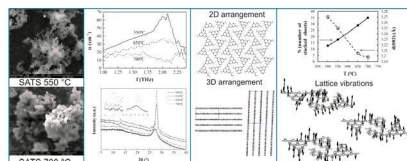
Zhilin Xie, Richard G. Blair, Nina Orlovskaya,
David A. Cullen and E. Andrew Payzant
page 210



The *in situ* high temperature XRD contour plot (A) and XRD patterns (B) of *h*-OsB₂ upon heating and cooling under an argon atmosphere.

2D to 3D transition of polymeric carbon nitride nanosheets

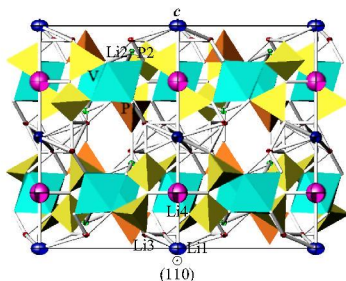
Pedro Chamorro-Posada, José Vázquez-Cabo, Francisco M. Sánchez-Arévalo, Pablo Martín-Ramos, Jesús Martín-Gil, Luis M. Navas-Gracia and Roberto C. Dante
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2D lattice mode vibrations and structural changes correlated with the so called "2D to 3D transition".

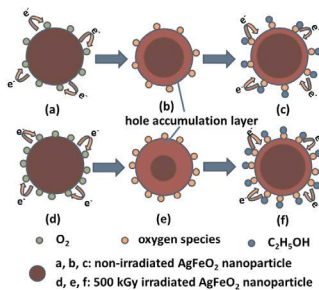
Crystal structures and electronic properties for the over-lithiated and Li–Ag substituted phases of Li₉V₃(P₂O₇)₃(PO₄)₂ insertion electrode system

Masashige Onoda, Makoto Inagaki and Hiroaki Saito
page 220



Gamma ray irradiated AgFeO₂ nanoparticles with enhanced gas sensor properties

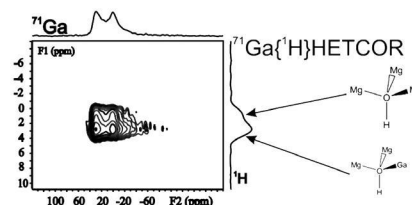
Xiuhua Wang, Zhijie Shi, Shangwu Yao, Fan Liao,
Juanjuan Ding and Mingwang Shao
page 228



Gamma ray irradiation improved the performance of gas sensor based on the AgFeO₂ nanoparticles including sensitivity and optimum operating temperature, which might be ascribed to the generation of defects.

Local environment and composition of magnesium gallium layered double hydroxides determined from solid-state ¹H and ⁷¹Ga NMR spectroscopy

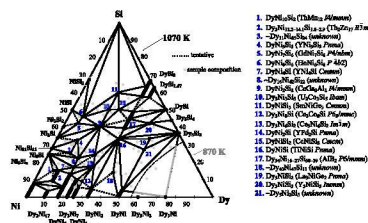
Line Boisen Petersen, Andrew S. Lipton, Vadim Zorin and Ulla Gro Nielsen
page 242



Two types of hydroxides groups are observed in magnesium gallium layered double hydroxides revealing an ordering of Ga in the cation layer.

The Dy–Ni–Si system as a representative of the rare earth–Ni–Si family: Its isothermal section and new rare-earth nickel silicides

Fang Yuan, Y. Mozharivskiy, A.V. Morozkin, A.V. Knotko,
V.O. Yapaskurt, M. Pani, A. Provino and P. Manfrinetti
page 247

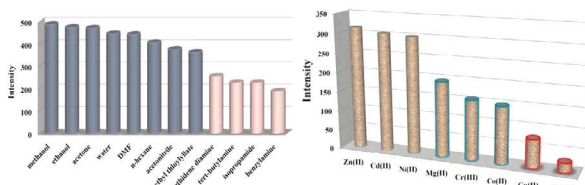


The Dy–Ni–Si system has been investigated at 1070 K by X-ray and microprobe analysis. The system contains the 12 known compounds DyNi₁₀Si₂, DyNi₅Si₃, DyNi₆Si₆, DyNi₄Si, DyNi₂Si₂, Dy₂Ni₃Si₅, DyNi₃Si₃, Dy₃Ni₆Si₂, DyNi₃Si₂, DyNiSi, Dy₃Ni₃Si₃, Dy₃Ni₂Si₂, and the new compounds Dy₃₄Ni_{16–27}Si_{50–39}, Dy₂Ni_{15.2–14.1}Si_{1.8–2.9}, ~Dy₁₁Ni₆₅Si₂₄, ~Dy₁₆Ni₆₂Si₂₂, DyNi₇Si₆, Dy₃Ni₈Si, DyNi₂Si, ~Dy₄₀Ni₁₄₇Si₁₃ and ~Dy₅Ni₂Si₃. Quasi-binary solid solutions were detected for Dy₂Ni₁₇, DyNi₅, DyNi₇, DyNi₃, DyNi₂, DyNi, DySi₂ and DySi_{1.67}. The crystal structures and magnetic properties of new phases RNi₇Si₆ (GdNi₇Si₆-type), R₃Ni₈Si (Ce₃Co₈Si-type), RNi₂Si (YPd₂Si-type) and R₃Ni₁₂Si₄ (Gd₃Ru₄Al₁₂-type), with R=Y, Gd–Tm, are also reported.

Syntheses, structures, molecular and cationic recognitions and catalytic properties of two lanthanide coordination polymers based on a flexible tricarboxylate

Yu Zhu, Yan-Mei Wang, Ji Xu, Pan Liu, H.A.B.M.D. Weththasinha, Yun-Long Wu, Xiao-Qing Lu and Ji-Min Xie

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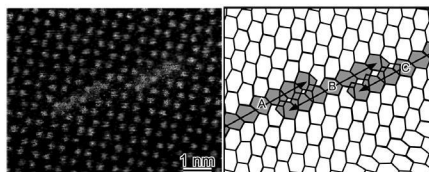


We have synthesized two isostructural 3D compounds based on H₃TTTA. They are chemical sensor of amine solvents and cations. They have higher yields and TOFs to catalyze cyanosilylation reactions.

Intergrowth structure of α -phase in β -type TmAlB₄ compound studied by high-angle annular detector dark-field scanning transmission electron microscopy

Kunio Yubuta, Takao Mori, Andreas Leithe-Jasper, Horst Borrmann, Yuri Grin, Shigeru Okada and Toetsu Shishido

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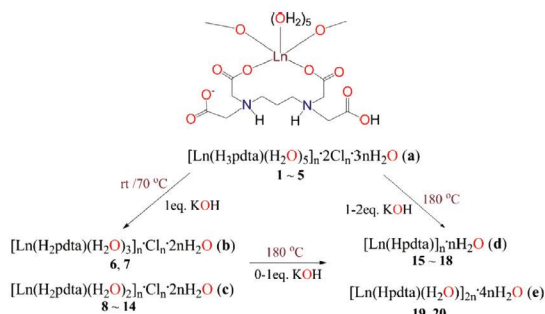


Nanostructure of a ThMoB₄-type (β -type) TmAlB₄ compound, in which YCrB₄-type (α -type) domains are locally intergrown, is studied by high-angle annular detector dark-field scanning transmission electron microscopy (HAADF-STEM). Z-contrast images by HAADF-STEM directly represent arrangements of Tm atoms located at centers of heptagonal atomic columns of B atoms as bright dots, and give us detailed information of the characteristic intergrowth structure of type domains in the matrix of the β -type phase.

Acidic 1,3-propanediaminetetraacetato lanthanides with luminescent and catalytic ester hydrolysis properties

Mao-Long Chen, Yan-Ru Shi, Yu-Chen Yang and Zhao-Hui Zhou

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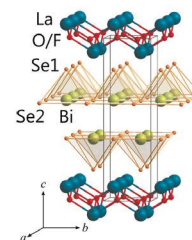
A series of water-soluble acidic 1,3-propanediaminetetraacetato lanthanides $[Ln(1,3-H_3pdta)(H_2O)_5]_n \cdot 2Cl_n \cdot 3nH_2O$ have been converted to their 2D and 3D lanthanides, which are active for the catalytic conversion of ester hydrolysis.

Rapid Communications

First single crystal growth and structural analysis of superconducting layered bismuth oxyseleide; La(O,F)BiSe₂

Masashi Tanaka, Masanori Nagao, Yoshitaka Matsushita, Masaya Fujioka, Saleem J. Denholme, Takahide Yamaguchi, Hiroyuki Takeya and Yoshihiko Takano

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Single crystal La(O,F)BiSe₂ has been prepared by a CsCl flux method. The structural analysis implies that La(O,F)BiSe₂ is a potential superconductor having a higher T_c under high pressure.

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