

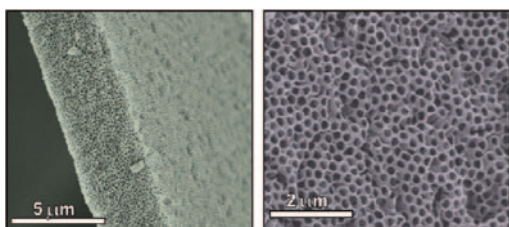
CONTENTS

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Regular Articles

Preparation of thin layer materials with macroporous microstructure for SOFC applications

D. Marrero-López, J.C. Ruiz-Morales, J. Peña-Martínez, J. Canales-Vázquez and P. Núñez
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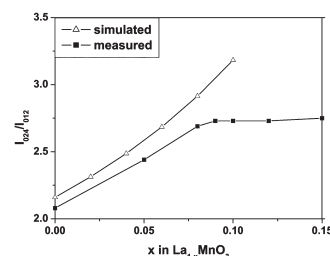


Thin films materials of mixed oxides with potential application in SOFC devices have been prepared with macroporous microstructure using PMMA microspheres as pore formers.

Regular Articles—Continued

Determination of A-site deficiency in lanthanum manganite by XRD intensity ratio

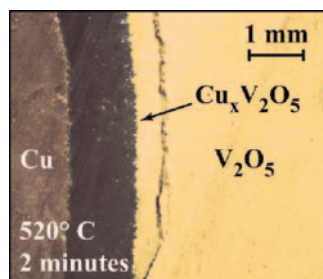
Yanbo Zuo, Jianheng Li, Jianxin Yi, Zhongbing Wang and Chusheng Chen
page 700



The X-ray diffraction intensity ratio of (024) and (012) reflections of $\text{La}_{1-x}\text{MnO}_{3\pm\delta}$ I_{024}/I_{012} increases with x until $x=0.09$ as predicted by the computer simulation, and at $x>0.09$ the intensity ratio levels off, showing that the maximum lanthanum deficiency is around 0.09.

Diffusion and phase transformations in spark plasma synthesized and sintered Cu–V₂O₅ couples

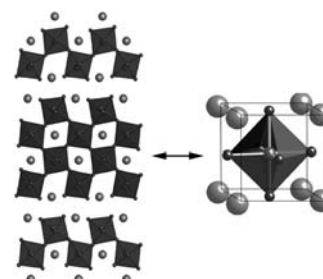
Jean-Philippe Monchoux and Jean Galy
page 693



Fast diffusion of Cu into V₂O₅ is studied on Cu–V₂O₅ diffusion couples sintered by spark plasma sintering. The shape of the diffusion profiles is explained by the influence of phase transitions and by the concentration dependence of the diffusion coefficient. High value of diffusion coefficient is measured ($D \approx 3 \times 10^{-8} \text{ m}^2/\text{s}$).

Phase and structural characterization of Sr₂Nb₂O₇ and SrNbO₃ thin films grown via pulsed laser ablation in O₂ or N₂ atmospheres

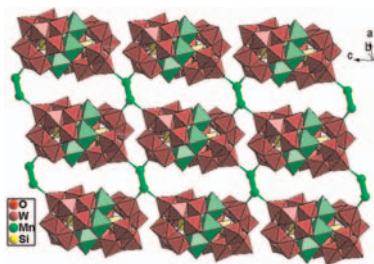
K.R. Balasubramaniam, Y. Cao, N. Patel, S. Havelia, P.J. Cox, E.C. Devlin, E.P. Yu, B.J. Close, P.M. Woodward and P.A. Salvador
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Phase selection of SrNbO₃ films is influenced primarily by the process gas (in the 1–100 mTorr pressure range). In oxygen, films adopt the Sr₂Nb₂O₇ (110)-layered perovskite structure (left). In nitrogen, films adopt the cubic perovskite SrNbO₃ structure (right). The films' microstructure depends, however, on the substrate type and temperature.

Structure and characterization of zero- to two-dimensional compounds built up of the sandwich-type clusters and transition-metal linkers

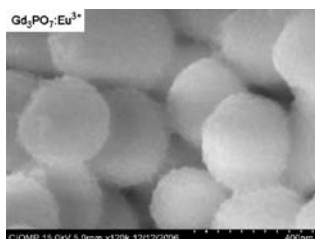
Zhiming Zhang, Shuang Yao, Enbo Wang, Chao Qin, Yanfei Qi, Yangguang Li and Rodolphe Clérac
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Five new compounds, from zero- to two-dimensional built up of the sandwich-type clusters and transition-metal linkers, have been obtained by the routine synthetic reactions in aqueous solution. This polyoxoanion framework architecture represents the first example of the 2D structure consisting of the sandwich-type polyoxoanion $[\text{Mn}_4(\text{H}_2\text{O})_2(\text{SiW}_9\text{O}_{34})]^{12-}$ and the binuclear $\{\text{Mn}_2(\text{H}_2\text{O})_6\}^{4+}$ group.

Synthesis of $\text{Gd}_3\text{PO}_7:\text{Eu}^{3+}$ nanospheres via a facile combustion method and optical properties

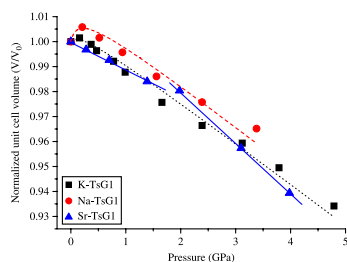
Ye Jin, Weiping Qin, Jisen Zhang, Xianmin Zhang, Yan Wang and Chunyan Cao
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SEM image of as-prepared $\text{Gd}_3\text{PO}_7:\text{Eu}^{3+}$ nanospheres.

Cation-dependent anomalous compression of gallosilicate zeolites with CGS topology: A high-pressure synchrotron powder diffraction study

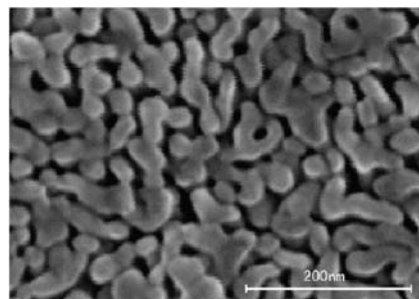
Yongjae Lee, Hyun-Hwi Lee, Dong Ryeol Lee, Sun Jin Kim and Chi-chang Kao
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Three different cation forms of gallosilicate CGS zeolites have been investigated using synchrotron X-ray powder diffraction and a diamond-anvil cell. Under hydrostatic conditions, unit-cell lengths and volume show anomalous compression behaviours depending on the non-framework cation type and initial hydration level, which implies different modes of pressure-induced hydration and channel distortion.

Facile synthesis of iron oxide with wormlike morphology and their application in water treatment

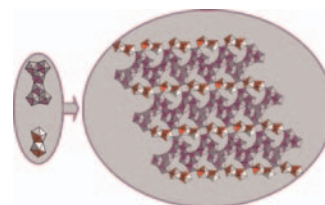
Lijuan Wan, Keying Shi, Xiqiang Tian and Honggang Fu
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A novel and facile synthesis route for the manufacture of transparent and uniform nanocrystalline $\alpha\text{-Fe}_2\text{O}_3$ (nc- Fe_2O_3) thin films or powders with wormlike morphology is reported, utilizing ferric nitrate as the inorganic source and triblock copolymer as the wormlike morphology-structure-directing agent through evaporation-induced assembly (EIA).

A new uranyl niobate sheet in the cesium uranyl niobate $\text{Cs}_9[(\text{UO}_2)_8\text{O}_4(\text{NbO}_5)(\text{Nb}_2\text{O}_8)_2]$

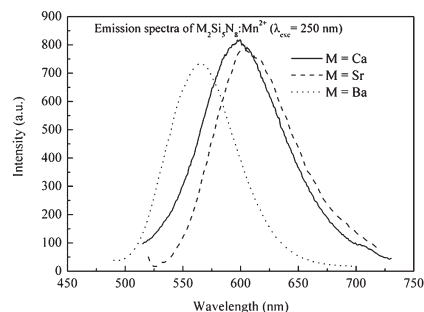
S. Saad, S. Obbade, S. Yagoubi, C. Renard and F. Abraham
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View of the ${}^2_{\infty}[\text{U}_8\text{O}_{36}]$ uranyl infinite layer formed by association of $[\text{U}_6\text{O}_{36}]$ and $[\text{U}_2\text{O}_{12}]$ uranyl blocks in $\text{Cs}_9[(\text{UO}_2)_8\text{O}_4(\text{NbO}_5)(\text{Nb}_2\text{O}_8)_2]$.

Preparation and photoluminescence properties of Mn^{2+} -activated $\text{M}_2\text{Si}_5\text{N}_8$ ($M = \text{Ca}, \text{Sr}, \text{Ba}$) phosphors

C.J. Duan, W.M. Otten, A.C.A. Delsing and H.T. Hintzen
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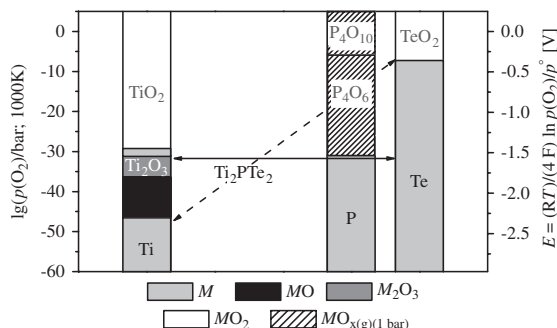


The luminescence properties of Mn^{2+} in $\text{M}_2\text{Si}_5\text{N}_8$ ($M = \text{Ca}, \text{Sr}, \text{Ba}$) have been investigated. All $\text{M}_2\text{Si}_5\text{N}_8:\text{Mn}^{2+}$ phosphors show narrow symmetric bands in the wavelength range of 500–700 nm with peak center at about 599, 606 and 567 nm for $M = \text{Ca}, \text{Sr}, \text{Ba}$, respectively. The observed band emission is ascribed to the ${}^4\text{T}_1({}^4\text{G}) \rightarrow {}^6\text{A}_1({}^6\text{S})$ transition of Mn^{2+} in $\text{M}_2\text{Si}_5\text{N}_8$ host lattice.

Continued

**Synthesis of the titanium phosphide telluride Ti_2PTe_2 :
A thermochemical approach**

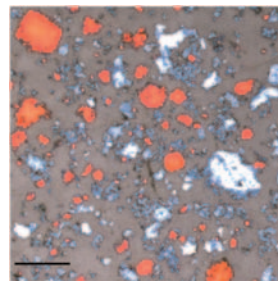
Frauke Philipp, Peer Schmidt, Edgar Milke,
Michael Binnewies and Stefan Hoffmann
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Oxygen partial pressure and electrochemical potential above the oxides of titanium, tellurium and phosphorus calculated at 1000 K, marked: level of equalisation of oxygen partial pressure.

Solid-state synthesis in the system $Na_{0.8}Nb_yW_{1-y}O_3$ with $0 \leq y \leq 0.4$: A new phase, $Na_{0.5}NbO_{2.75}$, with perovskite-type structure

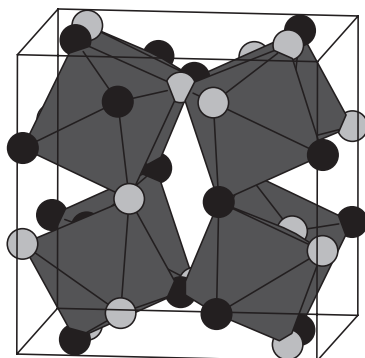
Tapas Debnath, Claus H. Rüscher, Thorsten M. Gesing,
Jürgen Koepeke and Altaf Hussain
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Optical micrograph of a polished sample of nominal composition $Na_{0.8}Nb_{0.4}W_{0.6}O_3$ showing a mixture of three different coloured crystals: red, light blue and white. The scale bar is 30 μm .

Structure and electrical transport properties of the ordered skutterudites $MGe_{1.5}S_{1.5}$ ($M = Co, Rh, Ir$)

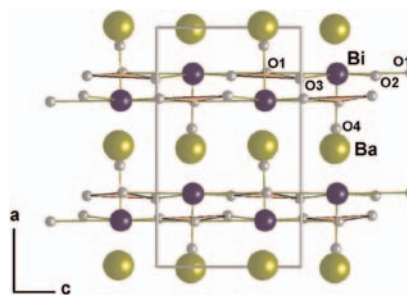
Paz Vaquero, Gerard G. Sobany and Martin Stindl
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The $MGe_{1.5}S_{1.5}$ phases exhibit an ordered skutterudite structure, in which the anions form diamond-like four-membered Ge_2S_2 rings.

Linear and nonlinear optical susceptibilities for a novel borate oxide $BaBiBO_4$: Theory and experiment

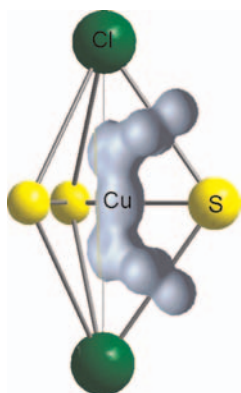
Ali Hussain Reshak, S. Auluck and I.V. Kityk
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Principal crystalline structure.

Structural aspects of fast copper mobility in Cu_6PS_5Cl —The best solid electrolyte from Cu_6PS_5X series

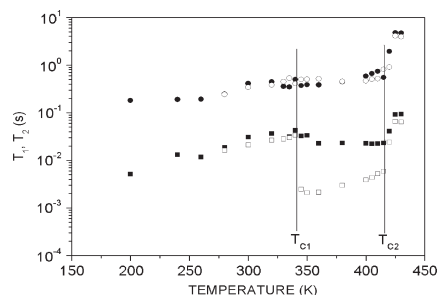
A. Gagor, A. Pietraszko and D. Kaynts
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Coordination of copper mobile ions in superionic phase of Cu_6PS_5Cl , $T = 435 K$.

A study of the phase transitions and proton dynamics of the superprotonic conductor $Cs_5H_3(SO_4)_4 \cdot 0.5H_2O$ single crystal with 1H and ^{133}Cs nuclear magnetic resonance

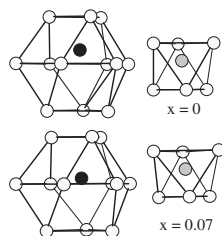
Ae Ran Lim
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The phase transitions and proton dynamics of $Cs_5H_3(SO_4)_4 \cdot 0.5H_2O$ were studied by the spin-lattice relaxation time and the spin-spin relaxation time of the 1H and ^{133}Cs nuclei. The “acid” and the “water” protons were distinguished. Our NMR study has provided new information about the roles of acid protons, water protons, and cesium nuclei in $Cs_5H_3(SO_4)_4 \cdot 0.5H_2O$ single crystals. Fig. Temperature dependences of T_1 and T_2 for acid and water protons in a $Cs_5H_3(SO_4)_4 \cdot H_2O$ single crystal (\bullet : T_1 and \blacksquare : T_2 for acid proton, \circ : T_1 and \square : T_2 for water proton).

Structure and magnetic properties of potassium doped bismuth ferrite

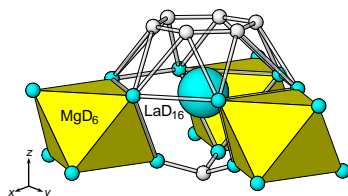
Ja. Dhahri, M. Boudard, S. Zemni, H. Roussel and M. Oumezzine
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$\text{Bi}_{1-x}\text{K}_x\text{FeO}_3$ ($0 \leq x \leq 0.07$) are described in $R3c$ space group. The average Fe (gray balls) and Bi/K (black balls) displacements decrease with K content reducing the polar character and leading to a change from rhombohedral to pseudo-cubic symmetry. Structural disorder results in strong diffuse scattering. The compounds remain antiferromagnetic at room temperature.

Mg substitution effect on the hydrogenation behaviour, thermodynamic and structural properties of the $\text{La}_2\text{Ni}_7\text{-H(D)}_2$ system

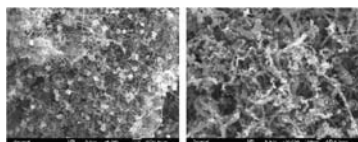
R.V. Denys, A.B. Riabov, V.A. Yartys, Masashi Sato and R.G. Delaplane
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Substitution of La by Mg in La_2Ni_7 occurs only in the Laves-type parts of the crystal structure to form LaMgNi_4 slabs within the $\text{La}_{1.5}\text{Mg}_{0.5}\text{Ni}_7$ crystal. Subsequent hydrogenation forms $\text{La}_{1.5}\text{Mg}_{0.5}\text{Ni}_7\text{D}_{9.1}$ with a nearly isotropic expansion of the unit cell that is in contrast to the large unilateral anisotropic expansion that takes place on hydrogenation of La_2Ni_7 . Contrary to $\text{La}_2\text{Ni}_7\text{D}_{6.5}$ where only LaNi_2 layers absorb hydrogen atoms leaving LaNi_5 slabs unmodified, in $\text{La}_{1.5}\text{Mg}_{0.5}\text{Ni}_7\text{D}_{9.1}$ both LaNi_5 and LaMgNi_4 layers become occupied; the effect of Mg substitution is the increase of the reversible hydrogenation storage capacity. Within the hydrogen sublattice inside the $\text{LaMgNi}_4\text{D}_{7.56}$ slab local ordering of Mg and La in the layer gives a packing of the MgD_6 octahedra and LaD_{16} polyhedra as shown.

Controlled modification of multiwalled carbon nanotubes with ZnO nanostructures

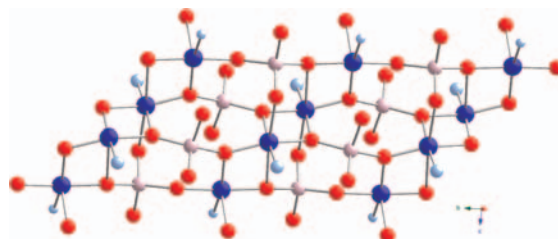
Xiuying Wang, Baiying Xia, Xingfu Zhu, Jiasheng Chen, Shilun Qiu and Jixue Li
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Multiwalled carbon nanotube (MWNT)/flower-like ZnO heterojunctions and MWNT/ZnO nanoparticle composites were prepared by zinc-ammonium complex ion covalently attached to the MWNTs through the C-N bonds via adjusting the reaction time. A growth mechanism has been proposed in which the soaking time plays a key role in controlling the size, morphology, and site of ZnO nanostructures.

Topologically novel copper molybdate phases based on 3,4'-dipyridylketone: Hydrothermal synthesis, structural characterization, and magnetic properties

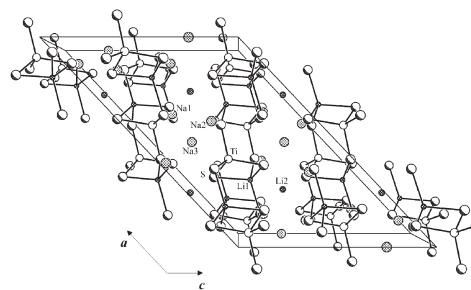
Matthew R. Montney and Robert L. LaDuca
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$[\text{Cu}_2(\text{MoO}_4)_2(3,4'\text{-dpk})(\text{H}_2\text{O})]$ (1, 3,4'-dpk = 3,4'-dipyridylketone) and $[\text{Cu}_4(3,4'\text{-dpk})_4(\text{Mo}_8\text{O}_{26})]$ (2) have been prepared by hydrothermal methods. 1 possesses 1-D $[\text{Cu}_2(\text{MoO}_4)_2(\text{H}_2\text{O})]_n$ ribbons containing magnetically interacting $\{\text{Cu}_4\text{O}_6\}$ tetramers. The ribbons are connected into 2-D by 3,4'-dpk ligands. The reduced phase 2 manifests an unprecedented 1-D "X-rail" chain motif.

Synthesis, structure, and ionic conductivity of $\text{Na}_5\text{Li}_3\text{Ti}_2\text{S}_8$

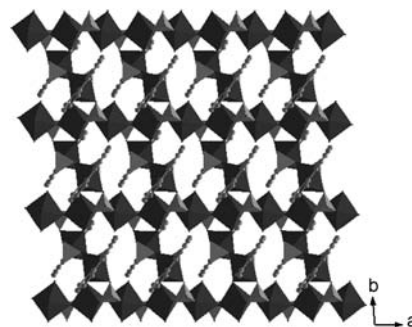
Fu Qiang Huang, Jiyong Yao, Zhanqiang Liu, Jianghua Yang and James A. Ibers
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The structure of $\text{Na}_5\text{Li}_3\text{Ti}_2\text{S}_8$ viewed down $[010]$. For the sake of clarity, the Na-S and Li(2)-S interactions are omitted.

(2,2'-bipy)[$\text{In}_2(\text{OH})_2(\text{H}_2\text{O})$](SO_4)₂: The first indium sulfate with a layer structure

Zhenfen Tian, Li Wang, Tianyou Song, Ying Wang, Liangliang Huang, Lirong Zhang and Suhua Shi
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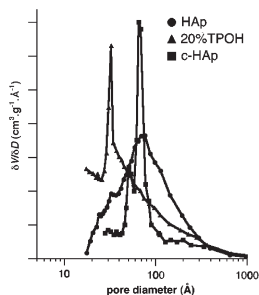


The two-dimensional layer structure of $(2,2'\text{-bipy})[\text{In}_2(\text{OH})_2(\text{H}_2\text{O})](\text{SO}_4)_2$ along $[001]$.

Organically modified porous hydroxyapatites: A comparison between alkylphosphonate grafting and citrate chelation

L. El-Hammari, H. Marroun, A. Laghzizil, A. Saoiabi, C. Roux, J. Livage and T. Coradin

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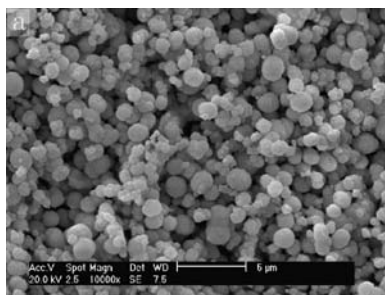


Evolution of pore size distribution of hydroxyapatite (HAp) after alkylphosphonate grafting (20% TPOH) or citrate addition (c-HAp) demonstrates the formation of organically modified mesoporous materials.

Hydrothermal synthesis and luminescence of $\text{CaMO}_4:\text{RE}^{3+}$ ($M = \text{W, Mo}$; $\text{RE} = \text{Eu, Tb}$) submicro-phosphors

Fang Lei and Bing Yan

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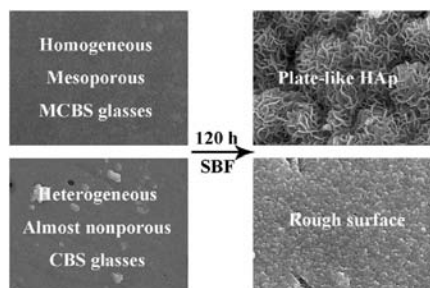


Submicro-crystalline Eu^{3+} -activated tungstate $\text{CaWO}_4:\text{RE}^{3+}$ phosphors with a sheelite structure have been synthesized via the hydrothermal process; the morphology was determined from the hydrothermal temperature. Scanning electron microscopy (SEM) images show that $\text{CaWO}_4:\text{Eu}^{3+}$ exhibits spherical particles, which can be controlled by the reaction parameters.

Comparisons between surfactant-templated mesoporous and conventional sol-gel-derived $\text{CaO-B}_2\text{O}_3\text{-SiO}_2$ glasses: Compositional, textural and in vitro bioactive properties

Tongping Xiu, Qian Liu and Jiacheng Wang

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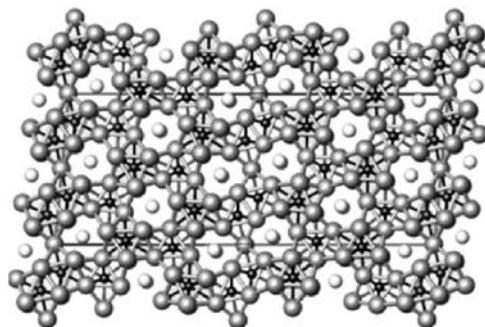


Surfactant-templated mesoporous $\text{CaO-B}_2\text{O}_3\text{-SiO}_2$ glasses (MCBS) are superior to conventional sol-gel-derived $\text{CaO-B}_2\text{O}_3\text{-SiO}_2$ glasses (CBS) in compositional homogeneity, textural properties and in vitro bioactivity.

$\text{Er}_{17}\text{Ru}_6\text{Te}_3$: A highly condensed metal-rich ternary telluride

Akash Mehta and John D. Corbett

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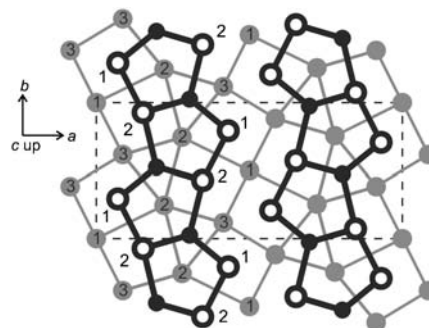


A 3D structure built of bi- and tricapped trigonal prisms centered by Ru or Te.

Rare earth-nickel-indides $\text{Dy}_5\text{Ni}_2\text{In}_4$ and $\text{RE}_4\text{Ni}_{11}\text{In}_{20}$ ($\text{RE} = \text{Gd, Tb, Dy}$)

Yuriy B. Tyvanchuk, Ute Ch. Rodewald, Yaroslav M. Kalychak and Rainer Pöttgen

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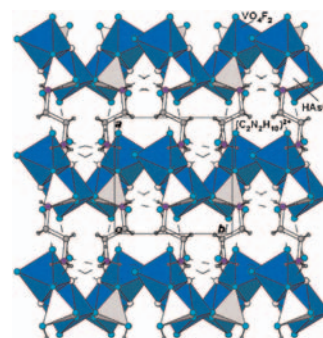


Crystal structure of $\text{Dy}_5\text{Ni}_2\text{In}_4$.

Hydrothermal synthesis, crystal structure, thermal behavior and spectroscopic and magnetic properties of two new organically templated fluoro-vanadyl-hydrogenarsenates: $(\text{R})_{0.5}[(\text{VO})(\text{HASO}_4)\text{F}]$ (R : Ethylenediammonium and piperazinium)

Teresa Berrocal, José L. Mesa, José L. Pizarro, Luis Lezama, Begoña Bazán, María I. Arriortua and Teófilo Rojo

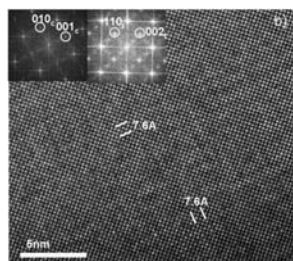
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Polyhedral view of the layered crystal structure of $(\text{C}_2\text{H}_{10}\text{N}_2)_{0.5}[(\text{VO})(\text{HASO}_4)\text{F}]$.

Structure, microstructure and magnetic properties of $\text{Sr}_{1-x}\text{Ca}_x\text{CrO}_3$ ($0 \leq x \leq 1$)

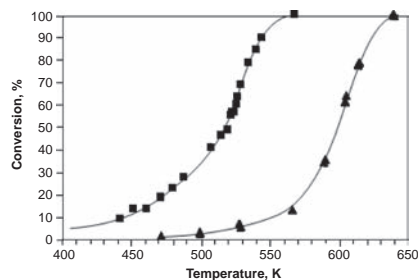
E. Castillo-Martínez, A. Durán and M.Á. Alario-Franco
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HRTEM image of a crystal of $\text{Sr}_{0.5}\text{Ca}_{0.5}\text{CrO}_3$ showing a random distribution of $2a_p \approx 7.6 \text{ \AA}$ all along the crystal that lacks long range order. Inset shows the FFT of the area of the image and of a tenth of that area showing the influence of the coherence length.

Surface properties and performance for VOCs combustion of $\text{LaFe}_{1-y}\text{Ni}_y\text{O}_3$ perovskite oxides

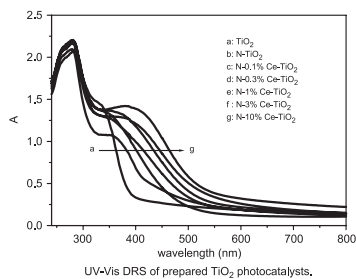
G. Pecchi, P. Reyes, R. Zamora, L.E. Cadús and J.L.G. Fierro
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LaFeO_3 , LaNiO_3 and substituted $\text{LaFe}_{1-y}\text{Ni}_y\text{O}_3$ ($y=0.1, 0.2$ and 0.3) perovskite-type oxides have been investigated as catalysts in the total combustion of ethanol and acetylacetate. The characterization indicate variation in specific surface area, crystal structure, reducibility and surface composition. The catalytic activity expressed as intrinsic activity ($\text{mol m}^{-2} \text{ h}^{-1}$) increases with nickel substitution. A synergy between Ni^{3+} and Fe^{3+} cations at the B position of the $\text{LaFe}_{1-y}\text{Ni}_y\text{O}_3$ perovskite for VOCs combustion was observed.

Characterization and activity of visible-light-driven TiO_2 photocatalyst codoped with nitrogen and cerium

Chao Liu, Xinhua Tang, Cehui Mo and Zhimin Qiang
page 913

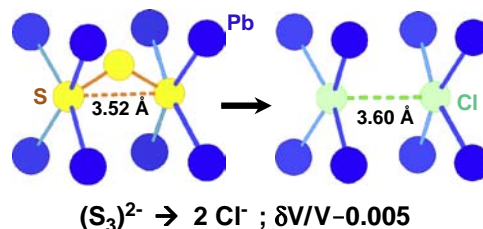


A novel TiO_2 photocatalyst codoped with nitrogen and cerium was synthesized and characterized. An enhanced visible light activity was achieved. UV-vis DRS results indicated that the optical absorption edge of the N-Ce codoped TiO_2 was obviously shifted to the visible light range as the Ce/Ti doping ratio increased.

Crystal structure of the new compound

$\text{Pb}_{3+x}\text{Sb}_{3-x}\text{S}_{7-x}\text{Cl}_{1+x}$ ($x \sim 0.45$): The homologous series $\text{Pb}_{(2+2N)}(\text{Sb}, \text{Pb})_{(2+2N)}\text{S}_{(2+2N)}(\text{S}, \text{Cl})_{(4+2N)}\text{Cl}_N$ and its polychalcogenide derivatives ($N=1-3$)

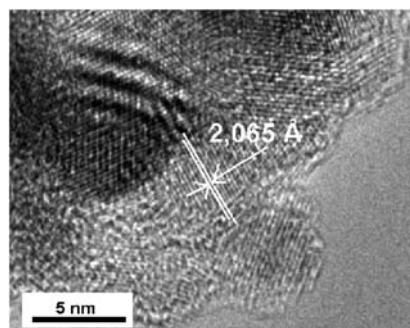
Charlotte Doussier, Yves Moëlo, Alain Meerschaut, Philippe Léone and Catherine Guillot-Deudon
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The title compound, $\text{Pb}_{3+x}\text{Sb}_{3-x}\text{S}_{7-x}\text{Cl}_{1+x}$, is derived from the homeotypic persulfide $\text{Pb}_6\text{Sb}_6\text{S}_{14}(\text{S}_3)$ by substituting two chlorine atoms for the S_3 trimer. This change is quite isovolumic.

High surface area V-Mo-N materials synthesized from amine intercalated foams

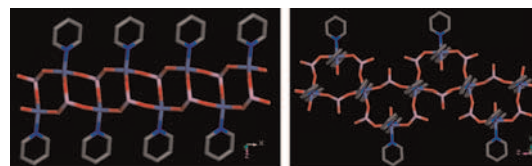
Piotr Krawiec, Rabi Narayan Panda, Emanuel Kockrick, Dorin Geiger and Stefan Kaskel
page 935



Nanocrystalline ternary V-Mo nitrides were prepared via nitridation of amine intercalated oxide foams or bulk ternary oxides. Foamed precursors were favorable for vanadium rich materials, while for molybdenum rich samples bulk ternary oxides resulted in higher specific surface areas.

Syntheses, structures and magnetic properties of two new one-dimensional cobalt (II) phosphites with organic amines acting as ligands

Gaijuan Li, Yan Xing and Shuyan Song
page 943

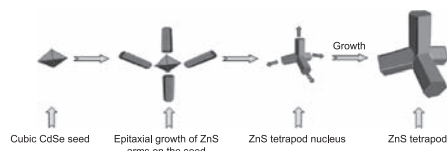


Two new 1D inorganic-organic hybrid cobalt (II) phosphites have been prepared under solvothermal conditions in the presence of pyridine. $\text{Co}(\text{HPO}_3)$ (py) possesses a 1D ladder-like framework constructed from CoO_3N tetrahedral, HPO_3 pseudo-pyramids and pyridine ligands (left); 1D-chain structure of $[\text{Co}(\text{OH})(\text{py})_3][\text{Co}(\text{py})_2][\text{HPO}_2(\text{OH})_3]$ consists of corner-shared six-membered rings (right).

Size-tunable synthesis of tetrapod-like ZnS nanopods by seed-epitaxial metal-organic chemical vapor deposition

Tianyou Zhai, Yang Dong, Yaobing Wang, Zongwei Cao, Ying Ma, Hongbing Fu and Jiannian Yao

page 950

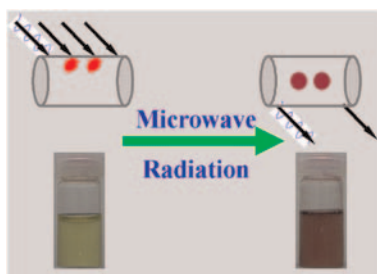


Single-crystalline tetrapod-like ZnS nanopods were synthesized by a one-step seed-epitaxial metal-organic chemical vapor deposition approach using cubic CdSe nanocrystals as the seeds. The diameters of the ZnS tetrapods can be easily tuned by changing the distances between the substrates and precursors.

Microwave-induced synthesis of highly dispersed gold nanoparticles within the pore channels of mesoporous silica

Jinlou Gu, Wei Fan, Atsushi Shimojima and Tatsuya Okubo

page 957

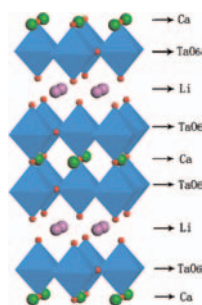


A facile and novel strategy has been developed to incorporate gold nanoparticles into the pore channels of mesoporous SBA-15 assisted by microwave radiation (MR) with mild reaction condition and rapid reaction speed. Due to the rapid and homogeneous nucleation, simultaneous propagation and termination by MR, the size of gold nanoparticles are effectively controlled.

Synthesis, crystal structure, and photocatalytic activity of a new two-layer Ruddlesden–Popper phase, $\text{Li}_2\text{CaTa}_2\text{O}_7$

Zhenhua Liang, Kaibin Tang, Qian Shao, Guocan Li, Suyuan Zeng and Huagui Zheng

page 964

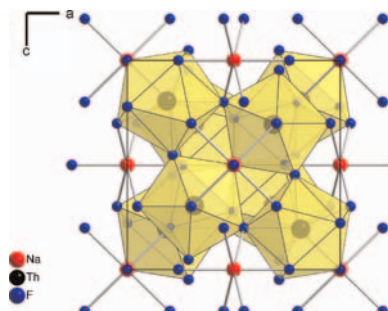


Crystal structure of a two-layer Ruddlesden–Popper phase $\text{Li}_2\text{CaTa}_2\text{O}_7$. A new two-layer Ruddlesden–Popper phase $\text{Li}_2\text{CaTa}_2\text{O}_7$ has been synthesized for the first time. $\text{Li}_2\text{CaTa}_2\text{O}_7$ crystallizes in the space group $Fm\bar{3}m$ determined by powder X-ray and electron diffraction. UV–visible diffuse reflection spectra and the photocatalytic degradation of RhB molecules in water under ultra visible light irradiation show that $\text{Li}_2\text{CaTa}_2\text{O}_7$ is a potential material in photocatalysis.

Twinned tetragonal structure and equation of state of NaTh_2F_9

Andrzej Grzechnik, Wolfgang Morgenroth and Karen Friese

page 971

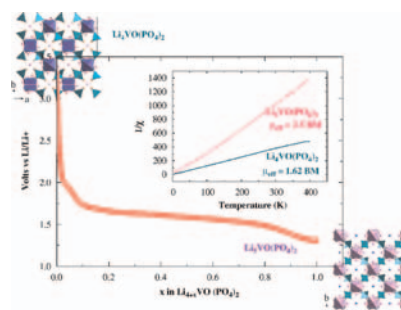


Crystal structure of NaTh_2F_9 ($I\bar{4}2m$, $Z=4$) at ambient conditions. The polyhedra around the Th atoms are drawn.

Topotactic insertion of lithium in the layered structure $\text{Li}_4\text{VO}(\text{PO}_4)_2$: The tunnel structure $\text{Li}_5\text{VO}(\text{PO}_4)_2$

M. Satya Kishore, V. Pralong, V. Caignaert, S. Malo, S. Hebert, U.V. Varadaraju and B. Raveau

page 976

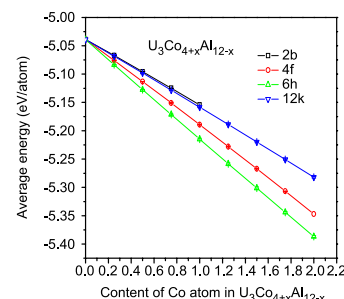


Electrochemical synthesis of a new 3D V(III) lithium phosphate, $\text{Li}_5\text{VO}(\text{PO}_4)_2$. Starting from the 2D $\text{Li}_4\text{VO}(\text{PO}_4)_2$, the topotactic reaction that take place during lithium intercalation is explained on the basis of the flexible coordinations of V^{4+} and V^{3+} species.

Atomistic simulation on the site preference and mechanical properties of $\text{Th}_3\text{Co}_{4+x}\text{Al}_{12-x}$ and $\text{U}_3\text{Co}_{4+x}\text{Al}_{12-x}$

Ping Qian, Hui-Jun Tian, Nan-Xian Chen and Jiang Shen

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It is seen from figure that the substitution of Co for Al at all the four sites 2b, 4f, 6h and 12k decrease the cohesive energy of $\text{U}_3\text{Co}_{4+x}\text{Al}_{12-x}$, which means that the Co atoms can play a role in stabilizing the structure. The Co atoms strongly prefer 6h sites.

Continued

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