

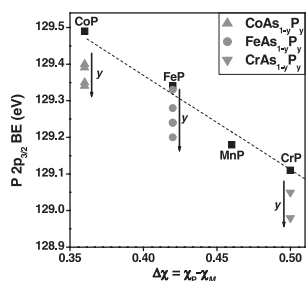
CONTENTS

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Regular Articles

Next-nearest neighbour contributions to the XPS binding energies and XANES absorption energies of P and As in transition-metal arsenide phosphides  $MA_{1-y}P_y$  having the MnP-type structure

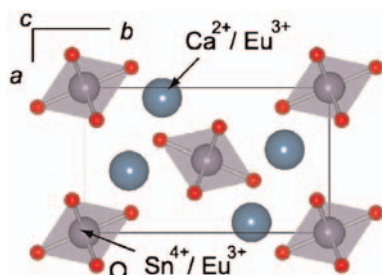
Andrew P. Grosvenor, Ronald G. Cavell and Arthur Mar  
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The metal arsenide phosphides  $CoAs_{1-y}P_y$ ,  $FeAs_{1-y}P_y$ , and  $CrAs_{1-y}P_y$  with the MnP-type structure have been studied by XPS and XANES. The shifts in the P 2p BEs observed for the metal arsenide phosphides compared to the binary metal phosphides cannot be explained by interaction of the nearest neighbours alone.

Preparation, crystal structure, and photoluminescence of  $Ca_2SnO_4 \cdot Eu^{3+}, Y^{3+}$

Hisanori Yamane, Yusuke Kaminaga, Shunsuke Abe and Takahiro Yamada  
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Rietveld analysis of the X-ray powder diffraction patterns revealed that  $Eu^{3+}$  replaced  $Ca^{2+}$  and  $Sn^{4+}$  in  $Ca_{2-x}Eu_xSn_{1-x}O_4$  ( $0 \leq x \leq 0.3$ ), and  $Eu^{3+}$  replaced  $Ca^{2+}$  and  $Y^{3+}$  replaced  $Sn^{4+}$  in  $Ca_{1.8}Y_{0.2}Eu_{0.2}Sn_{0.8}O_4$ . Red luminescence at 616 nm due to the  ${}^5D_0 \rightarrow {}^7F_2$  transition was observed in the photoluminescence spectra of these compounds.

Regular Articles—Continued

Synthesis and characterization of a new four-layer Aurivillius phase  $Bi_2SrNa_2Nb_4O_{15}$  and its protonated form

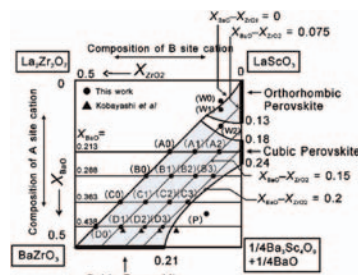
Zhenhua Liang, Kaibin Tang, Suyuan Zeng, Dong Wang, Tanwei Li and Huagui Zheng  
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A new four-layer Aurivillius phase  $Bi_2SrNa_2Nb_4O_{15}$  has been successfully synthesized. The powder X-ray diffraction shows that  $Bi_2SrNa_2Nb_4O_{15}$  crystallizes in the space group  $I4/mmm$  [ $a \sim 3.9021(1) \text{ \AA}$ ,  $c \sim 40.7554(10) \text{ \AA}$ ]. Protonated form of  $Bi_2SrNa_2Nb_4O_{15}$  was obtained by the substitution of bismuth oxide sheets with protons via acid treatment. The compositions of the protonated products was determined to be  $H_{1.8}[Sr_{0.8}Bi_{0.2}Na_2Nb_4O_{13}]$  by X-ray fluorescence spectroscopy and thermogravimetry.

Solid solutions of perovskite in the  $LaO_{1.5}-BaO-ScO_{1.5}-ZrO_2$  system at 1600 °C

Koichi Suehiro, Susumu Imashuku, Tetsuya Uda, Yoshitaro Nose and Yasuhiro Awakura  
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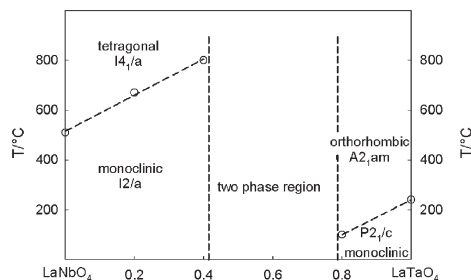
The phase boundary of solid solution between lanthanum scandate and barium zirconate at 1600 °C was clarified by establishing a partial pseudoquaternary phase diagram of the  $LaO_{1.5}-BaO-ScO_{1.5}-ZrO_2$  system at 1600 °C.

## Solid solubility and phase transitions in the system

### $\text{LaNb}_{1-x}\text{Ta}_x\text{O}_4$

Fride Vullum, Fabian Nitsche, Sverre Magnus Selbach and Tor Grande

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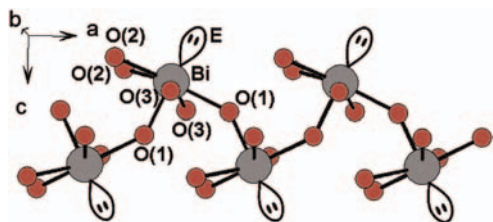


$\text{LaNb}_{1-x}\text{Ta}_x\text{O}_4$  ( $0 \leq x \leq 0.4$ ) with the monoclinic Fergusonite structure, was observed to transform to a tetragonal Scheelite, while monoclinic  $\text{LaNb}_{1-x}\text{Ta}_x\text{O}_4$  ( $0.8 \leq x \leq 1$ ) was shown to transform to an orthorhombic crystal structure.

## One-dimensional inorganic arrangement in the bismuth oxalate hydroxide $\text{Bi}(\text{C}_2\text{O}_4)\text{OH}$

Murielle Rivenet, Pascal Roussel and Francis Abraham

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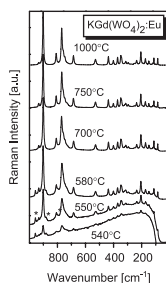


${}^{\infty}[\text{BiO}_5\text{E}]$  zig-zag chains running down [100] in  $\text{Bi}(\text{C}_2\text{O}_4)\text{OH}$ .

## The crystal structure, vibrational and luminescence properties of the nanocrystalline $\text{KEu}(\text{WO}_4)_2$ and $\text{KGd}(\text{WO}_4)_2:\text{Eu}^{3+}$ obtained by the Pechini method

L. Macalik, P.E. Tomaszewski, R. Lisiecki and J. Hanuza

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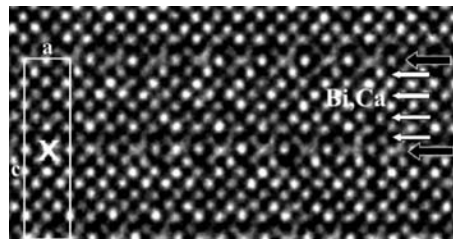
The luminescent nanocrystalline  $\text{KEu}(\text{WO}_4)_2$  and  $\text{KGd}_{0.98}\text{Eu}_{0.02}(\text{WO}_4)_2$  have been prepared by the Pechini method and characterised by using X-ray diffraction, infrared and Raman spectroscopy as well as optical spectroscopy. The crystal structure of  $\text{KEu}(\text{WO}_4)_2$  was refined in  $I2/c$  space group indicating the isostructurality to  $\text{KGd}(\text{WO}_4)_2$ . The size of the crystalline grains increases with the increase of the annealed temperature. The average size of crystallites of both crystals formed at 540°C was about 50 nm. X-ray diffraction, vibrational and optical studies showed that the structure of the synthesised nanocrystalline  $\text{KEu}(\text{WO}_4)_2$  and  $\text{KGd}(\text{WO}_4)_2:\text{Eu}$  is nearly the same as that found for the bulk material. The size-driven phase transitions were established for both compounds.

## Long-range ordering in the $\text{Bi}_{1-x}\text{Ae}_x\text{FeO}_{3-x/2}$ perovskites:

### $\text{Bi}_{1/3}\text{Sr}_{2/3}\text{FeO}_{2.67}$ and $\text{Bi}_{1/2}\text{Ca}_{1/2}\text{FeO}_{2.75}$

C. Lepoittevin, S. Malo, N. Barrier, N. Nguyen, G. Van Tendeloo and M. Hervieu

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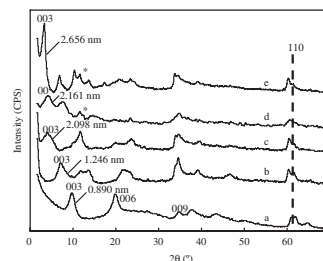


Complex long-range ordering of  $\text{Bi}/\text{Ae}$  cations and oxygen/vacancies consisting of 12-fold and 32-fold enlargement of the perovskite unit cell is observed in  $\text{Bi}_{1/3}\text{Sr}_{2/3}\text{FeO}_{2.67}$  and  $\text{Bi}_{1/2}\text{Ca}_{1/2}\text{FeO}_{2.75}$ , respectively.

## Layered double hydroxides as supports for intercalation and sustained release of antihypertensive drugs

Sheng-Jie Xia, Zhe-Ming Ni, Qian Xu, Bao-Xiang Hu and Jun Hu

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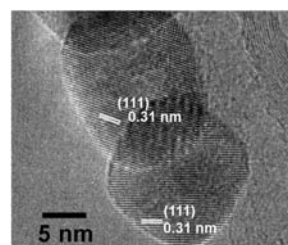


A series of antihypertensive drugs including Enalapril, Lisinopril, Captopril and Ramipril were intercalated into  $\text{Zn}/\text{Al}-\text{NO}_3$ -LDHs successfully by coprecipitation or ion-exchange technique. We focus on the structure, thermal property and low/controlled release property of as-synthesized drug-LDH composite intended for the possibility of applying these LDH-antihypertensive nanohybrids in drug delivery and controlled release systems.

## Controllable preparation and properties of composite materials based on ceria nanoparticles and carbon nanotubes

Changqing Li, Nijuan Sun, Jiangfeng Ni, Jinyong Wang, Haibin Chu, Henghui Zhou, Meixian Li and Yan Li

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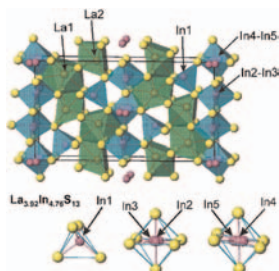


Composites based on carbon nanotubes (CNTs) and  $\text{CeO}_2$  nanoparticles were prepared with a mild hydrothermal treatment. Larger  $\text{CeO}_2$  nanoparticles were formed in the presence of CNTs. Grain size of  $\text{CeO}_2$  nanoparticles in composites could be reduced when  $\text{NaNO}_3$  was added. The size modulation mechanism was discussed. This  $\text{CeO}_2/\text{CNTs}$  composites could serve as promising anode materials for Li-ion batteries.

**Crystal structures of the  $Ln_{4-x}In_{5-y}S_{13}$  ( $Ln = La, Ce, Pr$  and  $Nd$ ;  $x = 0.08-0.12$ ,  $y = 0.21-0.24$ ),  $La_3In_{1.67}S_7$ ,  $Gd_3InS_6$  and  $La_4Ag_2In_4S_{13}$  compounds**

L.D. Gulay, M. Daszkiewicz and M.R. Huch

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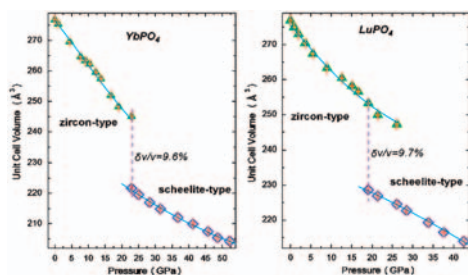


In the series of the  $Ln_{4-x}In_{5-y}S_{13}$  ( $Ln = La, Ce, Pr$  and  $Nd$ ;  $x = 0.08-0.12$ ,  $y = 0.21-0.24$ ) compounds the indium atoms occupy disordered position in the octahedral arrangement of the sulphur atoms. The tetrahedral position is ordered.

**Pressure-induced zircon-type to scheelite-type phase transitions in  $YbPO_4$  and  $LuPO_4$**

F.X. Zhang, M. Lang, R.C. Ewing, J. Lian, Z.W. Wang, J. Hu and L.A. Boatner

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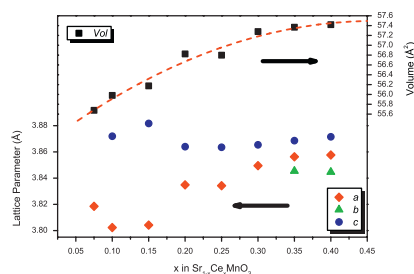


The tetragonal orthophosphates,  $YbPO_4$  and  $LuPO_4$ , show reversible phase transitions from the zircon structure-type to the scheelite structure-type at  $\sim 22$  and  $19$  Gpa, respectively. Coinciding with the phase transition, there is a  $\sim 10\%$  reduction in unit cell volume.

**Structural and electronic phase transitions in  $Sr_{1-x}Ce_xMnO_3$  perovskites**

Brendan J. Kennedy, Paul J. Saines, Qingdi Zhou, Zhaoming Zhang, Motohide Matsuda and Michihiro Miyake

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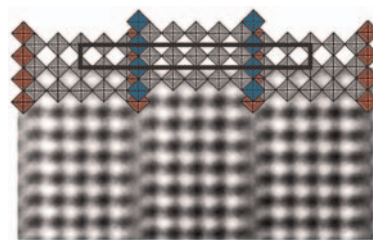


The presence of small amounts of trivalent Mn in the series  $Sr_{1-x}Ce_xMnO_3$  has a dramatic effect on the structure, with the structure changing from cubic to tetragonal and finally orthorhombic. The orbital ordering present at room temperature is lost upon heating.

**A series of aluminum tungsten oxides crystallizing in a new  $ReO_3$ -related structure type**

Frank Krumeich and Greta R. Patzke

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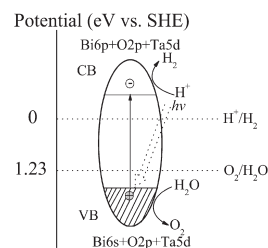


A structural model for  $Al_4W_{10}O_{32}$  was derived from electron diffraction, HRTEM and HAADF-STEM observations. The  $ReO_3$ -type structure of  $WO_3$  is sheared into five octahedra wide slabs that are connected via planes of  $AlO_6$  octahedra. Polytypes with different slab width exist and are frequently intergrown with each other.

**Electronic structure and photocatalytic properties of  $ABi_2Ta_2O_9$  ( $A = Ca, Sr, Ba$ )**

Yingxuan Li, Gang Chen, Hongjie Zhang, Zhonghua Li and Jingxue Sun

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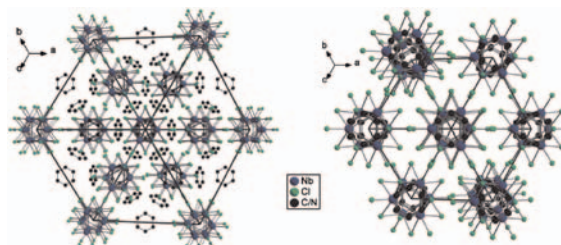
The valence band of the photocatalysts is consisted of  $O 2p$ ,  $Ta 5d$  and  $Bi 6s$  orbitals and the conduction band is from  $Bi 6p$ ,  $Ta 5d$  and  $O 2p$  orbitals. Photocatalytic properties of the photocatalyst for  $H_2$  evolution without using other co-catalysts from  $CH_3OH/H_2O$  solution and  $O_2$  evolution from  $AgNO_3/H_2O$  solution were observed under Hg lamp irradiation.

**Synthesis and structures of new niobium cluster compounds with pyridinium cations:  $(PyrH)_2[Nb_6Cl_{18}] \cdot EtOH$**

(Pyr: pyridine, Et: ethyl) and the cubic modification of  $(PyrH)_2[Nb_6Cl_{18}]$

Anke Flemming, Alessandra Hoppe and Martin Köckerling

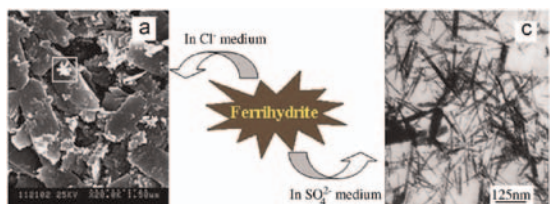
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The synthesis and structure of a second cubic modification of  $(PyrH)_2[Nb_6Cl_{18}]$  and of the new  $(PyrH)_2[Nb_6Cl_{18}] \cdot EtOH$  are reported, both of which contain isolated niobium halide cluster anions with an octahedral core of metal atoms.

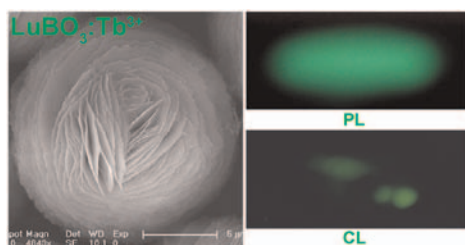
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**The transformation of ferrihydrite in the presence of trace Fe(II): The effect of the anionic media**  
 Hui Liu, Hui Guo, Ping Li and Yu Wei  
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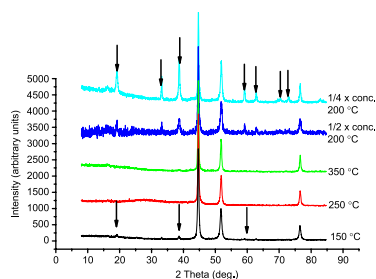
Fe(II)-induced transformation of ferrihydrite in sulfate-rich medium was studied. Lepidocrocite is a main ingredient in the product in Cl<sup>-</sup> medium at room temperature (RT), while goethite is the only product in SO<sub>4</sub><sup>2-</sup> medium. Goethite particles obtained in Cl<sup>-</sup> medium are star-like but rod-like in SO<sub>4</sub><sup>2-</sup> medium.

**Hydrothermal synthesis and luminescent properties of LuBO<sub>3</sub>:Tb<sup>3+</sup> microflowers**  
 Jun Yang, Cuimiao Zhang, Lili Wang, Zhiyao Hou, Shanshan Huang, Hongzhou Lian and Jun Lin  
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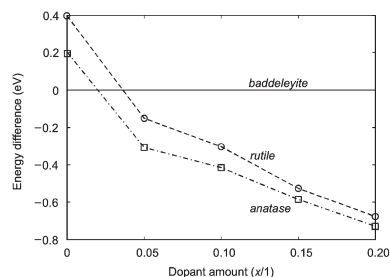
Hexagonal vaterite-type LuBO<sub>3</sub>:Tb<sup>3+</sup> microflower-like phosphors have been successfully prepared by a simple and mild hydrothermal process directly. The reaction mechanism has been considered as the dissolution/precipitation mechanism; the self-assembly evolution process has been proposed on homocentric layer-by-layer growth style. The luminescent properties of the as-obtained LuBO<sub>3</sub>:Tb<sup>3+</sup> samples have been investigated in detail, which shows it is a good green-emitting phosphor in fluorescent lamps and field emission displays potentially.

**Surfactant-free synthesis of nickel nanoparticles in near-critical water**  
 Peter Hald, Martin Bremholm, Steen Brummerstedt Iversen and Bo Brummerstedt Iversen  
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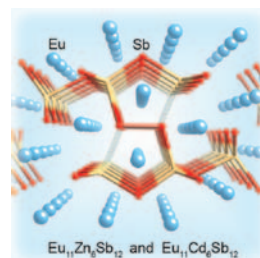
A surfactant-free synthesis route to nickel nanoparticles has been successfully transferred to near-critical water conditions reducing synthesis times from hours to seconds. Nickel nanoparticles in the 40–60 nm range have been synthesised from an ammonia stabilised hydrazine complex with the average size controlled by reaction temperature.

**A density-functional study on the stability of anatase-type phases in the system Mg–Ta–O–N**  
 Holger Wolff, Martin Lerch, Heikko Schilling, Carsten Bähz and Richard Dronskowski  
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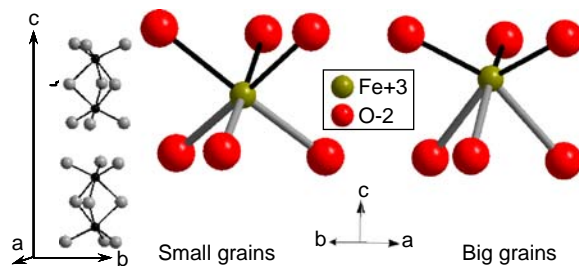
Density-functional total energy of Mg-doped TaON in several polymorphs, each in its most stable arrangement, as a function of the dopant amount.

**Synthesis, structure and physical properties of the new Zintl phases Eu<sub>11</sub>Zn<sub>6</sub>Sb<sub>12</sub> and Eu<sub>11</sub>Cd<sub>6</sub>Sb<sub>12</sub>**  
 Bayrammurad Saparov, Svilen Bobev, Arif Ozbay and Edmund R. Nowak  
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The synthesis, structure determination from single-crystal X-ray diffraction and magnetic properties of Eu<sub>11</sub>Zn<sub>6</sub>Sb<sub>12</sub> and Eu<sub>11</sub>Cd<sub>6</sub>Sb<sub>12</sub> are reported. Both compounds crystallize with the monoclinic space group C2/m, and their structure can be viewed as built of ZnSb<sub>4</sub> or CdSb<sub>4</sub> tetrahedra, which are connected through common corners and *exo*-bonds.

**Impact of structural features on pigment properties of α-Fe<sub>2</sub>O<sub>3</sub> haematite**  
 N. Pailhé, A. Wattiaux, M. Gaudon and A. Demourgues  
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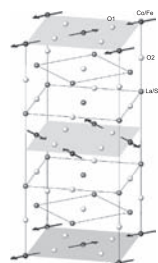
The reddish colour of Fe<sub>2</sub>O<sub>3</sub> haematite was analysed in regard to its structural features, especially in regard to the Fe<sup>3+</sup> octahedral site distortion, which is progressively less and less distorted from the centre towards the surface of the grains.

## Synthesis and characterization of the $K_2NiF_4$ phases

$La_{1+x}Sr_{1-x}Co_{0.5}Fe_{0.5}O_{4-\delta}$  ( $x = 0, 0.2$ )

H. El Shinawi and C. Greaves

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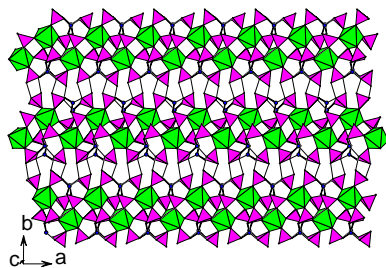


The reduced  $K_2NiF_4$  phases  $LaSrCo_{0.5}Fe_{0.5}O_{3.75}$  and  $La_{1.2}Sr_{0.8}Co_{0.5}Fe_{0.5}O_{3.85}$  accommodate disordered oxide ion vacancies confined to equatorial planes of the structure. Magnetic exchange results in AFM order at low temperature, which can be represented by a tetragonal noncollinear model for the moments.  $Co^{3+}$  ions, present in stoichiometric  $LaSrCo_{0.5}Fe_{0.5}O_4$  and  $La_{1.2}Sr_{0.8}Co_{0.5}Fe_{0.5}O_4$ , inhibit magnetic order and are assumed to be in the low-spin state.

## Synthesis, crystal structures, and luminescent properties of two types of lanthanide phosphonates

Ya-Qin Guo, Si-Fu Tang, Bing-Ping Yang and Jiang-Gao Mao

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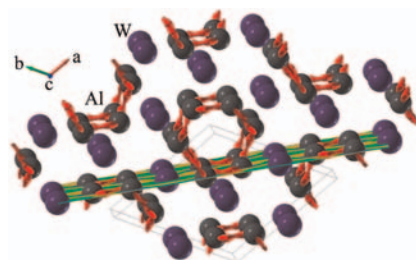


Two series of luminescent lanthanide phosphonates have been synthesized and structurally characterized. Their structures feature two different types of 2D sumpramolecular layers based on two types of 1D arrays interlinked via strong hydrogen bonds.

## Crystal structure and high-pressure studies of $WAl_2$ , an aluminide crystallizing with the $CrSi_2$ structure type

Q.F. Gu, D.Y. Jung, G. Krauss and W. Steurer

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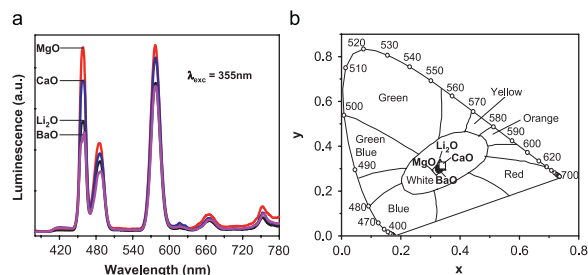


The novel compound  $WAl_2$  is the first aluminide crystallizing with the  $CrSi_2$  structure type. This compound is stable up to high pressures of at least 31.5 GPa. The chemical bonding analysis by means of the electron localization function (ELF) reveals a partially covalent bonding being responsible for the anisotropic compression behavior.

## White luminescence of Tm–Dy ions co-doped aluminoborosilicate glasses under UV light excitation

Shimin Liu, Gaoling Zhao, Xiaohua Lin, Hao Ying, Junbo Liu, Jianxun Wang and Gaorong Han

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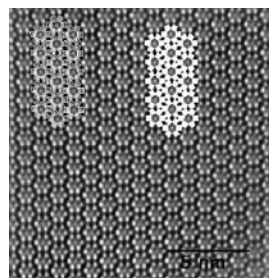


$Tm^{3+}$  and  $Dy^{3+}$  ions co-doped aluminoborosilicate glasses, which emit white light under UV light excitation, were prepared. The dependence of luminescence properties on glass compositions was studied, and results showed that the white color luminescence was not affected significantly with different network modifier oxides. This adjustability could broaden application areas.

## How isopolyanions self-assemble and condense into a 2D tungsten oxide crystal: HRTEM imaging of atomic arrangement in an intermediate new hexagonal phase

A. Chemseddine and U. Bloeck

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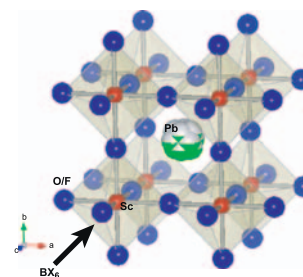


From the isopolyanion to the extended bulk tungsten oxide: HRTEM imaging.

## Synthesis of the novel perovskite-type oxyfluoride $PbScO_2F$ under high pressure and high temperature

Tetsuhiro Katsumata, Mamoru Nakashima, Hiroshi Umemoto and Yoshiyuki Inaguma

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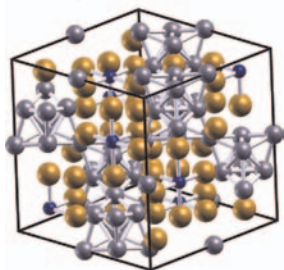
A novel perovskite-type oxyfluoride,  $PbScO_2F$ , was synthesized at high pressure (4 GPa) and temperature (1000 °C). This compound has a cubic perovskite-type structure in which the Pb ions are displaced along the  $\langle 110 \rangle$  direction from the ideal A-site position.

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### Pechini synthesis and characterization of molybdenum carbide and nickel molybdenum carbide

Arnold M. Stux, Christel Laberty-Robert and Karen E. Swider-Lyons

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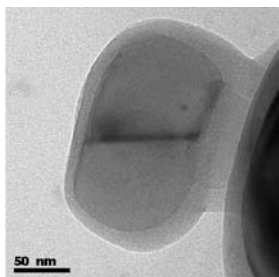


Ball and stick representation of the  $\eta$ -Ni<sub>6</sub>Mo<sub>6</sub>C crystal structure.

### Al<sub>2</sub>O<sub>3</sub> @ TiO<sub>2</sub>—A simple sol-gel strategy to the synthesis of low temperature sintered alumina-aluminium titanate composites through a core-shell approach

M. Jayasankar, S. Ananthakumar, P. Mukundan, W. Wunderlich and K.G.K. Warrior

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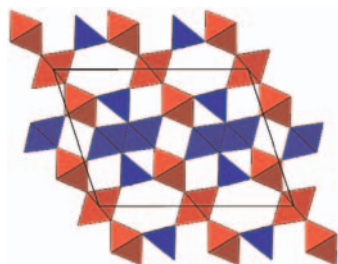


The article presents a simple sol-gel process through core-shell approach to the synthesis of low temperature sintered alumina-aluminium titanate. The lowering of the reaction temperature can be attributed to the maximisation of the contact surface between the reactant due to the core-shell approach. This material showed the better microstructure control compared to the standard solid-state mixing route.

### Formation and structural refinements of tunneled intergrowth phases in the Ga<sub>2</sub>O<sub>3</sub>-In<sub>2</sub>O<sub>3</sub>-SnO<sub>2</sub>-TiO<sub>2</sub> system

C.R. Maier, M. Charoenwongsa and D.D. Edwards

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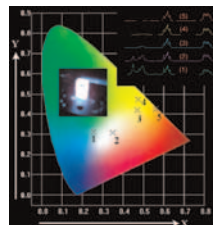


The structures of three beta-gallia-rutile intergrowths, expressed as (Ga,In)<sub>4</sub>(Sn,Ti)<sub>n-4</sub>O<sub>2n-2</sub>,  $n=6, 7,$  and  $9,$  were refined using Rietveld analysis of neutron time-of-flight powder diffraction data. The  $n=6$  phase Ga<sub>3.24</sub>In<sub>0.76</sub>Sn<sub>1.6</sub>Ti<sub>0.4</sub>O<sub>10</sub> crystallizes in  $P2_1/m$  whereas the  $n=7$  and  $9$  phases crystallize in  $C2/m$ . All structure are similar in that they possess hexagonal tunnels parallel to the [010] vector.

### Novel rare earth ions-doped oxyfluoride nano-composite with efficient upconversion white-light emission

Daqin Chen, Yuansheng Wang, Yunlong Yu, Ping Huang and Fangyi Weng

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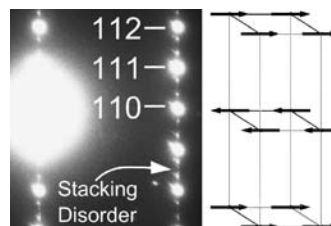


Under single 976 nm laser excitation, intense red, green and blue upconversion emissions were simultaneously observed owing to the successive energy transfer from Yb<sup>3+</sup> to Ho<sup>3+</sup> or Tm<sup>3+</sup>. Various colors of luminescence, including bright perfect white light with CIE- $X=0.351$  and CIE- $Y=0.306$ , can be easily tuned by adjusting the concentrations of the rare earth ions in the transparent oxyfluoride glass ceramics.

### Structural disorder, octahedral coordination and two-dimensional ferromagnetism in anhydrous alums

D.V. West, Q. Huang, H.W. Zandbergen, T.M. McQueen and R.J. Cava

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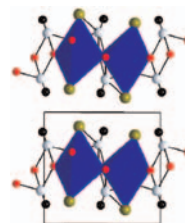


The anhydrous alums KCr(SO<sub>4</sub>)<sub>2</sub>, RbCr(SO<sub>4</sub>)<sub>2</sub> and KAl(SO<sub>4</sub>)<sub>2</sub> are characterized by X-ray and neutron powder diffraction and TEM diffraction. All compounds have octahedral coordination of the trivalent cations. Stacking disorder is observed, with the MO<sub>6</sub>-SO<sub>4</sub> network of polyhedra rotated in opposite directions between layers. Low-temperature NPD reveals ferromagnetic in-plane ordering, with antiferromagnetic ordering between planes below 3 K.

### Anomalous low-temperature behavior of the Co dimers in the oxo-halide CoSb<sub>2</sub>O<sub>3</sub>Br<sub>2</sub>

Zuzana Hugonin, Mats Johnsson, Sven Lidin, Dirk Wulferding, Peter Lemmens and Reinhard K. Kremer

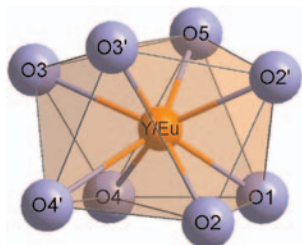
Page 2776



The synthesis, crystal structure determination, and magnetic properties of the new layered compound CoSb<sub>2</sub>O<sub>3</sub>Br<sub>2</sub> is reported. Structural Co-Co dimers are formed within the layers. The susceptibility below 25 K is typical for the onset of long-range antiferromagnetic correlations. Raman scattering and specific heat measurements both point to a structural instability leading to a loss of inversion symmetry below 6 K.

**Synthesis, crystal structures and luminescence properties of the  $\text{Eu}^{3+}$ -doped yttrium oxotellurates(IV)  $\text{Y}_2\text{Te}_4\text{O}_{11}$  and  $\text{Y}_2\text{Te}_5\text{O}_{13}$**

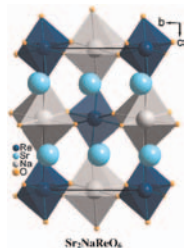
Patrick Höss, Andres Osvet, Frank Meister, Mirosław Batentschuk, Albrecht Winnacker and Thomas Schleid  
 Page 2783



The unique rare-earth metal(III) site in  $\text{Y}_2\text{Te}_4\text{O}_{11}$  coordinated by eight oxygen atoms in the shape of a distorted trigonal dodecahedron where also the  $\text{Eu}^{3+}$  cations of the doped compound reside.

**Crystal growth and structural investigation of  $\text{A}_2\text{BReO}_6$  ( $A = \text{Sr}, \text{Ba}$ ;  $B = \text{Li}, \text{Na}$ )**

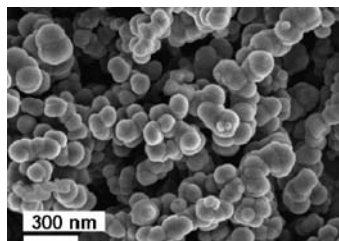
M. Bharathy and H.-C. zur Loye  
 Page 2789



Single-crystal structure analyses of double perovskite rhenates,  $\text{Sr}_2\text{LiReO}_6$ ,  $\text{Ba}_2\text{LiReO}_6$  and  $\text{Ba}_2\text{NaReO}_6$  indicate cubic symmetry while that of  $\text{Sr}_2\text{NaReO}_6$  shows monoclinic symmetry.

**One-step catalyst-free generation of carbon nanospheres via laser-induced pyrolysis of anthracene**

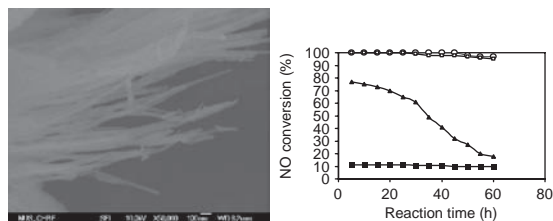
M. Bystrzejewski, H. Lange, A. Huczko, P. Baranowski, H.-W. Hübers, T. Gemming, T. Pichler, B. Büchner and M.H. Rummeli  
 Page 2796



Carbon nanospheres with diameters between 100 and 400 nm have been successfully synthesized via low-power laser assisted pyrolysis of anthracene in a nitrogen atmosphere. The developed facile route yields homogeneous nanoparticles and requires no supplementary carbon feedstock or catalyst. The sharp thermal gradient afforded by the laser results in two kinds of carbon products that differ in crystallinity and mean particle size. Our detailed findings point to the carbon nanospheres being comprised of nanosized unclosed aromatic layers that are connected together by simple organic linkers.

**The direct decomposition of NO over the  $\text{La}_2\text{CuO}_4$  nanofiber catalyst**

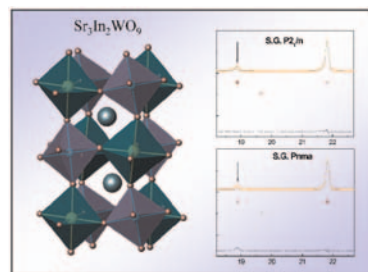
Lizhen Gao, Hui Tong Chua and Sibudjing Kawi  
 Page 2804



$\text{La}_2\text{CuO}_4$  nanofibers, made by use of single walled carbon nanotubes as templates under mild hydrothermal conditions, could catalytically decompose NO completely into nitrogen and oxygen at the low temperature of 300 °C.

**Order-disorder in  $\text{In}^{3+}$  perovskites: The example of  $\text{A}(\text{In}_{2/3}\text{B}'_{1/3})\text{O}_3$  ( $A = \text{Ba}, \text{Sr}$ ;  $B' = \text{W}, \text{U}$ )**

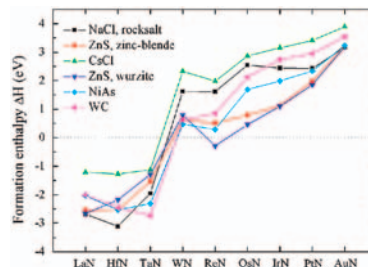
S.A. Larrérgola, J.A. Alonso, R.M. Pinacca, M.C. Viola and J.C. Pedregosa  
 Page 2808



The structure of the new uranium-based double perovskite  $\text{Sr}_3\text{In}_2\text{UO}_9$  is described and the true symmetry of the other title compounds are revisited. The presence of long-range ordering in the Sr samples, by contrast with the Ba perovskites, is related with the smaller unit cell and B-B distances in the Sr oxides, promoting the electrostatic repulsions between highly charged  $\text{W}^{6+}$  and  $\text{U}^{6+}$  cations as driving force for the long-range B-site ordering.

**Electronic and mechanical properties of 5d transition metal mononitrides via first principles**

Erjun Zhao and Zhijian Wu  
 Page 2814

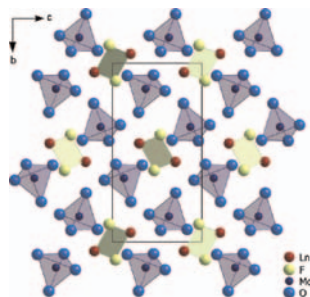


Formation enthalpy per formula unit  $\Delta H$  (eV) for all the considered structures of 5d transition metal mononitrides  $\text{MN}$  ( $M = \text{La}-\text{Au}$ ). It was shown that the formation enthalpy increases from  $\text{LaN}$  to  $\text{AuN}$ . The nitrides with negative values indicate that they can be synthesized experimentally at ambient conditions.

## Crystal structure, spectroscopic properties, and magnetic behavior of the fluoride-derivatized lanthanoid(III) ortho-oxomolybdates(VI) $LnF[MoO_4]$ ( $Ln = Sm-Tm$ )

Ingo Hartenbach, Sabine Strobel, Peter K. Dorhout and Thomas Schleid

Page 2828

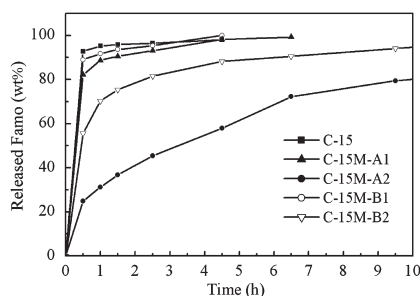


View at the crystal structure of  $LnF[MoO_4]$  ( $Ln = Sm-Tm$ ) along [100] with special emphasis on the isolated  $[MoO_4]^{2-}$  tetrahedra (blue) and the  $[F_2Ln]^{4+}$  rhombuses (green).

## Controlled drug release from bifunctionalized mesoporous silica

Wujun Xu, Qiang Gao, Yao Xu, Dong Wu, Yuhuan Sun, Wanling Shen and Feng Deng

Page 2837

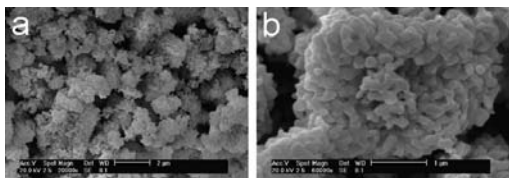


Trimethylsilyl-carboxyl bifunctionalized SBA-15 has been studied as carrier for controlled release of drug famotidine. To load drug with large capacity, SBA-15 with high content of carboxyl groups was successfully synthesized. After grafting trimethylsilyl groups on the surface of carboxyl functionalized SBA-15, the release of Famo was greatly delayed with the increasing content of TMS groups.

## Solid-state synthesis, characterization and luminescent properties of $Eu^{3+}$ -doped gadolinium tungstate and molybdate phosphors: $Gd_{(2-x)}MO_6:Eu_x^{3+}$ ( $M = W, Mo$ )

Fang Lei, Bing Yan and Hao-Hong Chen

Page 2845

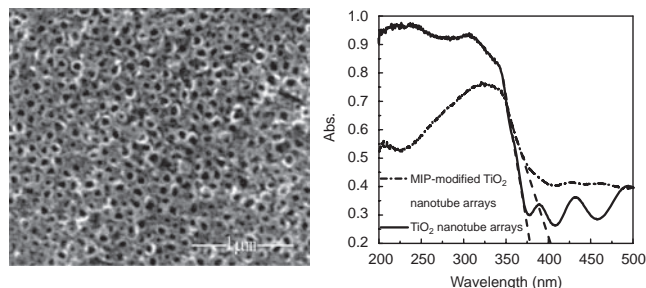


Excellent red phosphors gadolinium tungstate and molybdate with the formula  $Gd_{(2-x)}MO_6:Eu_x^{3+}$  ( $M = Mo, W$ ) were synthesized by the conventional solid-state reaction at 900 and 1300°C for 4 h, respectively. SEM images indicate that the morphology of  $Gd_{1.96}WO_6:Eu_{0.04}^{3+}$  has 3D micro-pore network structures better than the block-like  $Gd_{1.96}MoO_6:Eu_{0.04}^{3+}$ . Their quantum efficiency has been investigated.

## Synthesis of molecular imprinted polymer modified $TiO_2$ nanotube array electrode and their photoelectrocatalytic activity

Na Lu, Shuo Chen, Hongtao Wang, Xie Quan and Huimin Zhao

Page 2852

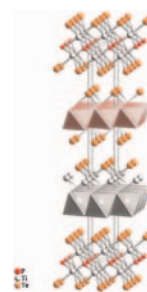


A tetracycline hydrochloride molecularly imprinted polymer modified  $TiO_2$  nanotube array electrode was prepared via surface molecular imprinting. It showed improved response to simulated solar light and higher adsorption capability for tetracycline hydrochloride, thereby exhibiting increased PEC activity under simulated solar light irradiation. The apparent first-order rate constant was 1.2-fold of that on  $TiO_2$  nanotube array electrode.

## The layered metal $Ti_2PTE_2$

Frauke Philipp, Peer Schmidt, Michael Ruck, Walter Schnelle and Anna Isaeva

Page 2859

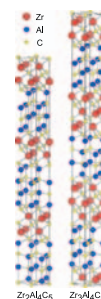


Crystal structure of  $Ti_2PTE_2$  with stacking sequence of the hexagonal layers of anions and cations. Highlighted in red is the octahedral coordination of phosphorus by titanium, and in grey the octahedral coordination of titanium by phosphorus and tellurium.

## Syntheses, crystal structures and Si solubilities of new layered carbides $Zr_2Al_4C_5$ and $Zr_3Al_4C_6$

Keita Sugiura, Tomoyuki Iwata, Hideto Yoshida, Shinobu Hashimoto and Koichiro Fukuda

Page 2864



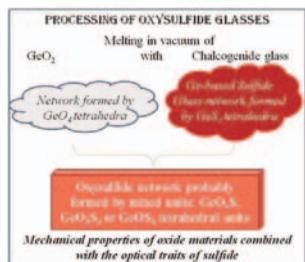
Crystal structures of new layered carbides  $(ZrC)_2Al_4C_3$  and  $(ZrC)_3Al_4C_3$ .



## Processing and characterization of new oxysulfide glasses in the Ge–Ga–As–S–O system

C. Maurel, L. Petit, M. Dussauze, E.I. Kamitsos, M. Couzi, T. Cardinal, A.C. Miller, H. Jain and K. Richardson

Page 2869

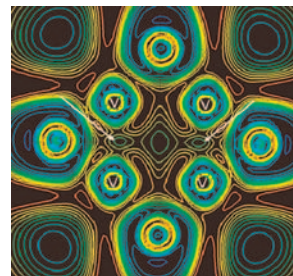


In this paper, we explain how new oxysulfide glasses are prepared in the Ge–Ga–As system employing a two-step process: (1) the processing of the chalcogenide glass (ChG) and (2) the re-melting of the ChG with GeO<sub>2</sub> powder. Raman, infrared and XPS spectroscopies show the formation of new oxysulfide structural units.

## Quantum chemical study and low-temperature calorimetry of phase transition in V<sub>4</sub>S<sub>9</sub>Br<sub>4</sub>

S.G. Kozlova, S.P. Gabuda, G.A. Berezovskii, D.P. Pischur, Y.V. Mironov, A. Simon and V.E. Fedorov

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Dysynaptic basins of electron spin pairing in low-temperature phase V<sub>4</sub>S<sub>9</sub>Br<sub>4</sub> (arrows).

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