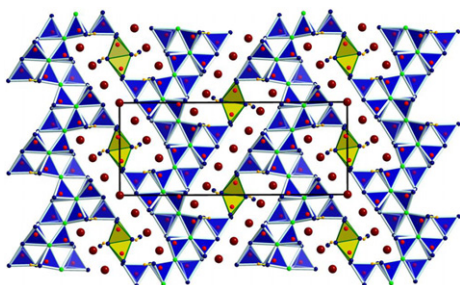


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Regular Articles

The new high-pressure borate $\text{Co}_7\text{B}_{24}\text{O}_{42}(\text{OH})_2 \cdot 2\text{H}_2\text{O}$ —Formation of edge-sharing BO_4 tetrahedra in a hydrated borate

Stephanie C. Neumair, Reinhard Kaindl and Hubert Huppertz
page 1

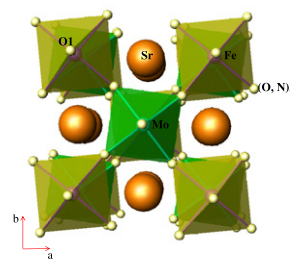


The new high-pressure borate hydrate $\text{Co}_7\text{B}_{24}\text{O}_{42}(\text{OH})_2 \cdot 2\text{H}_2\text{O}$ is built up from corner-sharing BO_4 tetrahedra forming corrugated layers, that are interconnected among each other by two edge-sharing BO_4 tetrahedra (B_2O_6 units). In this paper we report on synthesis, structural details, and properties of the new compound $\text{Co}_7\text{B}_{24}\text{O}_{42}(\text{OH})_2 \cdot 2\text{H}_2\text{O}$.

Regular Articles

Double perovskite $\text{Sr}_2\text{FeMoO}_{6-x}\text{N}_x$ ($x = 0.3, 1.0$) oxynitrides with anionic ordering

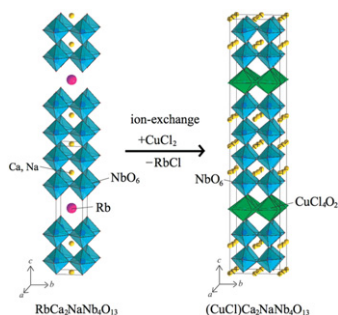
M. Retuerto, C. de la Calle, M.J. Martínez-Lope, F. Porcher, K. Krezhov, N. Menéndez and J.A. Alonso
page 18



We have synthesized and studied the new oxynitride double perovskites $\text{Sr}_2\text{FeMoO}_{6-x}\text{N}_x$. They present anionic ordering between O and N. The nitridation process improves the long-range Fe/Mo ordering. They show a ferrimagnetic transition with a reduced saturation magnetization compared to $\text{Sr}_2\text{FeMoO}_6$, due to the different nature of the double exchange interactions through Fe–N–Mo–N–Fe in contrast to Fe–O–Mo–O–Fe. We suggest a shift towards a configuration $\text{Fe}^{4+}(3d^4, S=2):\text{Mo}^{5+}(4d^1, S=1/2)$.

Quadruple-layered perovskite $(\text{CuCl})\text{Ca}_2\text{NaNb}_4\text{O}_{13}$

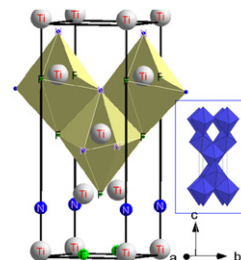
A. Kitada, Y. Tsujimoto, T. Yamamoto, Y. Kobayashi, Y. Narumi, K. Kindo, A.A. Aczel, G.M. Luke, Y.J. Uemura, Y. Kiuchi, Y. Ueda, K. Yoshimura, Y. Ajiro and H. Kageyama
page 10



We present a quadruple-layered copper oxyhalide $(\text{CuCl})\text{Ca}_2\text{NaNb}_4\text{O}_{13}$ synthesized through a topotactic ion-exchange reaction of $\text{RbCa}_2\text{NaNb}_4\text{O}_{13}$ with CuCl_2 . The compound has a well-defined superstructure. Magnetic studies suggest the absence of magnetic order even at 2 K.

Electronic structure and anisotropic chemical bonding in TiNF from ab initio study

Samir F. Matar
page 25

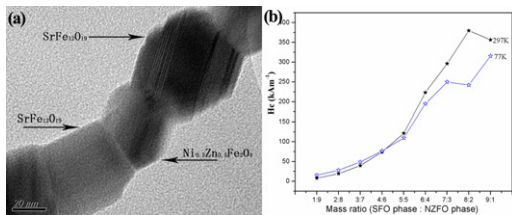


The geometry optimized ground state anatase derived TiNF structure with arrangement of open faceted TiN_3F_3 distorted octahedra. The insert shows the arrangement of octahedra in anatase TiO_2 .

Microstructure, magnetic properties and exchange-coupling interactions for one-dimensional hard/soft ferrite nanofibers

Fuzhan Song, Xiangqian Shen, Mingquan Liu and Jun Xiang

page 31

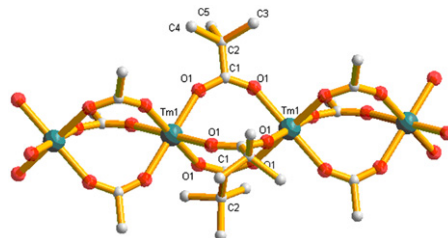


SrFe₁₂O₁₉ (SFO)/Ni_{0.5}Zn_{0.5}Fe₂O₄ (NZFO) composite ferrite nanofibers with a uniform phase distribution show competition of the exchange-coupling interaction and the dipolar interaction in the composite nanofibers.

Novel 1D coordination polymer {Tm(Piv)₃}_n: Synthesis, structure, magnetic properties and thermal behavior

Irina Fomina, Zhanna Dobrokhotova, Grygory Aleksandrov, Anna Emelina, Mikhail Bykov, Irina Malkerova, Artem Bogomyakov, Lada Puntus, Vladimir Novotortsev and Igor Eremenko

page 49

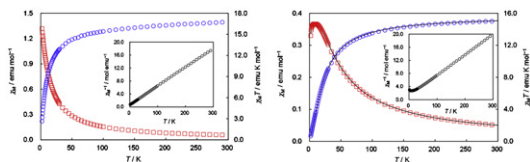


Novel 1D coordination polymer {Tm(Piv)₃}_n was synthesized and studied by X-ray diffraction. The magnetic, luminescence properties, the thermal behavior and the volatility for the compound {Tm(Piv)₃}_n were investigated.

Two coordination polymers of manganese(II) isophthalate and their preparation, structures, and magnetic properties

Jinxi Chen, Jingjing Wang and Masaaki Ohba

page 37

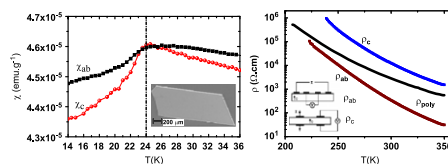


Three-dimensional porous and two-dimensional layered manganese isophthalates have been prepared. Magnetic susceptibility measurements exhibit overall weak antiferromagnetic interactions between the Mn(II) ions in both compounds.

Revisiting the properties of delafossite CuCrO₂: A single crystal study

Maria Poienar, Vincent Hardy, Bohdan Kundys, Kiran Singh, Antoine Maignan, Françoise Damay and Christine Martin

page 56

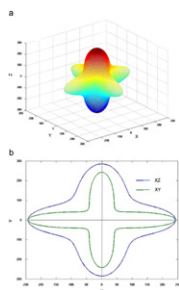


3R-CuCrO₂ platelet-like single crystals have been successfully grown by the flux method. As revealed by $\chi(T)$ and $C(T)$ measurements, their properties are characterised by a unique antiferromagnetic transition at $T_N=24$ K. Interestingly, despite a very small magnetic anisotropy, a large one is evidenced by the resistivity ratio, $\rho_c/\rho_{ab}\sim 35$, at 300 K. This suggests an easier charge hopping in the [CrO₂] planes rather than along c axis.

Theoretical investigations of the physical properties of zircon-type YVO₄

Zuocai Huang, Jing Feng and Wei Pan

page 42

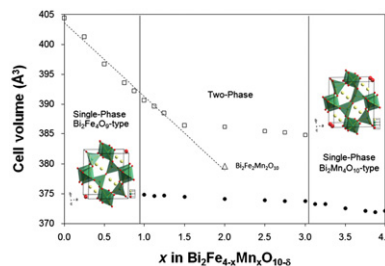


(a) Directional dependence of Young's modulus in zircon-type YVO₄ and (b) projections of the directional dependent Young's modulus in different planes for zircon-type YVO₄. The units are in GPa.

Mixed crystal formation and structural studies in the mullite-type system Bi₂Fe₄O₉-Bi₂Mn₄O₁₀

Zachary R. Kann, Jeffrey T. Auletta, Eric W. Hearn, Sven-U. Weber, Klaus D. Becker, Hartmut Schneider and Michael W. Lufaso

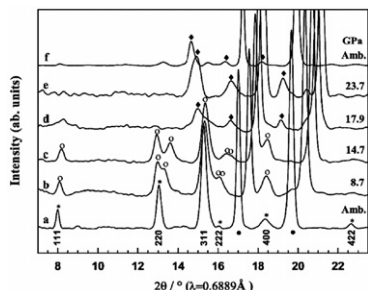
page 62



Single-phase regions are found near each end-member and a two-phase region is observed at intermediate compositions, extending from about $x=1$ to 3, according to the general formula of the mixed crystals Bi₂Fe_{4-x}Mn_xO₁₀₋₅.

Pressure-induced phase transition of Fe₂TiO₄: X-ray diffraction and Mössbauer spectroscopy

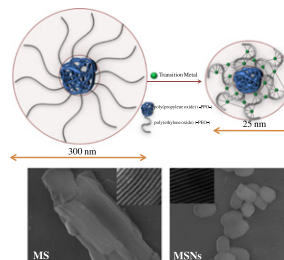
Ye Wu, Xiang Wu and Shan Qin
page 72



A series of phase transition of Fe₂TiO₄ occurs from cubic (a) to tetragonal (b and c) then to orthorhombic phase (d-f) at high pressure.

Transition metal-chelating surfactant micelle templates for facile synthesis of mesoporous silica nanoparticles

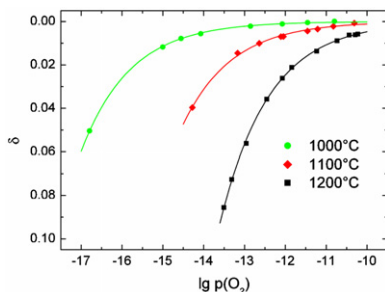
Hye Sun Lee, Won Hee Kim, Jin Hyung Lee, Doo Jin Choi, Young-Keun Jeong and Jeong Ho Chang
page 89



Metal-chelating surfactant micelle templates support a simple and facile preparations of size-tunable ordered MSNs.

Nonstoichiometry, point defects and magnetic properties in Sr₂FeMoO_{6-δ} double perovskites

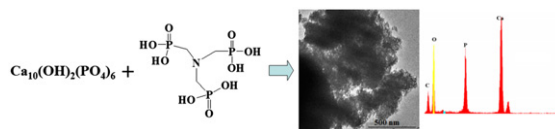
R. Kircheisen and J. Töpfer
page 76



Nonstoichiometry δ of Sr₂FeMoO_{6- δ} as function of oxygen partial pressure at 1000, 1100, and 1200 °C.

Synthesis and characterization of nanoapatites organofunctionalized with aminotriphosphonate agents

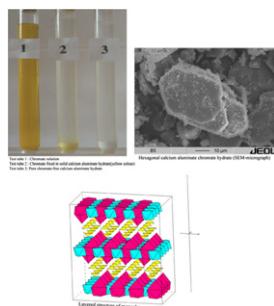
Sanaâ Saoiabi, Sanae El Asri, Abdelaziz Laghzizil, Sylvie Masse and Jerome L. Ackerman
page 95



Hydroxyapatite in the form of naturally occurring phosphate rock is converted in the presence of nitrilotris(methylene)triphosphonate (NTP) to high surface area apatite nanoparticles (dimensions measured by TEM) with NTP-functionalized surfaces.

Cr⁶⁺-containing phases in the system CaO–Al₂O₃–CrO₄²⁻–H₂O at 23 °C

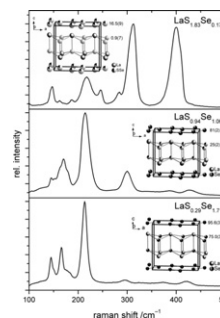
Herbert Pöllmann and Stephan Auer
page 82



Chromate can be incorporated in LDH-phases with compositions like: 3CaO · Al₂O₃ · 1/2CaCrO₄ · 1/2Ca(OH)₂ · nH₂O, 3CaO · Al₂O₃ · CaCrO₄ · nH₂O, 3CaO · Al₂O₃ · 1/6CaCrO₄ · 5/6Ca(OH)₂ · nH₂O, 3CaO · Al₂O₃(0-x)CaCrO₄(1-x) Ca(OH)₂ · 12H₂O, (0 < x < 0.17).

Ternary lanthanum sulfide selenides α-LaS_{2-x}Se_x (0 < x < 2) with mixed dichalcogenide anions X₂²⁻ (X = S, Se)

Christian Bartsch and Thomas Doert
page 101

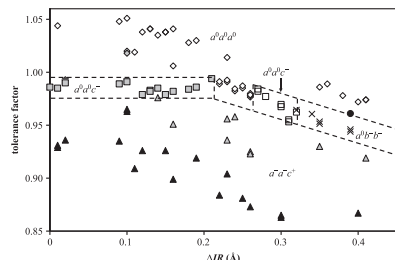


Raman spectra and site occupancies in the structures of selected lanthanum sulfide selenides.

Structures of ordered tungsten- or molybdenum-containing quaternary perovskite oxides

Bradley E. Day, Nicholas D. Bley, Heather R. Jones, Ryan M. McCullough, Hank W. Eng, Spencer H. Porter, Patrick M. Woodward and Paris W. Barnes

page 107

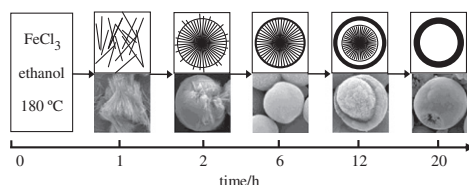


A survey of the tolerance factor of 41 Mo/W- and 52 Nb/Ta-containing quaternary perovskites plotted as a function of the difference between the two six-coordinate M -cation ionic radii. Compounds with cubic symmetry are represented by diamonds, those with tetragonal symmetry are represented by squares, those with $I2/m$ monoclinic symmetry are represented by \times , and those with $P2_1/n$ monoclinic symmetry are represented by triangles. White symbols represent compositions where $A = \text{Ba}^{2+}$, gray symbols represent compositions where $A = \text{Sr}^{2+}$, and black symbols represent where $A = \text{Ca}^{2+}$. The filled circle represents rhombohedral $\text{Ba}_2\text{BiTaO}_6$ ($t = 0.961$; space group— $R\bar{3}c$; tilt system— $a^-a^-a^-$). References for the compounds included in this figure are listed in the Supporting Information File.

Hematite homogeneous core/shell hierarchical spheres: Surfactant-free solvothermal preparation and their improved catalytic property of selective oxidation

Suoyuan Lian, Haitao Li, Xiaodie He, Zhenhui Kang, Yang Liu and Shuitong Lee

page 117

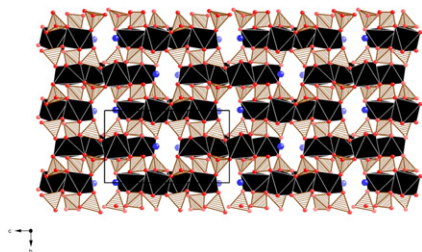


Fe_2O_3 homogeneous core/shell hierarchical microspheres were synthesized by solvothermal method. Owing to the special structure, the synthesized Fe_2O_3 microspheres exhibit a superior catalytic activity in benzyl oxidation.

Synthesis, structure, and optical properties of $\text{CsU}_2(\text{PO}_4)_3$

George N. Oh, Emilie Ringe, Richard P. Van Duyne and James A. Ibers

page 124

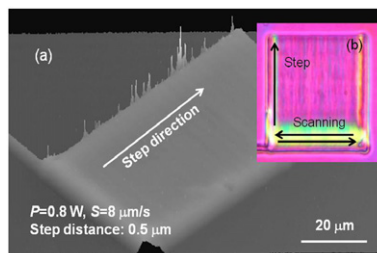


Stacking of the layers in $\text{CsU}_2(\text{PO}_4)_3$, viewed along [100].

Laser patterning and preferential orientation of two-dimensional planar $\beta\text{-BaB}_2\text{O}_4$ crystals on the glass surface

F. Suzuki, K. Ogawa, T. Honma and T. Komatsu

page 130

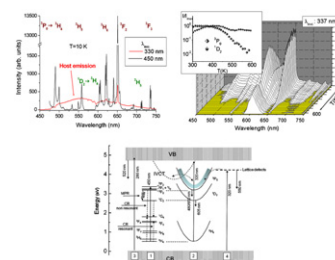


This figure shows confocal scanning laser microscope and polarized optical microscope photographs for $\beta\text{-BaB}_2\text{O}_4$ crystals obtained by laser irradiations. The laser scanning was repeated with a step of $0.5\ \mu\text{m}$ between the lines using the condition of the power of $P = 0.8\ \text{W}$ and a laser scanning speed of $S = 8\ \mu\text{m/s}$. It is suggested that $\beta\text{-BaB}_2\text{O}_4$ crystals in the overlapped laser-irradiated region are highly oriented and the c -axis direction of $\beta\text{-BaB}_2\text{O}_4$ crystals is perpendicular to the laser scanning direction.

Optical spectroscopy and excited state dynamics of $\text{CaMoO}_4:\text{Pr}^{3+}$

Enrico Cavalli, Fabio Angiuli, Philippe Boutinaud and Rachid Mahiou

page 136

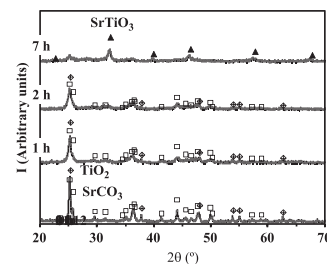


A general scheme is proposed in order to account for the complex dependence of the luminescence properties of the $\text{CaMoO}_4:\text{Pr}^{3+}$ system on the experimental parameters including excitation wavelength, temperature, doping concentration, etc.

Thermodynamic restrictions on mechanochemical synthesis of strontium titanate

J.F. Monteiro, A.A.L. Ferreira, I. Antunes, D.P. Fagg and J.R. Frade

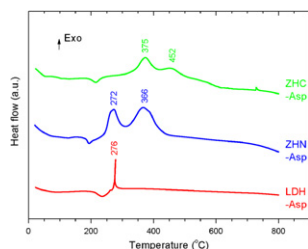
page 143



X-Ray diffractograms of the starting TiO_2 (anatase) + SrCO_3 mixture and after mechanical activation at 650 rpm, for 1, 2, and 7 h. Different symbols are used to identify reflections ascribed to anatase (diamonds), SrCO_3 (squares) and SrTiO_3 (triangles).

Intercalation studies of zinc hydroxide chloride: Ammonia and amino acids

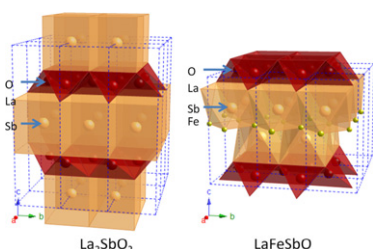
Gregorio Guadalupe Carbajal Arizaga
page 150



The zinc hydroxide chloride (ZHC) with formula $Zn_5(OH)_8Cl_2 \cdot 2H_2O$ was tested as intercalation matrix. In comparison with the well-known zinc hydroxide nitrate (ZHN) and layered double hydroxides (LDH), ZHC was the best matrix for thermal protection of Asp combustion, presenting exothermic peaks even at 452 °C, while the highest exothermic event in ZHN was at 366 °C, and in the LDH it was at 276 °C.

The hunt for LaFeSbO: Synthesis of La_2SbO_2 and a case of mistaken identity

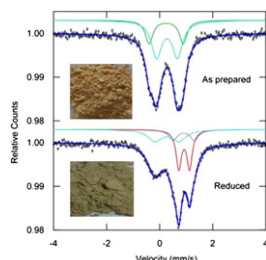
Sean Muir, Jason Vielma, Guenter Schneider, A.W. Sleight and M.A. Subramanian
page 156



The layered oxypnictide compounds La_2SbO_2 and $La_{1.9}Sr_{0.1}SbO_2$ have been synthesized and investigated. Both crystallize in a $ThCr_2Si_2$ type configuration and are semiconducting. Stability of the unreported compound LaFeSbO has been investigated using density functional theory. A case of mistaken identity in the literature regarding the composition LaNiBiO is addressed.

Investigation of the iron site localization in doped ZnO

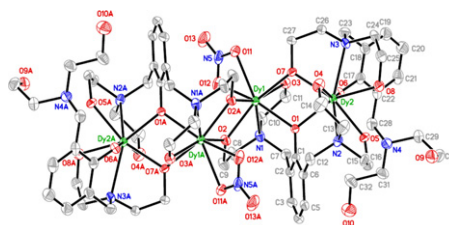
M.D. Carvalho, L.P. Ferreira, R.P. Borges and M. Godinho
page 160



$Zn_{0.95}Fe_{0.05}O$ obtained by a combustion method and after reduction under hydrogen atmosphere.

The synthesis, structure, magnetic and luminescent properties of a new tetranuclear dysprosium (III) cluster

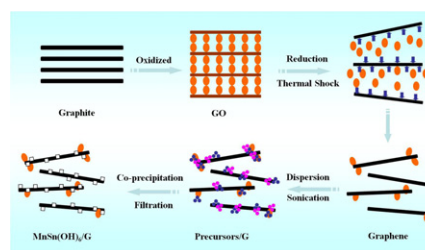
Yen-Han Chen, Yun-Fan Tsai, Gene-Hsian Lee and En-Che Yang
page 166



A new tetranuclear dysprosium (III) complex $[Dy_4(dhampH_3)_4(NO_3)_2](NO_3)_2$ is synthesized and reported in this paper. This molecule has luminescence and can potentially act as a SMM.

Controlled synthesis of $MnSn(OH)_6$ /graphene nanocomposites and their electrochemical properties as capacitive materials

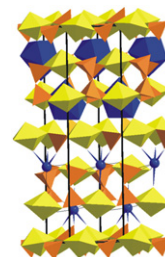
Gongkai Wang, Xiang Sun, Fengyuan Lu, Qingkai Yu, Changsheng Liu and Jie Lian
page 172



Graphite oxide (GO) can be synthesized by oxidizing graphite using Hummers method. Graphene was reduced from GO by thermal exfoliation. In this work, $MnSn(OH)_6$ /graphene nanocomposites were synthesized by a simple co-precipitation method and their electrochemical performances have been explored.

$[La(UO_2)V_2O_7][(UO_2)(VO_4)]$ the first lanthanum uranylvanadate with structure built from two types of sheets based upon the uranophane anion-topology

A. Mer, S. Obbade, M. Rivenet, C. Renard and F. Abraham
page 180

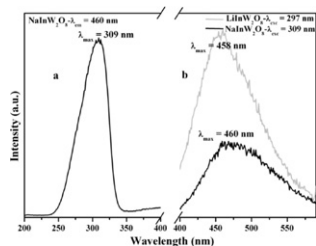


A view of the three-dimensional structure of $[La(UO_2)V_2O_7][(UO_2)(VO_4)]$.

Continued

Photoluminescence properties of rare earths (Eu^{3+} , Tb^{3+} , Dy^{3+} and Tm^{3+}) activated NaInW_2O_8 wolframite host lattice

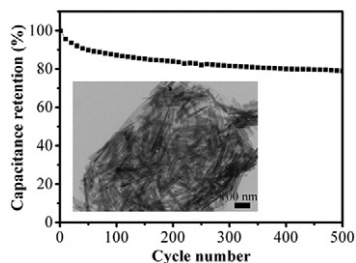
S. Asiri Naidu, S. Boudin, U.V. Varadaraju and B. Raveau
page 187



NaInW_2O_8 double tungstate doped with Eu^{3+} , Dy^{3+} , Tb^{3+} and Tm^{3+} shows characteristic emission of intense red for Eu^{3+} , yellow for Dy^{3+} , green for Tb^{3+} and blue for Tm^{3+} .

Synthesis and characterization of a nanocomposite of goethite nanorods and reduced graphene oxide for electrochemical capacitors

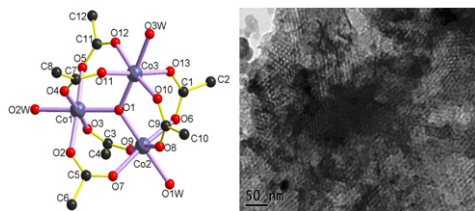
Qingliang Shou, Jipeng Cheng, Li Zhang, Bradley J. Nelson and Xiaobin Zhang
page 191



The reduced graphene oxide sheets are decorated with goethite nanorods. The as-prepared composite exhibits a high electrochemical capacitance with good recycling capability, which is promising for supercapacitor applications.

Synthesis of Co-containing mesoporous carbon foams using a new cobalt-oxo cluster as a precursor

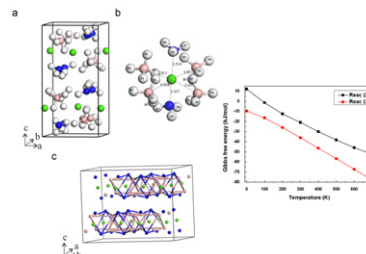
Yao-Kang Lv, Yun-Long Feng, Li-Hua Gan, Ming-Xian Liu, Liang Xu, Cao Liu, Hao-Wen Zheng and Jie Li
page 198



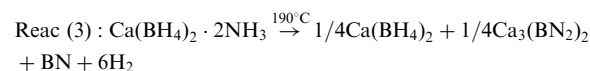
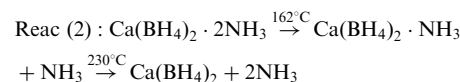
A new trinuclear cobalt-oxo cluster, $2[\text{Co}_3\text{O}(\text{Ac})_6(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}$ (1), was obtained and further used as a precursor to synthesize Co-containing mesoporous carbon foams (Co-MCFs) which exhibit improved electrochemical behaviors.

Structural, energetic and thermodynamic analyses of $\text{Ca}(\text{BH}_4)_2 \cdot 2\text{NH}_3$ from first principles calculations

Peng-Fei Yuan, Fei Wang, Qiang Sun, Yu Jia and Zheng-Xiao Guo
page 206

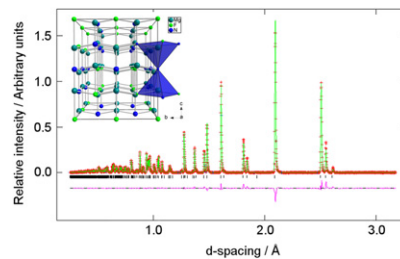


The crystal structure of this compound and the calculated decomposition reaction free energy for two different reactions:



Structural studies of magnesium nitride fluorides by powder neutron diffraction

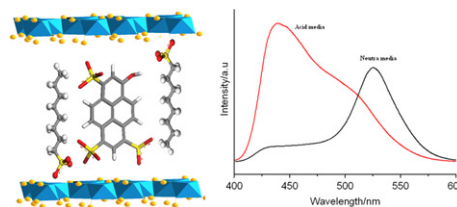
Michael A. Brogan, Robert W. Hughes, Ronald I. Smith and Duncan H. Gregory
page 213



Definitive structures of the ternary magnesium nitride fluorides Mg_3NF_3 and the lower temperature polymorph of Mg_2NF have been determined from powder neutron diffraction data. The nitride halides are essentially ionic and exhibit weak temperature independent paramagnetic behaviour.

8-Hydroxypyrene-1,3,6-trisulphonate and octanesulphonate co-assembled layered double hydroxide and its controllable solid-state luminescence by hydrothermal synthesis

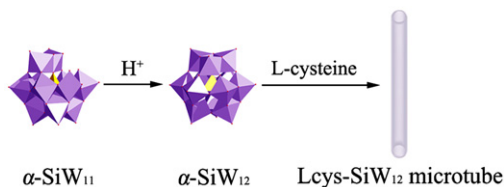
Sile Dang, Dongpeng Yan and Jun Lu
page 219



8-Hydroxy-pyrene-1,3,6-trisulphonate and octanesulphonate co-intercalated ZnAl layered double hydroxide can exhibit tunable solid-state blue and green fluorescence by treating the sample at acid and neutral media under hydrothermal condition.

Preparation and application of L-cysteine-doped Keggin polyoxometalate microtubes

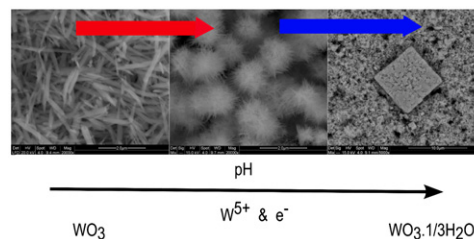
Yan Shen, Jun Peng, Huanqiu Zhang, Cuili Meng and Fang Zhang
page 225



The Lcys-SiW₁₂ microtubes were formed during transformation of the monolacunary Keggin-type [$\alpha\text{-SiW}_{11}\text{O}_{39}$]⁸⁻ to the saturated Keggin-type [$\alpha\text{-SiW}_{12}\text{O}_{40}$]⁴⁻, meanwhile L-cysteine molecules were doped during the growth of the microtubes.

One-dimensional WO₃ and its hydrate: One-step synthesis, structural and spectroscopic characterization

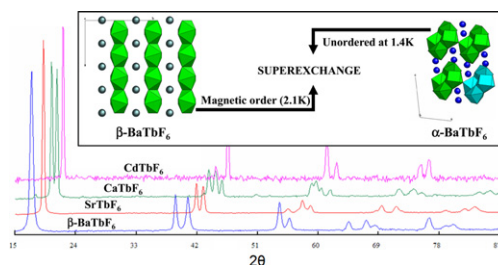
Kingsley O. Iwu, Augustinas Galeckas, Protima Rauwel, Andrej Y. Kuznetsov and Truls Norby
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The figure illustrates the role of pH in morphological and absorption edge evolution of WO₃ (hydrate) as well as the variation in the concentration of defect electrons between anhydrous and hydrated WO₃.

Magnetic behaviour of the MTbF₆ fluoroterbates (M = Cd, Ca, Sr, (α/β)-Ba)

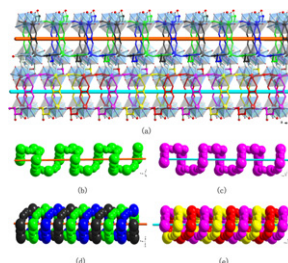
M. Josse, M. El-Ghozzi, D. Avignant, G. André, F. Bourée and O. Isnard
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Powder neutron diffraction revealed magnetic order in four of the five investigated fluoroterbates, while crystal chemical analyses of α and β forms of BaTbF₆ evidenced the existence of superexchange interactions.

Two types of rare earth-organic frameworks constructed by racemic tartaric acid

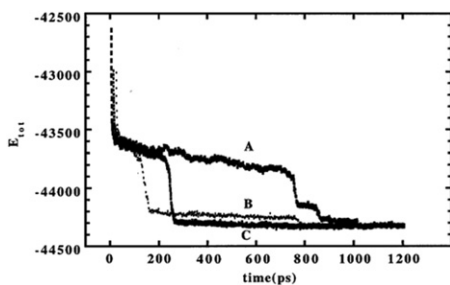
Zhan-Guo Jiang, Yao-Kang Lv, Jian-Wen Cheng and Yun-Long Feng
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[R₂(tar)₂(C₂O₄)(H₂O)₂]_n · 4nH₂O (R = La (2), Nd (3)) display rare fsx-4,5-*P*₂₁/*c* topology containing hydrophilic channels bounded by triple helical chains along *a* axis.

Molecular dynamics simulations of solid state recrystallization I: Observation of grain growth in annealed iron nanoparticles

Jinfan Huang and Lawrence S. Bartell
page 238

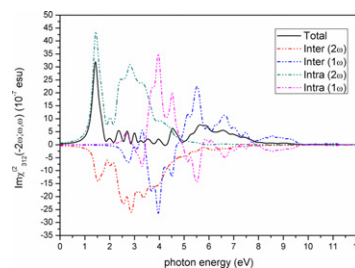


Time dependence of energy per atom in the quenching of liquid nanoparticles A–C of iron. Nanoparticle C freezes directly into a single crystal but A and B freeze to solids with two grains. A and B eventually recrystallize into single crystals.

Rapid Communication

Ab initio study of the linear and nonlinear optical properties of chalcopyrite CdGeAs₂

You Yu, Beijun Zhao, Shifu Zhu, Tao Gao, Haijun Hou and Zhiyu He
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Calculated total imaginary part of $\chi_{312}^{(2)}(-2\omega; \omega, \omega)$ spectra along with the intra-(2 ω)/(1 ω) and inter-(2 ω)/(1 ω) band contributions.

Continued

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