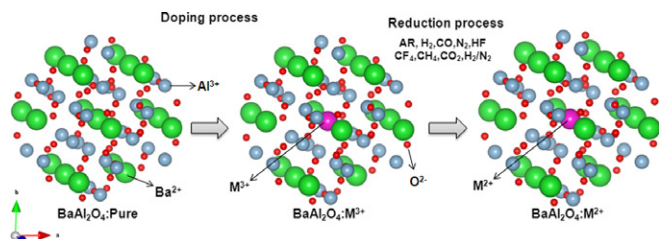


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### Regular Articles

#### Computer modelling of the reduction of rare earth dopants in barium aluminate

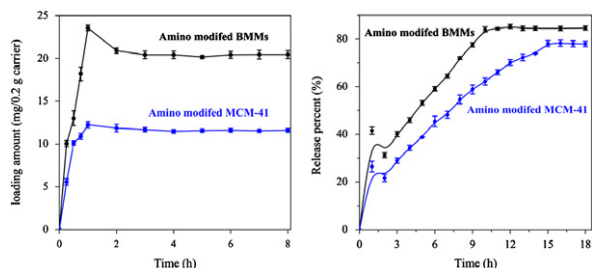
Marcos V. dos S. Rezende, Mário E.G. Valerio and Robert A. Jackson  
page 1903



The doping and subsequent reduction of a rare earth ion into the barium aluminate lattice.

#### Functionalized bimodal mesoporous silicas as carriers for controlled aspirin delivery

Lin Gao, Jihong Sun and Yuzhen Li  
page 1909

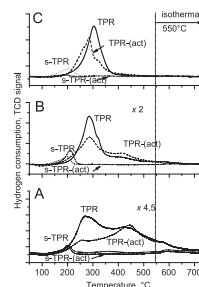


Loading (A) and release profiles (B) of aspirin in N-BMMs and N-MCM-41 indicated that BMMs have more drug loading capacity and faster release rate than that MCM-41.

### Regular Articles—Continued

#### TPR investigations on the reducibility of Cu supported on Al<sub>2</sub>O<sub>3</sub>, zeolite Y and SAPO-5

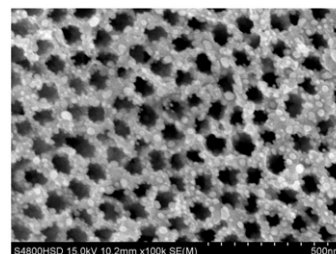
Dang Lanh Hoang, Thi Thuy Hanh Dang, Jana Engeldinger, Matthias Schneider, Jörg Radnik, Manfred Richter and Andreas Martin  
page 1915



TPR, TPR-(act), s-TPR and s-TPR-(act) profiles of (1.36)Cu/SAPO-5 (A), (4.55)Cu/SAPO-5 (B) and (9.19)Cu/SAPO-5 (C) samples. The intensities of TCD signals in (A) and (B) are multiplied by 4.5 and 2, respectively.

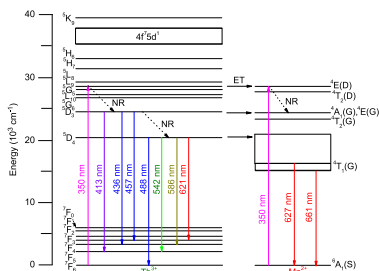
#### Design of highly ordered Ag–SrTiO<sub>3</sub> nanotube arrays for photocatalytic degradation of methyl orange

Yue Sun, Jiawen Liu and Zhonghua Li  
page 1924



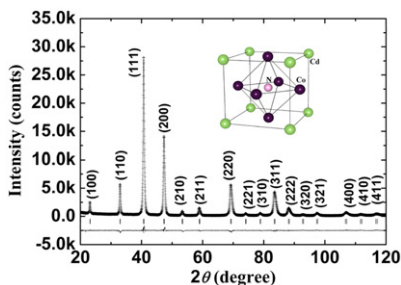
Ag–SrTiO<sub>3</sub> nanotube arrays were successfully prepared. The photocatalytic activity was evaluated by degradation of methyl orange under ultraviolet irradiation.

**Photoluminescence and energy transfer in Tb<sup>3+</sup>/Mn<sup>2+</sup> co-doped ZnAl<sub>2</sub>O<sub>4</sub> glass ceramics**  
Gandham Lakshminarayana and Lothar Wondraczek  
*page 1931*



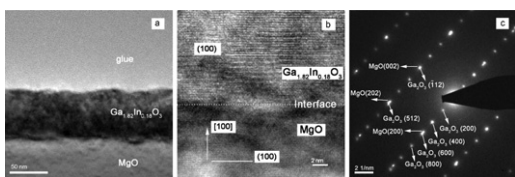
In the prepared Tb<sup>3+</sup>/Mn<sup>2+</sup> co-doped glass ceramics containing gahnite (ZnAl<sub>2</sub>O<sub>4</sub>) nanocrystals, the luminescence color is changed from green light to yellowish-red light with an increase in Mn<sup>2+</sup> concentration due to enhanced energy transfer from Tb<sup>3+</sup> to Mn<sup>2+</sup> ions. This tunability should have potential applications in solid state lighting to produce white light, which can be obtained by appropriately optimizing the ratio of Tb<sup>3+</sup>/Mn<sup>2+</sup> ions under UV(350 nm) excitation.

**Preparation and physical properties of antiperovskite-type compounds CdNC<sub>3-z</sub>Ni<sub>z</sub> (0 ≤ z ≤ 3)**  
Bing He, Cheng Dong, Lihong Yang, Linhui Ge and Hong Chen  
*page 1939*



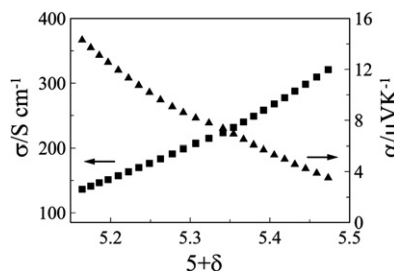
CdNC<sub>3</sub> is a new ternary nitride with antiperovskite structure, and it can form a complete solid solution series with CdNNi<sub>3</sub>.

**Structural and optical properties of Ga<sub>2</sub>O<sub>3</sub>:In films deposited on MgO (1 0 0) substrates by MOCVD**  
Lingyi Kong, Jin Ma, Caina Luan and Zhen Zhu  
*page 1946*



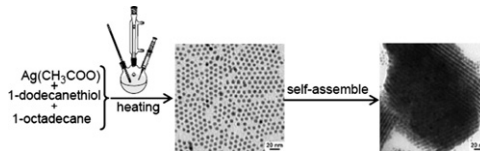
Low magnification XTEM (a), HRTEM (b) and SAED (c) micrographs of the interface area between Ga<sub>1.82</sub>In<sub>0.18</sub>O<sub>3</sub> film and MgO substrate have showed the Ga<sub>1.82</sub>In<sub>0.18</sub>O<sub>3</sub> is an epitaxial film.

**High-temperature electron-hole transport in PrBaCo<sub>2</sub>O<sub>5+δ</sub>**  
A.Yu. Suntsov, I.A. Leonidov, M.V. Patrakeev and V.L. Kozhevnikov  
*page 1951*



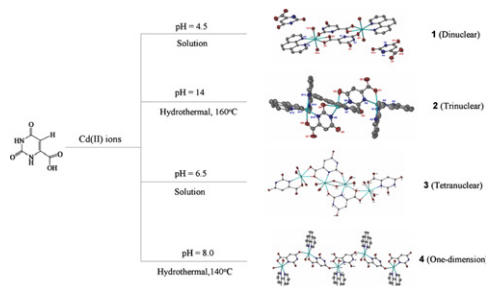
Electrical properties in PrBaCo<sub>2</sub>O<sub>5+δ</sub> depending on oxygen content at 800 °C.

**One-pot synthesis, optical property and self-assembly of monodisperse silver nanospheres**  
Aiwei Tang, Shengchun Qu, Yanbing Hou, Feng Teng, Yongsheng Wang and Zhanguo Wang  
*page 1956*



Different sized and monodisperse silver nanospheres were prepared using a one-pot approach with no pre-synthesis of organometallic precursors, and the silver nanospheres can self-assemble into highly ordered superlattices.

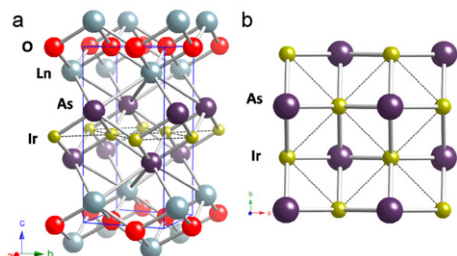
**Di-, tri-, tetranuclear clusters and polymeric cadmium compounds: Syntheses, structures and fluorescent properties with various linking fashions and high stability of orotates under the condition of strong bases**  
Xing Li, Yue Bing, Mei-Qin Zha, Dong-Jie Wang, Lei Han and Rong Cao  
*page 1963*



Assembly of orotic acid and Cd(II) salts result in four new compounds under different reaction conditions, the compounds possess strong photoluminescence emissions and high thermal stability.

## Synthesis and electronic properties of $LnRhAsO$ and $LnIrAsO$ compositions

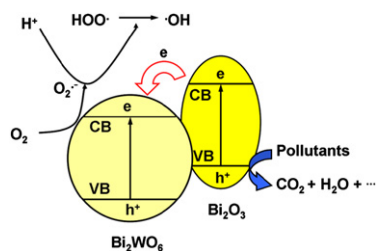
Sean Muir, A.W. Sleight and M.A. Subramanian  
page 1972



$LnIrAsO$  ( $Ln = La, Ce, Nd$ ) and  $LnRhAsO$  ( $Ln = Ce, Rh$ ) have been synthesized. These new transition metal oxypnictide compositions are isostructural to  $LaFeAsO$ . The  $5d$  Ir compositions demonstrate a shorter metal-metal interaction than the  $4d$  Rh compositions.

## Preparation and visible light photocatalytic activity of $Bi_2O_3/Bi_2WO_6$ heterojunction photocatalysts

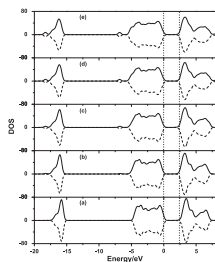
Ming-Sheng Gui, Wei-De Zhang, Qing-Xi Su and Cai-Hong Chen  
page 1977



The  $Bi_2O_3/Bi_2WO_6$  heterojunction catalysts were constructed with improved photocatalytic activity, which can be ascribed to their improved light absorption property and the reduced recombination rate between photoexcited electrons and holes.

## Investigation of the silicon concentration effect on Si-doped anatase $TiO_2$ by first-principles calculation

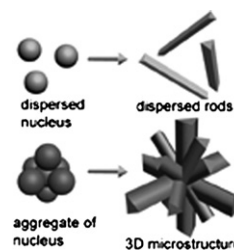
Weimei Shi, Qifeng Chen, Yao Xu, Dong Wu and Chun-fang Huo  
page 1983



The total density of states (TDOS) of  $Ti_{1-x}Si_xO_2$  with (a)  $x=0$ , (b)  $x=0.03125$ , (c)  $x=0.0625$ , (d)  $x=0.09375$  and (e)  $x=0.125$ .

## Phase-controlled solvothermal synthesis and characterization of nickel sulfides with good single crystalline nature

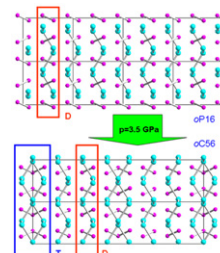
Shuguang Chen, Kai Zeng, Haibin Li and Fujin Li  
page 1989



Rhombohedral NiS dispersed rods and 3D flower-like microstructures are evolved from dispersed nucleus and aggregate of nucleus, respectively, and the cross-sections of such rods are in equilateral triangle-like shape.

## Pressure-induced development of bonding in NiAs type compounds and polymorphism of NiP

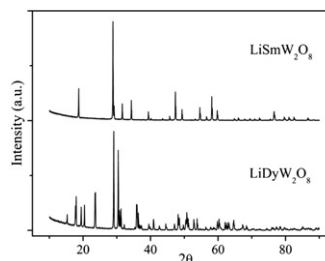
Przemyslaw Dera, John D. Lazarz and Barbara Lavina  
page 1997



A reversible, pressure-induced phase transition has been found in nickel monophosphide NiP at 3.5 GPa by means of in situ single-crystal X-ray diffraction. The high-pressure phase is a commensurately modulated superstructure of the NiAs aristotype involving gradual conversion from the net of isolated  $P_2$  dimers found in the ambient NiP, towards zig-zag polymeric  $P_\infty$  chains found in MnP.

## Crystal structure of $LiLnW_2O_8$ ( $Ln = \text{lanthanides and Y}$ ): An X-ray powder diffraction study

J.M. Postema, W.T. Fu and D.J.W. IJdo  
page 2004

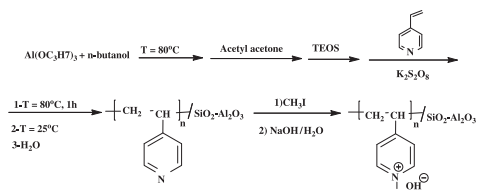


Part of the X-ray diffraction patterns of  $LiSmW_2O_8$  and  $LiDyW_2O_8$  representing two structure types in  $LiLnW_2O_8$ : the scheelite with  $Ln = La-Gd$  and wolframite with  $Ln = Dy-Lu$  and Y. In  $LiTbW_2O_8$  both the scheelite and the wolframite structures occur at high and low temperatures, respectively.

Continued

## Preparation, characterization and catalyst application of ternary interpenetrating networks of poly 4-methyl vinyl pyridinium hydroxide–SiO<sub>2</sub>–Al<sub>2</sub>O<sub>3</sub>

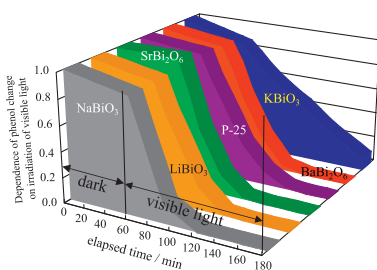
Roozbeh Javad Kalbasi, Majid Kolahdoozan and Sedigheh Mozafari Vanani  
page 2009



In this paper, we report the synthesis of poly 4-methyl vinyl pyridinium hydroxide–SiO<sub>2</sub>–Al<sub>2</sub>O<sub>3</sub>. The novelty of this procedure is at easy preparation together with using inexpensive materials.

## Photocatalytic activities of various pentavalent bismuthates under visible light irradiation

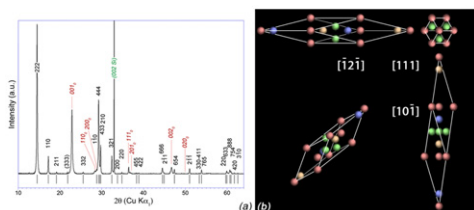
Takahiro Takei, Rie Haramoto, Qiang Dong, Nobuhiro Kumada, Yoshinori Yonesaki, Nobukazu Kinomura, Takayuki Mano, Shunsuke Nishimoto, Yoshikazu Kameshima and Michihiro Miyake  
page 2017



Nine pentavalent bismuthates were synthesized and were examined for their photocatalytic activities by decomposition of phenol under visible light irradiation. NaBiO<sub>3</sub>, LiBiO<sub>3</sub>, SrBi<sub>2</sub>O<sub>6</sub> and BaBi<sub>2</sub>O<sub>6</sub> indicated faster decomposition rate than that of anatase (P25) under UV–vis light irradiation.

## A very promising piezoelectric property of Ta<sub>2</sub>O<sub>5</sub> thin films. I: Monoclinic–trigonal phase transition

M. Audier, B. Chenevier, H. Roussel, L. Vincent, A. Peña and A. Lintanf Salaün  
page 2023



(a)  $\theta/2\theta$  X-ray pattern of the tantalum oxide layer prepared by i-MOCVD, cooled down at 5 °C min<sup>-1</sup> after a thermal treatment at 850 °C under N<sub>2</sub> for 1 h. (b) Rhombohedral cell of the Ta<sub>2</sub>O<sub>5</sub> trigonal structure of R3 space-group decorated with its 10 Ta sites.

## A very promising piezoelectric property of Ta<sub>2</sub>O<sub>5</sub> thin films. II: Birefringence and piezoelectricity

M. Audier, B. Chenevier, H. Roussel, L. Vincent, A. Peña and A. Lintanf Salaün  
page 2033

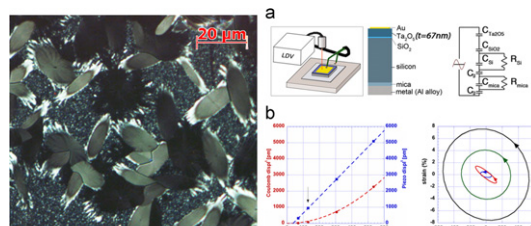
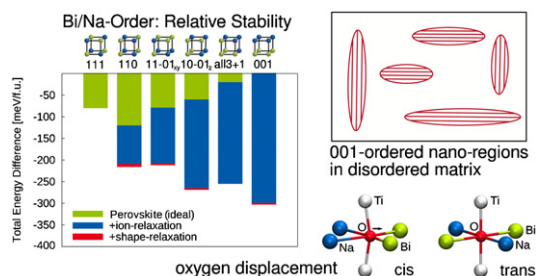


Image of cross-polarized optical microscopy showing grains of trigonal structure embedded in the monoclinic phase (on the left); (a) mounting of the sample for Laser Doppler Vibrometry, sample constituted of several layers and its equivalent electrical circuit; (b) longitudinal displacements due to converse piezoelectric and Coulomb effects and corresponding piezoelectric strain– $U_{app}$  hystereses.

## Chemical order and local structure of the lead-free relaxor ferroelectric Na<sub>1/2</sub>Bi<sub>1/2</sub>TiO<sub>3</sub>

Melanie Gröting, Silke Hayn and Karsten Albe  
page 2041



First-principles calculations give relative stabilities of different chemically ordered structures. The results suggest a new model for the local structure of Na<sub>1/2</sub>Bi<sub>1/2</sub>TiO<sub>3</sub> with 001-ordered nano-regions embedded in a chemically disordered matrix. Chemical order/disorder additionally induces displacive disorder within the oxygen sublattice.

## Morphology evolution of ZrB<sub>2</sub> nanoparticles synthesized by sol–gel method

Yun Zhang, Ruixing Li, Yanshan Jiang, Bin Zhao, Huiping Duan, Junping Li and Zhihai Feng  
page 2047

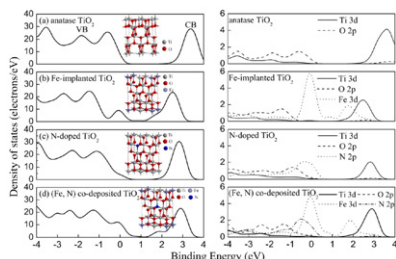


Increasing the gelation temperature, the particle shapes changed from sphere-like particles at 65 °C to a particle chain at 75 °C, and then form rod-like particles at 85 °C.



**Characterization and photocatalytic activity of Fe- and N-co-deposited TiO<sub>2</sub> and first-principles study for electronic structure**

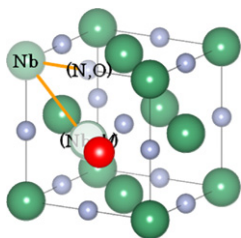
Chung-Chih Yen, Da-Yung Wang, Li-Shin Chang and Han C. Shih  
page 2053



The electronic properties of (Fe, N) co-deposited TiO<sub>2</sub> films determined by theoretical calculations is graphically shown; Fe and N preferentially substitute the Ti and O site, to form impurity level.

**Preparation, crystal structure, and superconductive characteristics of new oxynitrides (Nb<sub>1-x</sub>M<sub>x</sub>)(N<sub>1-y</sub>O<sub>y</sub>) where M=Mg, Si, and x ≈ y**

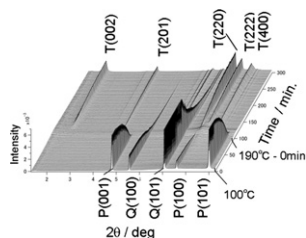
Yoshio Ohashi, Teruki Motohashi, Yuji Masubuchi, Toshihiro Moriga, Keiichiro Murai and Shinichi Kikkawa  
page 2061



Doped silicon ions substituting Nb in (Nb<sub>0.87</sub>Si<sub>0.09</sub>□<sub>0.04</sub>)(N<sub>0.87</sub>O<sub>0.13</sub>) introduced a large displacement at the 4a site mainly because of the accompanied vacancy. The silicon ions may also be slightly shifted from the regular octahedral 4a site (green) towards the interstitial tetrahedral site (red) statistically in the rock-salt type lattice.

**Effects of quartz particle size and water-to-solid ratio on hydrothermal synthesis of tobermorite studied by in-situ time-resolved X-ray diffraction**

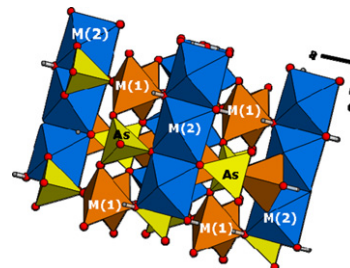
J. Kikuma, M. Tsunashima, T. Ishikawa, S. Matsuno, A. Ogawa, K. Matsui and M. Sato  
page 2066



Time-resolved XRD data set was obtained at up to 190 °C under a saturated steam pressure. Tobermorite (5CaO · 6SiO<sub>2</sub> · 5H<sub>2</sub>O) formation reaction was investigated in detail for several different starting materials.

**Magnetostructural correlations in the antiferromagnetic Co<sub>2-x</sub>Cu<sub>x</sub>(OH)AsO<sub>4</sub> (x=0 and 0.3) phases**

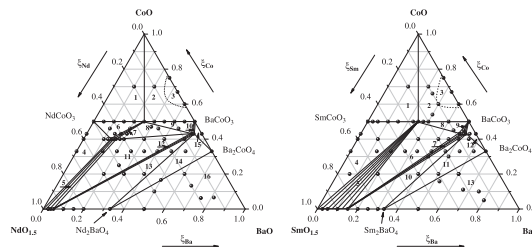
I. de Pedro, J.M. Rojo, J.L. Pizarro, J. Rodríguez Fernández, M.I. Arriortua and T. Rojo  
page 2075



Schematic drawing of the Co<sub>2-x</sub>Cu<sub>x</sub>(OH)AsO<sub>4</sub> (x=0 and 0.3) crystal structure view along the [0 1 0] direction. Polyhedra are occupied by the M(II) ions (M=Co and Cu) and the AsO<sub>4</sub> groups are represented by tetrahedra. Open circles correspond to the oxygen atoms, and small circles show the hydrogen atoms.

**Phase equilibria and crystal structure of the complex oxides in the Ln-Ba-Co-O (Ln=Nd, Sm) systems**

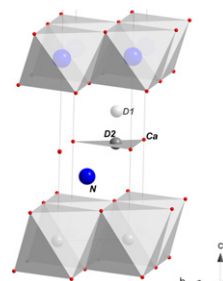
L.Ya. Gavrilova, T.V. Aksenova, N.E. Volkova, A.S. Podzorova and V.A. Cherepanov  
page 2083



Projections of isobaric isothermal phase diagrams of the Nd-Ba-Co-O system and Sm-Ba-Co-O system.

**Order and disorder in Ca<sub>2</sub>ND<sub>0.90</sub>H<sub>0.10</sub>-A structural and thermal study**

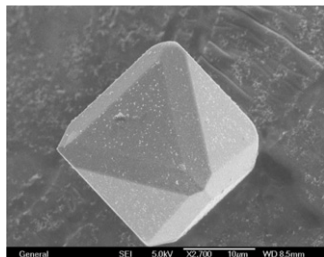
Maarten C. Verbraeken, Emmanuelle Suard and John T.S. Irvine  
page 2088



Ca<sub>2</sub>ND<sub>0.90</sub>H<sub>0.10</sub> forms a mixture of ordered and disordered phases when synthesised at 600 °C. The ordered phase disappears at high temperature upon release of structural deuterium/hydrogen, leaving a single, partially disordered phase.

## One-step green synthesis of cuprous oxide crystals with truncated octahedra shapes *via* a high pressure flux approach

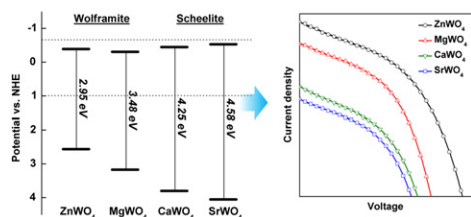
Benxian Li, Xiaofeng Wang, Dandan Xia, Qingxin Chu, Xiaoyang Liu, Fengguo Lu and Xudong Zhao  
page 2097



The Cu<sub>2</sub>O crystals with truncated octahedral shape were one-step synthesized in high yield via high pressure flux method for the first time, which is green and environmentally friendly. The mechanisms of synthesis and crystal growth were discussed in this paper.

## Electronic band structures and photovoltaic properties of MWO<sub>4</sub> (M = Zn, Mg, Ca, Sr) compounds

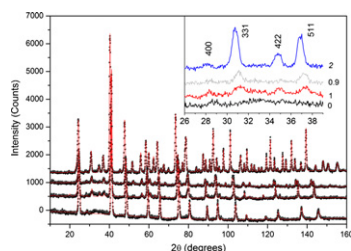
Dong Wook Kim, In-Sun Cho, Seong Sik Shin, Sangwook Lee, Tae Hoon Noh, Dong Hoe Kim, Hyun Suk Jung and Kug Sun Hong  
page 2103



The electronic band structures of divalent metal tungstates are described from the combination of experimental results and theoretical calculations, and their electronic structure-dependent photovoltaic performances are also studied.

## The fluorite-pyrochlore transformation of Ho<sub>2-y</sub>Nd<sub>y</sub>Zr<sub>2</sub>O<sub>7</sub>

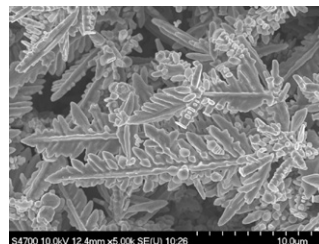
Richard Clements, James R. Hester, Brendan J. Kennedy, Chris D. Ling and Anton P.J. Stampfl  
page 2108



Neutron diffraction profiles for Nd<sub>2-y</sub>Ho<sub>y</sub>Zr<sub>2</sub>O<sub>7</sub> type oxides reveal details of the transformation from the ordered pyrochlore structure ( $y = 0$ ) to the disordered fluorite structure ( $y = 2$ ).

## Special fractal growth of dendrite copper using a hydrothermal method

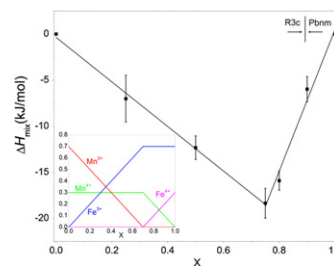
Yan Zheng, Zhejuan Zhang, Pingsheng Guo, Pingang He and Zhuo Sun  
page 2114



Uniform dendritic Cu are grown through controlling  $V_{\text{glycerol/water}}$  in range of 0.6–1.2 and the concentration of H<sub>3</sub>PO<sub>3</sub> in range of 0.06–0.3 M. The rhombic cluster Cu are obtained by decreasing the amount of glycerol.

## Thermochemistry of La<sub>0.7</sub>Sr<sub>0.3</sub>Mn<sub>1-x</sub>Fe<sub>x</sub>O<sub>3</sub> solid solutions (0 < x < 1)

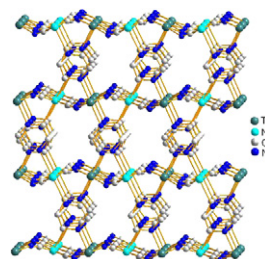
Nihan Kemik, Yayoi Takamura and Alexandra Navrotsky  
page 2118



Enthalpy of mixing ( $\Delta H_{\text{mix}}$ ) of La<sub>0.7</sub>Sr<sub>0.3</sub>Mn<sub>1-x</sub>Fe<sub>x</sub>O<sub>3-y</sub> solid solution at room temperature as a function of Fe/(Fe + Mn) ratio,  $x$ . Linear fits for the two regions at low and high  $x$  are shown as solid lines. The inset shows the content of Mn<sup>3+</sup>, Mn<sup>4+</sup>, Fe<sup>3+</sup> and Fe<sup>4+</sup> as a function of  $x$  based on the work by Jonker [18]. The redox reactions between different valence states of Fe and Mn dominate the energetic behavior of the solid solution.

## Synthesis and characterization of T[Ni(CN)<sub>4</sub>] · 2pyz with T = Fe, Ni; pyz = pyrazine: Formation of T-pyz-Ni bridges

A.A. Lemus-Santana, J. Rodríguez-Hernández, M. González, S. Demeshko, M. Ávila, M. Knobel and E. Reguera  
page 2124



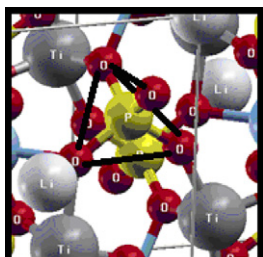
Rippled sheets structure for the pillared solids T[Ni(CN)<sub>4</sub>] · 2pyz. The pyrazine molecule is found forming T-pyz-Ni bridges between neighboring layers.

**Electronic band structure and optical properties of titanium oxyphosphates  $\text{Li}_{0.50}\text{Co}_{0.25}\text{TiO}(\text{PO}_4)$  single crystals:**

**An *ab-initio* calculations**

Ali Hussain Reshak, H. Kamarudin, I.V. Kityk, R. Khenata and S. Auluck

page 2131

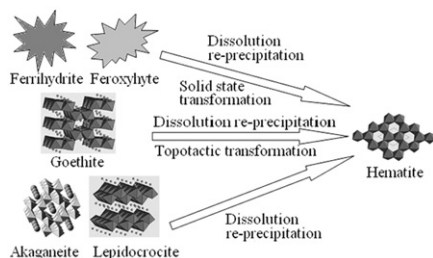


It is shown that P is tetrahedrally coordinated by four O ions.

**Comparison study on transformation of iron oxyhydroxides: Based on theoretical and experimental data**

Bin Lu, Hui Guo, Ping Li, Hui Liu, Yu Wei and Denglu Hou

page 2139

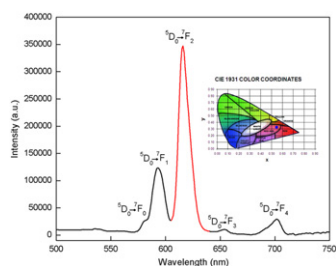


The transformation of various iron oxyhydroxides in the presence of trace Fe(II) was compared based on experimental results, thermodynamic stability, crystalline structure, and transformation mechanism.

**Novel  $\text{Eu}^{3+}$ -doped lead telluroborate glasses for red laser source applications**

M.V. Vijaya Kumar, B.C. Jamalaih, K. Rama Gopal and R.R. Reddy

page 2145

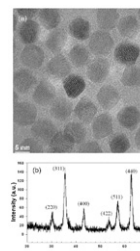


Luminescence spectrum of the PTBEu20 glass with CIE coordinates.

**Seed-mediated synthesis, properties and application of  $\gamma\text{-Fe}_2\text{O}_3\text{-CdSe}$  magnetic quantum dots**

Alex W.H. Lin, Chung Yen Ang, Pranab K. Patra, Yu Han, Hongwei Gu, Jean-Marie Le Breton, Jean Juraszek, Hubert Chiron, Georgia C. Papaefthymiou, Subramanian Tamil Selvan and Jackie Y. Ying

page 2150

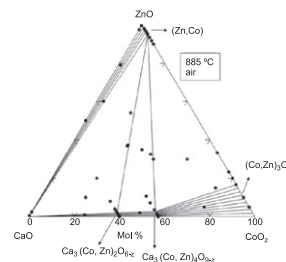


(a) HRTEM image of oleic acid capped MPs. The size of MPs ranges from 8 to 10 nm. (b) XRD pattern of  $\gamma\text{-Fe}_2\text{O}_3$  MPs.

**Phase diagram, crystal chemistry and thermoelectric properties of compounds in the Ca-Co-Zn-O system**

W. Wong-Ng, T. Luo, W. Xie, W.H. Tang, J.A. Kaduk, Q. Huang, Y. Yan, S. Chattopadhyay, X. Tang and T. Tritt

page 2159



Phase diagram of the  $\text{CaO-CoO}_x\text{-ZnO}$  system at  $885^\circ\text{C}$  in air, showing the limits of various solid solutions, and the tie-line relationships of various phases.

**Structural behavior and thermoelectric properties of the brownmillerite system  $\text{Ca}_2(\text{Zn}_x\text{Fe}_{2-x})\text{O}_5$**

Emily Asenath-Smith, Scott T. Misture and Doreen D. Edwards

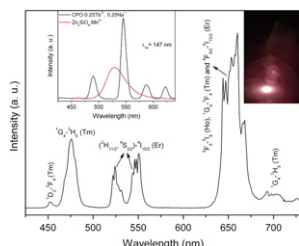
page 2167



Preferential substitution by zinc for iron at the tetrahedral sites of brownmillerite dicalcium ferrite modifies the high temperature  $\text{Imma}(0\ 0\ \gamma)00$  phase from incommensurate to commensurate.

**Vacuum ultraviolet and near-infrared excited luminescence properties of  $\text{Ca}_3(\text{PO}_4)_2:\text{RE}^{3+}$ ,  $\text{Na}^+$  ( $\text{RE} = \text{Tb}$ ,  $\text{Yb}$ ,  $\text{Er}$ ,  $\text{Tm}$ , and  $\text{Ho}$ )**

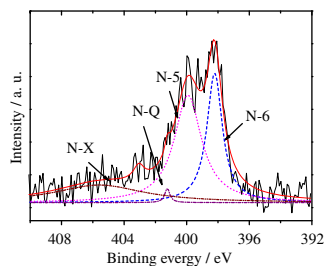
Jia Zhang, Yuhua Wang, Linna Guo, Feng Zhang, Yan Wen, Bitao Liu and Yan Huang  
page 2178



The  $\text{CPO}:0.25\text{Tb}^{3+}$ ,  $0.25\text{Na}^+$  exhibits a comparable brightness to the commercial  $\text{Zn}_2\text{SiO}_4:\text{Mn}^{2+}$  upon 147 nm excitation. Good white light color is achieved in  $\text{CPO}:\text{Yb}^{3+}-\text{Tm}^{3+}-\text{Er}^{3+}-\text{Ho}^{3+}$  under 980 nm excitation.

**Effect of nitrogen-containing groups on enhanced capacitive behaviors of multi-walled carbon nanotubes**

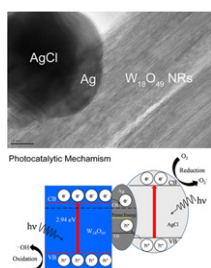
Ji-Il Kim and Soo-Jin Park  
page 2184



The  $\text{N}_{1s}$  spectra of nitrogen functionalized multi-walled carbon nanotubes are measured by X-ray photoelectron spectroscopy.

**$\text{W}_{18}\text{O}_{49}$  nanorods decorated with  $\text{Ag}/\text{AgCl}$  nanoparticles as highly-sensitive gas-sensing material and visible-light-driven photocatalyst**

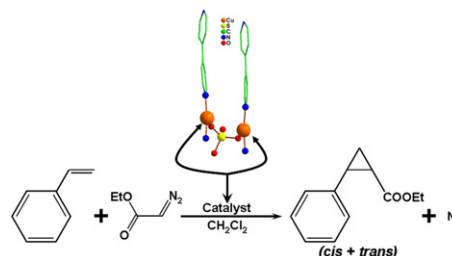
Shibin Sun, Xueting Chang, Lihua Dong, Yidong Zhang, Zhenjiang Li and Yanyan Qiu  
page 2190



The  $\text{Ag}/\text{AgCl}$  nanoparticles adhered well to the  $\text{W}_{18}\text{O}_{49}$  nanorod. The  $\text{Ag}$  could act as transfer center of the photoexcited carriers, prohibiting their recombinations in both  $\text{W}_{18}\text{O}_{49}$  and  $\text{AgCl}$ .

**Metal-organic framework based on copper(I) sulfate and 4,4'-bipyridine catalyzes the cyclopropanation of styrene**

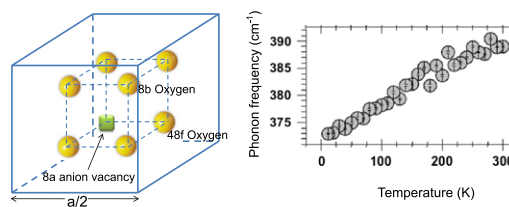
Fa-Nian Shi, Ana Rosa Silva and João Rocha  
page 2196



A new MOF structure built up of 4,4'-bipyridine, sulphate and  $\text{Cu(I)}$ , is an active heterogeneous catalyst for cyclopropanation of styrene with ethyldiazoacetate.

**Pyrochlore “dynamic spin-ice”  $\text{Pr}_2\text{Sn}_2\text{O}_7$  and monoclinic  $\text{Pr}_2\text{Ti}_2\text{O}_7$ : A comparative temperature-dependent Raman study**

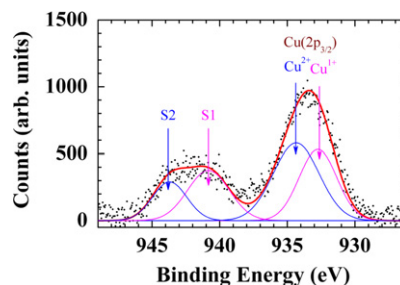
Surajit Saha, Sudakshina Prusty, Surjeet Singh, R. Suryanarayanan, A. Revcolevschi and A.K. Sood  
page 2204



The phonon-phonon anharmonic interaction which is responsible for the temperature-dependent anomalous behavior of phonons, arise due to the inherent vacant sites in the pyrochlore structure.

**Low cost, surfactant-less, one pot synthesis of  $\text{Cu}_2\text{O}$  nano-octahedra at room temperature**

Asar Ahmed, Namdeo S. Gajbhiye and Amish G. Joshi  
page 2209

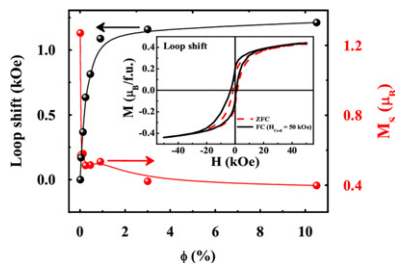


$\text{Cu}_2\text{O}$  octahedra were found to have thin layer of  $\text{CuO}$ , due to oxidation of surface  $\text{Cu}^+$  atoms by the surfactant O atoms.



**Multifunctional properties of CoNi alloy embedded in the SiO<sub>2</sub> host: Role of interparticle interaction**

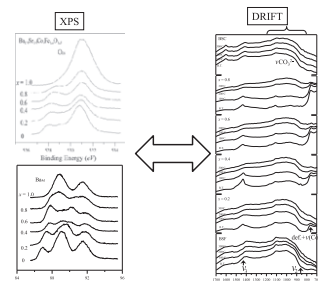
S. Das, S. Majumdar and S. Giri  
page 2215



Plot of loop shift (left axis) and saturation magnetization (right axis) with volume fraction ( $\phi$ ). Inset: loop shift after field-cooling with 50 kOe field and no shift after zero-field-cooling.

**X-ray photoelectron (XPS) and Diffuse Reflectance Infra Fourier Transformation (DRIFT) study of**

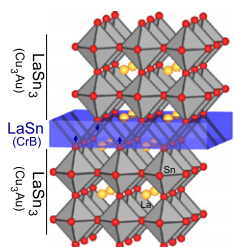
**Ba<sub>0.5</sub>Sr<sub>0.5</sub>Co<sub>x</sub>Fe<sub>1-x</sub>O<sub>3- $\delta$</sub>  (BSCF:  $x = 0-0.8$ ) ceramics**  
Jae-Il Jung and Doreen D. Edwards  
page 2238



The bonding of CO<sub>3</sub><sup>2-</sup> to the surface of BSCF perovskite and the bonding state between cations vs. oxygen have been suggested.

**The binary tin-rich lanthanum stannides La<sub>2</sub>Sn<sub>5</sub> and La<sub>3</sub>Sn<sub>7</sub>—A structural and bond theoretical study**

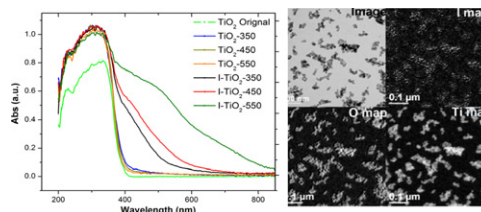
Ines Dürr, Michael Schwarz and Caroline Röhr  
page 2220



La<sub>2</sub>Sn<sub>5</sub> and La<sub>3</sub>Sn<sub>7</sub>, stacking variants of LaSn<sub>3</sub> (Cu<sub>3</sub>Au type, *close* clusters) and LaSn (CrB type, *zig-zag* chains).

**Enhanced visible-light absorption and dopant distribution of iodine-TiO<sub>2</sub> nanoparticles synthesized by a new facile two-step hydrothermal method**

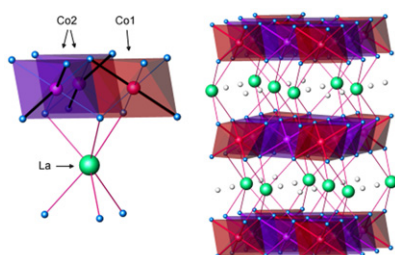
Xiaoting Hong, Zhiping Luo and James D. Batteas  
page 2244



As-synthesized I-TiO<sub>2</sub> nanoparticles show significantly enhanced visible-light absorption, with the dopant iodine homogeneously dispersed on each I-TiO<sub>2</sub> nanostructure based on EELS elemental mapping.

**Structure and properties of a novel cobaltate La<sub>0.30</sub>CoO<sub>2</sub>**

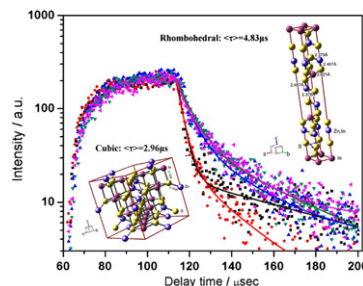
K. Knížek, J. Hejtmánek, M. Maryško, E. Šantavá, Z. Jiráček, J. Buršík, K. Kirakci and P. Beran  
page 2231



Optimized superstructure of La<sub>0.30</sub>CoO<sub>2</sub> obtained by LDA calculation.

**Insights into photoluminescence property and photocatalytic activity of cubic and rhombohedral ZnIn<sub>2</sub>S<sub>4</sub>**

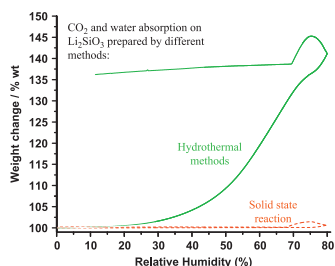
Shaohua Shen, Penghui Guo, Liang Zhao, Yuanchang Du and Liejin Guo  
page 2250



Rhombohedral ZnIn<sub>2</sub>S<sub>4</sub> showed a superior photocatalytic activity for H<sub>2</sub> evolution than cubic ZnIn<sub>2</sub>S<sub>4</sub>, which was proved to be related with their different dynamics of photogenerated carriers.

## Surfactant-assisted hydrothermal crystallization of nanostructured lithium metasilicate ( $\text{Li}_2\text{SiO}_3$ ) hollow spheres: II—Textural analysis and $\text{CO}_2$ - $\text{H}_2\text{O}$ sorption evaluation

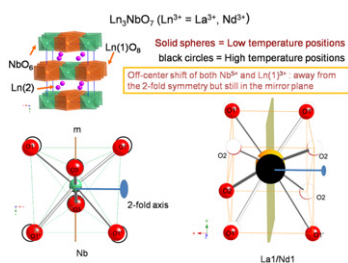
José Ortiz-Landeros, Carlos Gómez-Yáñez and Heriberto Pfeiffer  
page 2257



$\text{Li}_2\text{SiO}_3$  varied significantly its capacity of  $\text{CO}_2$  absorption as a function of the microstructural properties and by the water presence.

## Synchrotron and neutron powder diffraction study of phase transition in weberite-type $\text{Nd}_3\text{NbO}_7$ and $\text{La}_3\text{NbO}_7$

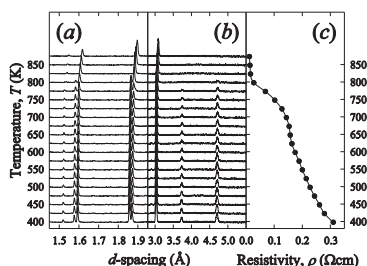
Lu Cai and Juan C. Nino  
page 2263



The phase transition of  $\text{La}_3\text{NbO}_7$  and  $\text{Nd}_3\text{NbO}_7$  upon cooling primarily involves the off-center shifting of  $\text{Nb}^{5+}$  ions inside the  $\text{NbO}_6$  octahedra, combined with shifts of one third of the  $\text{Ln}^{3+}$  ( $\text{Ln}^{3+} = \text{La}^{3+}$  and  $\text{Nd}^{3+}$ ) ions at the center of the  $\text{LnO}_8$  polyhedra towards off-center positions. Above the phase transition temperature,  $\text{Ln}^{3+}$  and  $\text{Nb}^{5+}$  sit at a position with mirror symmetry and 2-fold axis. Below the phase transition temperature,  $\text{Ln}^{3+}$  and  $\text{Nb}^{5+}$  shift away from the 2-fold axis but still in the mirror plane.

## A high temperature diffraction-resistance study of chalcopyrite, $\text{CuFeS}_2$

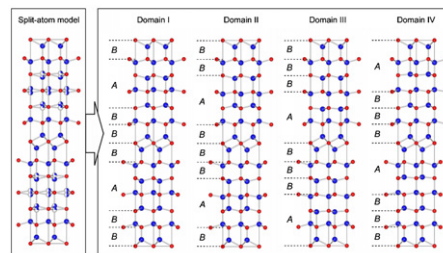
T.E. Engin, A.V. Powell and S. Hull  
page 2272



Structural, magnetic and electrical properties of  $\text{CuFeS}_2$  to 873 K have been investigated using DC resistance measurements, performed in-situ during the collection of powder neutron diffraction data.

## Synthesis and structural characterization of $\text{Al}_7\text{C}_3\text{N}_3$ -homeotypic aluminum silicon oxycarbonitride,

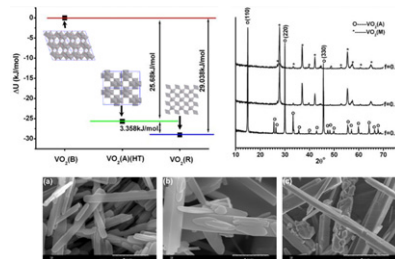
$(\text{Al}_{7-x}\text{Si}_x)(\text{O}_y\text{C}_z\text{N}_{6-y-z})$  ( $x \sim 1.2$ ,  $y \sim 1.0$  and  $z \sim 3.5$ )  
Daisuke Urushihara, Motoaki Kaga, Toru Asaka,  
Hiromi Nakano and Koichiro Fukuda  
page 2278



A new oxycarbonitride discovered in the Al-Si-O-C-N system,  $(\text{Al}_{7-x}\text{Si}_x)(\text{O}_y\text{C}_z\text{N}_{6-y-z})$  ( $x \sim 1.2$ ,  $y \sim 1.0$  and  $z \sim 3.5$ ). The crystal is composed of four types of domains (I, II, III and IV), and hence the structure is represented by a split-atom model. Individual crystal structures can be regarded as layered structures, which consist of *A*-type  $[(\text{Al}, \text{Si})_4(\text{O}, \text{C}, \text{N})_4]$  unit layers and *B*-type  $[(\text{Al}, \text{Si})(\text{O}, \text{C}, \text{N})_2]$  single layers.

## Selective formation of $\text{VO}_2(\text{A})$ or $\text{VO}_2(\text{R})$ polymorph by controlling the hydrothermal pressure

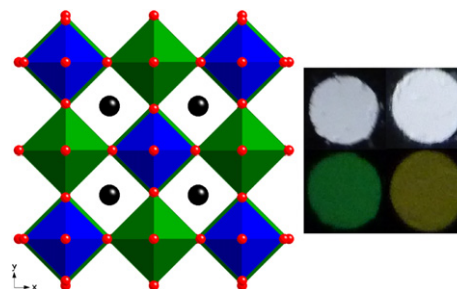
Shidong Ji, Feng Zhang and Ping Jin  
page 2285



Selective formation of  $\text{VO}_2(\text{A})$  or  $\text{VO}_2(\text{R})$  could be achieved by controlling the system pressure through varying the filling ratio during hydrothermal treatment.

## Crystal growth, structures, and optical properties of the cubic double perovskites $\text{Ba}_2\text{MgWO}_6$ and $\text{Ba}_2\text{ZnWO}_6$

Daniel E. Bugaris, Jason P. Hodges, Ashfia Huq and Hans-Conrad zur Loye  
page 2293

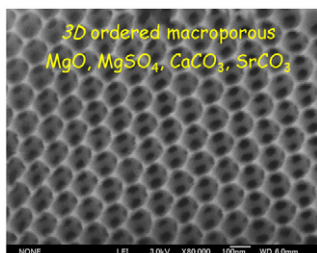


$\text{Ba}_2\text{MgWO}_6$  and  $\text{Ba}_2\text{ZnWO}_6$  adopt the cubic double perovskite structure. Both compounds luminesce under UV irradiation, with green and yellow emissions, respectively.

**Preparation and formation mechanism of three-dimensionally ordered macroporous (3DOM) MgO, MgSO<sub>4</sub>, CaCO<sub>3</sub>, and SrCO<sub>3</sub>, and photonic stop band properties of 3DOM CaCO<sub>3</sub>**

Masahiro Sadakane, Rika Kato, Toru Murayama and Wataru Ueda

page 2299

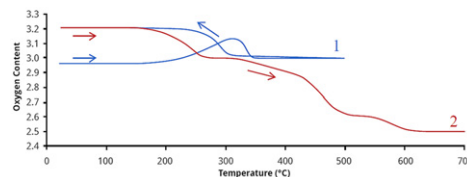


Well-ordered 3-dimensionally ordered macroporous MgO, MgSO<sub>4</sub>, CaCO<sub>3</sub>, and SrCO<sub>3</sub> materials were obtained in a high pore fraction.

**Synthesis and oxygen content dependent properties of hexagonal DyMnO<sub>3+δ</sub>**

S. Remsen, B. Dabrowski, O. Chmaissem, J. Mais and A. Szewczyk

page 2306



Thermogravimetric annealing in 21% O<sub>2</sub> after initial synthesis of DyMnO<sub>3+δ</sub> in argon (curve 1) and subsequent reduction in 42% H<sub>2</sub> to Dy<sub>2</sub>O<sub>3</sub> and MnO (curve 2).

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