

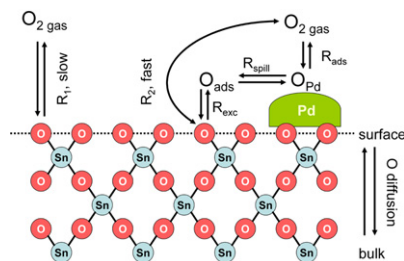
Abstracted/indexed in BioEngineering Abstracts, Chemical Abstracts, Coal Abstracts, Current Contents/Physics, Chemical, & Earth Sciences, Engineering Index, Research Alert, SCISEARCH, Science Abstracts, and Science Citation Index. Also covered in the abstract and citation database SciVerse SCOPUS[®]. Full text available on SciVerse ScienceDirect[®].

Regular Articles

Oxygen exchange on nanocrystalline tin dioxide modified by palladium

D.D. Frolov, Y.N. Kotovshchikov, I.V. Morozov, A.I. Boltalin, A.A. Fedorova, A.V. Marikutsa, M.N. Rumyantseva, A.M. Gaskov, E.M. Sadovskaya and A.M. Abakumov

page 1



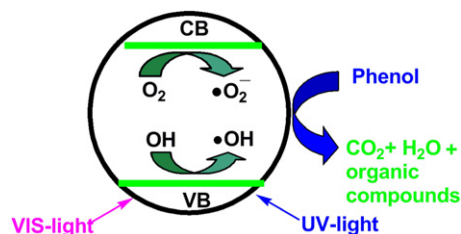
Nanocrystalline SnO₂ modification by Pd essentially influences the interaction with gas phase molecules. A temperature programmed isotopic exchange study revealed that Pd promotes oxygen exchange of the material by facilitating oxygen dissociation and spill-over on the surface of active clusters.

Regular Articles—Continued

A green chemical approach to the synthesis of photoluminescent ZnO hollow spheres with enhanced photocatalytic properties

Greta Patrinoiu, Madalina Tudose, Jose Maria Calderón-Moreno, Ruxandra Birjega, Petru Budrugaec, Ramona Ene and Oana Carp

page 17

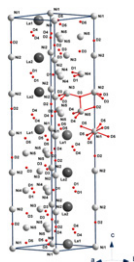


The photocatalytic reaction initiated by the photoexcitation of the semiconductor (ZnO), leads to the formation of electron-hole, while part of the electron-hole pairs recombine, some holes combine with water to form •OH radicals and some electrons convert oxygen to super oxide radical (•O₂⁻).

Hydrogen atom distribution and hydrogen induced site depopulation for the La_{2-x}Mg_xNi₇-H system

Matylda N. Guzik, Bjørn C. Hauback and Klaus Yvon

page 9

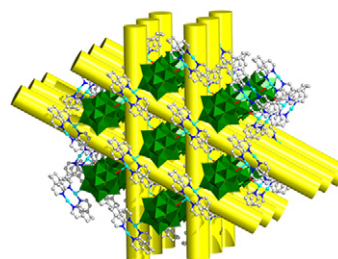


The detailed D atoms arrangement in La_{1.63}Mg_{0.37}Ni₇D_{8.8} differs significantly from the previously reported La_{1.5}Mg_{0.5}Ni₇D_{8.9(9.1)}. The present model consists of only five deuterium sites as opposed to nine proposed for La_{1.5}Mg_{0.5}Ni₇D_{8.9(9.1)}. The reported four remaining deuterium atom positions in La_{1.5}Mg_{0.5}Ni₇D_{8.9(9.1)} were not found in the investigated La_{1.63}Mg_{0.37}Ni₇D_{8.8}. The five Ni atoms have deuterium among their nearest neighbors, which surround them in a way similar to configurations observed in some complex transition metal hydrides and already reported for metallic hydrides. In the presented deuterium-rich phase, deformed tetrahedron, rigid trigonal pyramids as well as disordered and deformed saddle-like configuration are observed.

An unusual mono-substituted Keggin anion-chain based 3D framework with 24-membered macrocycles as linker units

Haijun Pang, Huiyuan Ma, Yan Yu, Ming Yang, Ye Xun and Bo Liu

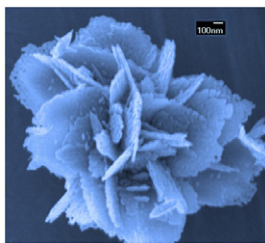
page 23



An unusual example of mono-substituted Keggin anion-chain based hybrid compound that possesses a 3D structure has been synthesized, which offers a feasible route for synthesis of such compounds.

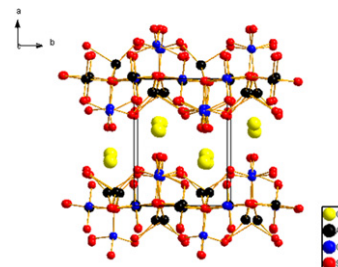
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Biomolecule-assisted synthesis and gas-sensing properties of porous nanosheet-based corundum In_2O_3 microflowers
Wen-Hui Zhang and Wei-De Zhang
page 29



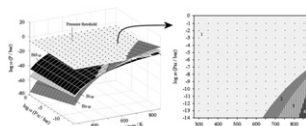
Nanosheets-based corundum In_2O_3 microflowers were fabricated by one-pot hydrothermal treatment of D-fructose/ $\text{In}(\text{NO}_3)_3$ mixture followed by calcination, which show high performance for formaldehyde sensing.

Synthesis, structure, and electronic structure of $\text{CsAgGa}_2\text{Se}_4$
Dajiang Mei, Wenlong Yin, Kai Feng, Lei Bai, Zheshuai Lin, Jiyong Yao and Yicheng Wu
page 54



$\text{CsAgGa}_2\text{Se}_4$ contains two-dimensional ${}^2_{\infty}[\text{AgGa}_2\text{Se}_4]^-$ layers with a novel chain-sublayer-chain structure.

Thermochemical and kinetic aspects of the sulfurization of Cu-Sb and Cu-Bi thin films
Diego Colombara, Laurence M. Peter, Keith D. Rogers and Kyle Hutchings
page 36



Example of 3D plot showing the equilibrium pressure surfaces of species potentially escaping from chalcogenide films as a function of temperature and sulfur partial pressure. Bi_2 , Bi , and BiS are the gaseous species in equilibrium with solid Bi_2S_3 considered in this specific example. The pressure threshold plane corresponds to the pressure limit above which the elemental losses from $1 \mu\text{m}$ thick films exceeds 10% of the original content per cm^2 area of film and dm^3 capacity of sulfurization furnace under static atmosphere conditions. The sulfurization temperature/sulfur partial pressure boundaries required to minimise the elemental losses below a given value can be easily read from the 2D projection of the intersection curves onto the T - P_{S_2} plane.

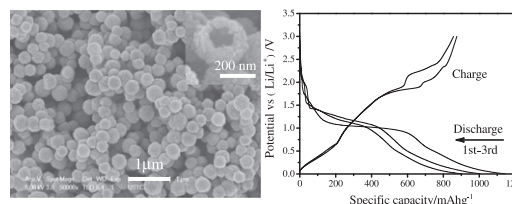
Example of 3D plot showing the equilibrium pressure surfaces of species potentially escaping from chalcogenide films as a function of temperature and sulfur partial pressure.

$\text{Bi}_{(g)}$, $\text{Bi}_{2(g)}$, and $\text{BiS}_{(g)}$ are the gaseous species in equilibrium with solid $\text{Bi}_2\text{S}_{3(s)}$ considered in this specific example.

The pressure threshold plane corresponds to the pressure limit above which the elemental losses from $1 \mu\text{m}$ thick films exceeds 10% of the original content per cm^2 area of film and dm^3 capacity of sulfurization furnace under static atmosphere conditions.

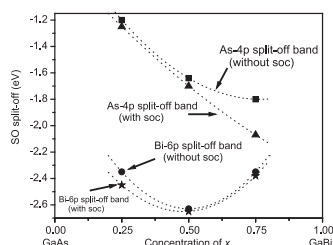
The sulfurization temperature/sulfur partial pressure boundaries required to minimise the elemental losses below a given value can be easily read from the 2D projection of the intersection curves into the T - P_{S_2} plane.

New strategy to the controllable synthesis of CuInS_2 hollow nanospheres and their applications in lithium ion batteries
Weixin Zhang, Hui Zeng, Zeheng Yang and Qiang Wang
page 58



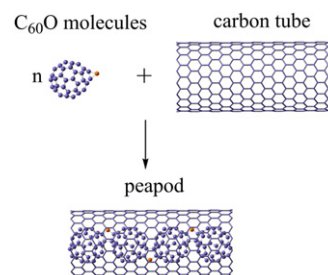
CuInS_2 hollow nanospheres was successfully prepared from Cu_2O solid nanospheres in the absence of any surfactant, which can deliver a large initial discharge capacity of 1144 mAh g^{-1} and exhibit good cycle performance.

Bismuth in gallium arsenide: Structural and electronic properties of $\text{GaAs}_{1-x}\text{Bi}_x$ alloys
Ali Hussain Reshak, H. Kamarudin, S. Auluck and I.V. Kityk
page 47



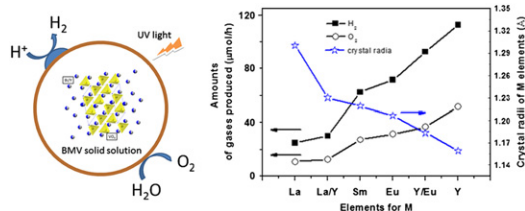
Bowing effect of spin-orbit split-off band values versus Bi content with and without spin-orbit coupling for $\text{GaAs}_{1-x}\text{Bi}_x$ (at $x = 0.25, 0.50$ and 0.75). Calculations are done with GGA.

Structure and electronic properties of the nanopapods—One dimensional C_{60}O polymer encapsulated in single-walled carbon nanotubes
Weiye Qiao, Xinqian Li, Hongcun Bai, Ying Zhu and Yuanhe Huang
page 64



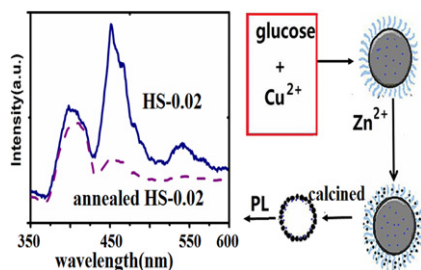
Formation of the novel peapod—1D C_{60}O polymer encapsulated inside single-walled carbon nanotube.

Roles of Bi, M and VO₄ tetrahedron in photocatalytic properties of novel Bi_{0.5}M_{0.5}VO₄ (M = La, Eu, Sm and Y) solid solutions for overall water splitting
 Hui Liu, Jian Yuan, Zhi Jiang, Wenfeng Shangguan, Hisahiro Einaga and Yasutake Teraoka
 page 70



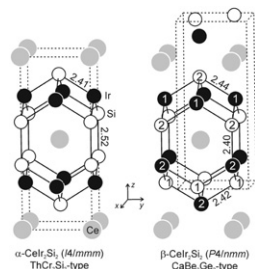
Novel Bi_{0.5}M_{0.5}VO₄ (M = La, Eu, Sm and Y) solid solutions showed the high and stable photocatalytic activities for overall water splitting with their crystal radii of M elements.

CuO–ZnO heterometallic hollow spheres: Morphology and defect structure
 Xuemin Shi, Xuzhuang Yang, Xiaojun Gu and Haiquan Su
 page 76



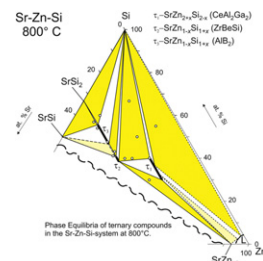
CuO–ZnO hollow spheres were obtained using Cu-embedded carbon spheres as template, and the photoluminescent spectra afforded the evidence regarding the oxygen vacancies in the hollow spheres.

Electronic structure and chemical bonding of α- and β-CeIr₂Si₂ intermediate valence compounds
 Samir F. Matar, Rainer Pöttgen and Bernard Chevalier
 page 81



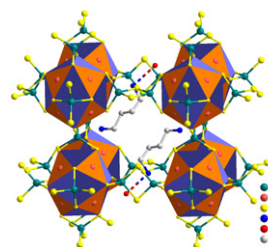
The crystal structures of α- and β-CeIr₂Si₂. Relevant interatomic distances (Å), the three-dimensional [Ir₂Si₂] networks and the crystallographically independent iridium and silicon sites are indicated.

The systems Sr–Zn–{Si,Ge}: Phase equilibria and crystal structure of ternary phases
 V.V. Romaka, M. Falmbigl, A. Grytsiv and P. Rogl
 page 87



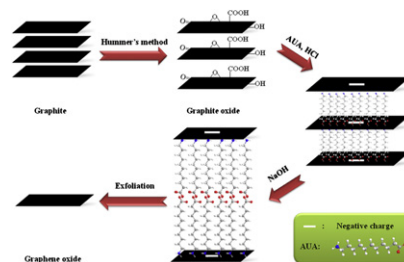
Phase equilibria of ternary compounds in the Sr–Zn–Si-system at 800 °C.

Synthesis and characterization of (H₂dab)₂Cu₈Ge₄S₁₄ · 2H₂O: An expanded framework based on icosahedral Cu₈S₁₂ cluster
 Ren-Chun Zhang, Chi Zhang, Shou-Hua Ji, Min Ji and Yong-Lin An
 page 94



Compound 1 contains a 3D expanded framework constructed from icosahedral Cu₈S₁₂ clusters linked by GeS₄ and dimeric Ge₂S₆ units, with diprotonated 1,4-dab and H₂O molecules located in the channels.

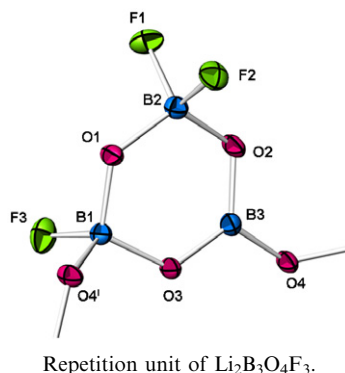
Influence of pH condition on colloidal suspension of exfoliated graphene oxide by electrostatic repulsion
 Long-Yue Meng and Soo-Jin Park
 page 99



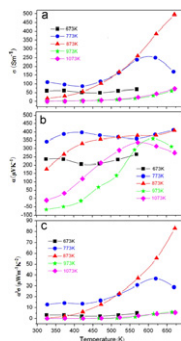
A stable graphene oxide suspension could be quickly prepared by exfoliating a graphite oxide suspension by a host–guest electrostatic repulsion in aqueous solution.

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Li₂B₃O₄F₃, a new lithium-rich fluoroxyborate
 Thomas Pilz, Hanne Nuss and Martin Jansen
 page 104

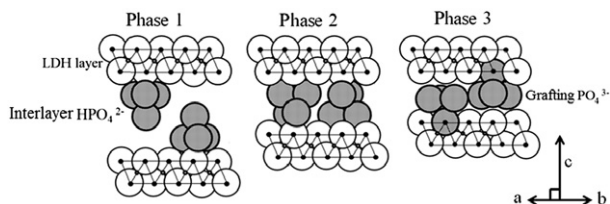


Preparation and thermoelectric properties of ternary superionic conductor CuCrS₂
 Yue-Xing Chen, Bo-Ping Zhang, Zhen-Hua Ge and Peng-Peng Shang
 page 109



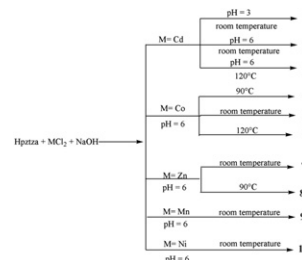
The samples sintered above 873 K, both of the Seebeck coefficient and electrical conductivity exhibit an increase tendency with increasing temperature, which is due to the mechanism of mix-conduction for CuCrS₂.

Direct observation of grafting interlayer phosphate in Mg/Al layered double hydroxides
 Akihiro Shimamura, Eiji Kanezaki, Mark I. Jones and James B. Metson
 page 116



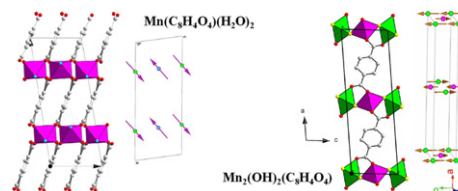
The cross section of the synthetic Mg, Al layered double hydroxides in Phase 1, with interlayer hydrogen phosphate Phase 2, and with grafted phosphate, Phase 3.

A set of new transition metal-based coordination complexes dependent upon Hpztza ligand (Hpztza = 2-(5-(pyrazin-2-yl)-2H-tetrazol-2-yl) acetic acid)
 Jie Yang, Lei Shen, Gao-Wen Yang, Qiao-Yun Li, Wei Shen, Jian-Ning Jin, Jing-Jing Zhao and Jian Dai
 page 124



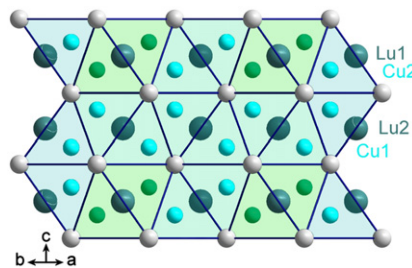
Ten new coordination polymers with 2-(5-(pyrazin-2-yl)-2H-tetrazol-2-yl) acetic acid (Hpztza) ligand have been synthesized and their structures have been characterized. All of the complexes show photoluminescence at room temperature.

Magnetic measurements and neutron diffraction study of the layered hybrid compounds Mn(C₈H₄O₄)(H₂O)₂ and Mn₂(OH)₂(C₈H₄O₄)
 Romain Sibille, Adel Mesbah, Thomas Mazet, Bernard Malaman, Silvia Capelli and Michel François
 page 134



The macroscopic magnetic properties and magnetic structures of two metal-organic frameworks based on manganese (II) and terephthalate molecules are presented.

Crystal structure of ~RCu₃S₃ and ~RCuTe₂ (R = Gd–Lu) compounds
 L.D. Gulay, M. Daszkiewicz and V.Ya. Shemet
 page 142

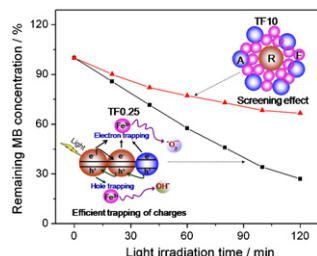


In the series of the ~RCu₃S₃ and ~RCuTe₂ compounds the R and Cu atoms occupy disordered positions. The S (Te) atoms are stacked in a close packed arrangement with the layers in the sequence AB.

A novel approach for enhanced visible light activity in doped nanosize titanium dioxide through the excitons trapping

Kanakkanmavudi B. Jaimy, K.V. Baiju, Swapankumar Ghosh and K.G.K. Warrier

page 149

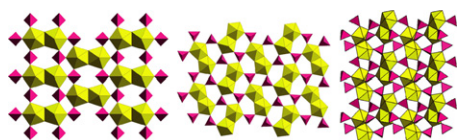


Model explaining the transfer and trapping of e^-/h^+ pairs in mixed phase titania by Fe^{3+} ions suggests the reason for the increased lifetime of e^-/h^+ pairs and enhanced photocatalytic activity.

Synthesis and characterization of uranyl chromate sheet compounds containing edge-sharing dimers of uranyl pentagonal bipyramids

Daniel K. Unruh, Michelle Baranay, Laura Pressprich, Megan Stoffer and Peter C. Burns

page 158

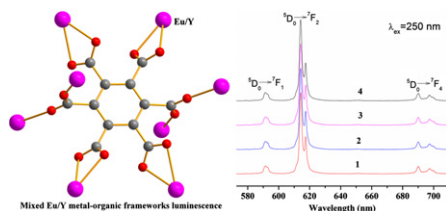


Eight uranyl chromate compounds containing sheet structural units built from uranyl pentagonal bipyramids and $(CrO_4)^{2-}$ tetrahedra are reported. Relationships between sheet topologies and interstitial constituents is examined.

Hydrothermal synthesis, crystal structures and photoluminescence properties of mixed europium–yttrium organic frameworks

Yinfeng Han, Lianshe Fu, Luis Mafra and Fa-Nian Shi

page 165

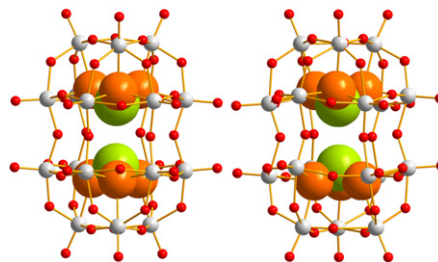


Three mixed europium and yttrium organic frameworks: $Eu_{2-x}Y_x(Mel)(H_2O)_6$ ($Mel = \text{mellitic acid}$) have been synthesized and characterized. All the compounds contain a 3-D net with (4, 8)-flu topology. The study indicates that the photoluminescence properties are effectively affected by the different ratios of europium and yttrium ions, the quantum efficiency is increased and the Eu^{3+} lifetime becomes longer in these MOFs than those of the Eu analog.

Spectroscopic studies of sulfite-based polyoxometalates at high temperature and high pressure

Raul Quesada Cabrera, Steven Firth, Christopher S. Blackman, De-Liang Long, Leroy Cronin and Paul F. McMillan

page 171

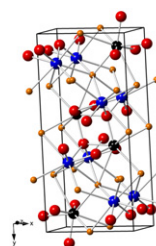


Structural changes occurring within non-conventional Dawson-type $[\alpha/\beta-Mo_{18}O_{54}(SO_3)_2]^{4-}$ polyanions in the form of tetrapentylammonium salts were studied by a combination of IR, Raman and visible spectroscopy at high temperature and high pressure. Evidence of the formation of bronze-type materials above 400 K and also upon pressurization to 8 GPa is presented. This conclusion is suggested to be a general result for polyoxometalate compounds subjected to extreme conditions and it opens opportunities for the design of new materials with interesting optical and electronic properties.

Syntheses and crystal structures of the quaternary uranium lanthanide oxyselenides $UYb_2O_2Se_3$ and $U_2Ln_2O_4Se_3$ ($Ln = Pr, Sm, Gd$)

Adam D. Raw and James A. Ibers

page 177

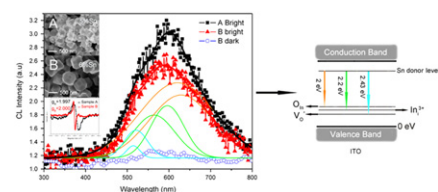


The $U_2Ln_2O_4Se_3$ ($Ln = Pr, Sm, Gd$) structure: primarily U sites are in black, primarily Ln sites are in blue, O red, Se orange.

Sn-doped polyhedral In_2O_3 particles: Synthesis, characterization, and origins of luminous emission in wide visible range

Yunqing Zhu and Yiqing Chen

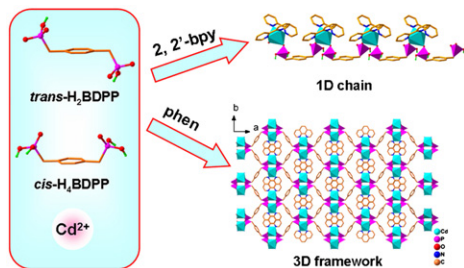
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With more oxygen vacancies and tin doping. ITO particles can exhibit a better CL performance. Sn donor level near the conduction band edge plays an important role in luminous emission in wide visible range.

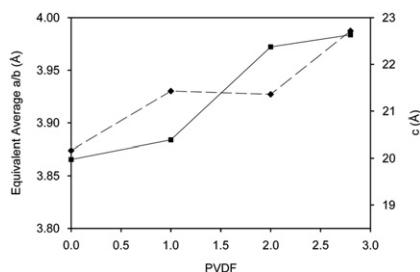
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Hydrothermal syntheses, structures and characterizations of two luminescent cadmium(II) complexes with *p*-xylenediphosphonic acid and N-donor ligands
 Yan-Qiong Sun, Jin Hu, Han-Hui Zhang and Yi-Ping Chen
 page 189



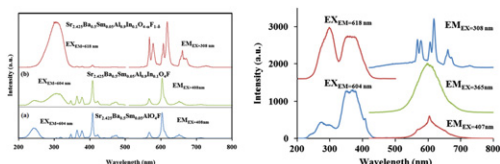
Two new cadmium diphosphonates were obtained by using two different auxiliary ligands. The influence of the N-donor ligands on the structure of the complexes is discussed.

Low temperature fluorination of Sr₃Fe₂O_{7-x} with polyvinylidene fluoride: An X-ray powder diffraction and Mössbauer spectroscopy study
 Cathryn A. Hancock, Tirma Herranz, Jose F. Marco, Frank J. Berry and Peter R. Slater
 page 195



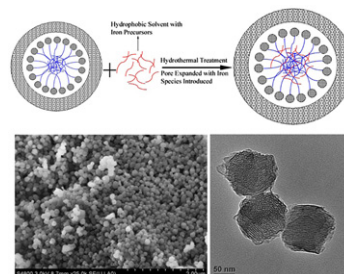
Low temperature (375 °C) fluorination of Sr₃Fe₂O_{7-x} with poly(vinylidene fluoride) leads to the production of three new Ruddlesden Popper oxide fluorides with progressive filling of the anion sites within the structure.

Structure-composition-luminescence correlations in Sr_{2.5-3x/2}Ba_{0.5}Sm_xAl_{1-y}In_yO₄F (0.001 ≤ x, y ≤ 0.1) oxyfluorides
 Sangmoon Park
 page 204



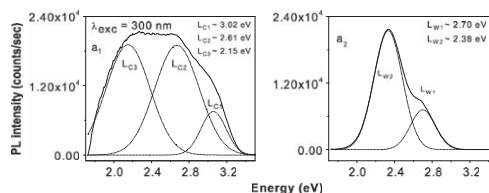
After the replacement of Sr²⁺ and Al³⁺ ions by Sm³⁺ and In³⁺ ions in Sr_{2.5}Ba_{0.5}AlO₄F host structure, a novel charge-transfer band centered around 304 nm shifted from 240 nm is monitored; moreover, sharp and well-resolved emission peaks in the ⁴G_{5/2} → ⁶H_J transitions of the Sm³⁺ activator are observed (Figure, Left). The diverse excitation and emission photoluminescence spectra of Sr_{2.5-3x/2}Ba_{0.5}Sm_xAl_{1-y}In_yO₄₋₂F_{1-δ} (0.001 ≤ x, y ≤ 0.1) phosphors originated by the charge-transfer of the host to the Sm³⁺ activator, the *f-f* transitions in the Sm³⁺ ions, and the defect-induced self-activation are also introduced (Figure, Right).

Simultaneous pore enlargement and introduction of highly dispersed Fe active sites in MSNs for enhanced catalytic activity
 Jin Lou Gu, Xu Dong, S.P. Elangovan, Yongsheng Li, Wenru Zhao, Toshio Iijima, Yasuo Yamazaki and Jian Lin Shi
 page 208



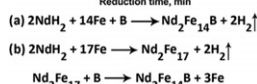
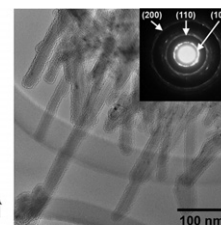
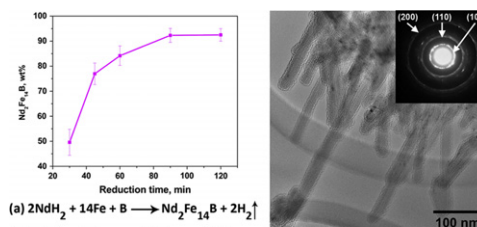
Uniform MSNs with iron active centers and large pore size have been prepared by a newly developed strategy, which demonstrates enhanced catalytic performance for benzylation of benzene by benzyl chloride.

Photoluminescence and Raman evidence for mechano-chemical interaction of polyaniline-emeraldine base with ZnS in cubic and hexagonal phase
 M. Scocioreanu, M. Baibarac, I. Baltog, I. Pasuk and T. Velula
 page 217



Photoluminescence spectra of ZnS with cubic (a₁) and wurtzite (a₂) structure.

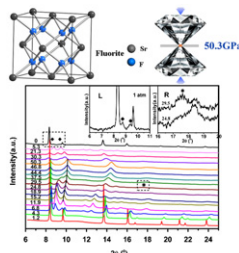
The reaction mechanism of formation of chemically synthesized Nd₂Fe₁₄B hard magnetic nanoparticles
 P.K. Deheri, S. Shukla and R.V. Ramanujan
 page 224



The kinetics, reaction mechanism and morphology of Nd₂Fe₁₄B magnetic nanoparticles synthesized by sol-gel followed by reduction-diffusion at 800 °C.

Structural phase transitions of SrF₂ at high pressure

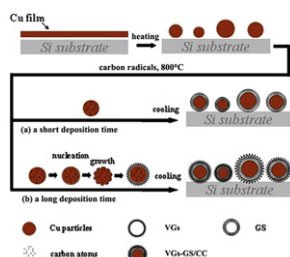
J.S. Wang, C.L. Ma, D. Zhou, Y.S. Xu, M.Z. Zhang, W. Gao, H.Y. Zhu and Q.L. Cui
page 231



The high-pressure behavior of SrF₂ has been investigated by angle-dispersive synchrotron X-ray powder diffraction measurement up to 50.3 GPa at room temperature.

Controllable synthesis of a novel hedgehog-like core/shell structure

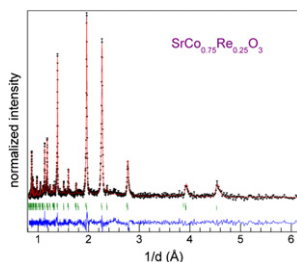
Shumin Wang, Hongwei Tian, Yanhui Pei, Qingnan Meng, Jianli Chen, Huan Wang, Yi Zeng, Weitao Zheng and Yichun Liu
page 235



With increasing deposition time, graphene sheets extend from the surface of GS/CC, causing the multilayer graphene encapsulated copper to be converted into vertically aligned graphene sheets-graphene shell/copper core structure.

Structural and physical properties of Re substituted B-site ordered and disordered SrCo_{1-x}Re_xO_{3-δ} (x = 0.1, 0.25, 0.5)

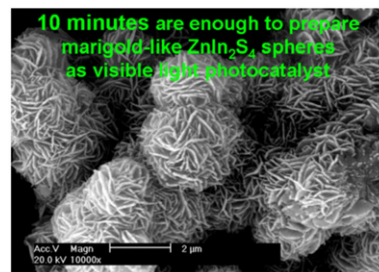
A. Baszczuk, B. Dabrowski, S. Kolesnik, O. Chmaissem and M. Avdeev
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Neutron diffraction pattern for SrCo_{0.75}Re_{0.25}O₃. SrCo_{0.75}Re_{0.25}O₃ is not a partially cation ordered Sr₄Co₃ReO₁₂ phase, but a mixture of two structural and magnetic phases with disordered SrCo_{1-xd}Re_{xd}O₃ and ordered SrCo_{1-xo}Re_{xo}O₃ compositions where xd > 0.1 and xo < 0.5.

Microwave-assisted hydrothermal synthesis of marigold-like ZnIn₂S₄ microspheres and their visible light photocatalytic activity

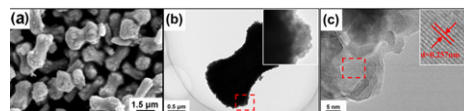
Zhixin Chen, Danzhen Li, Guangcan Xiao, Yunhui He and Yi-Jun Xu
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Marigold-like ZnIn₂S₄ microspheres were synthesized by a fast microwave-assisted hydrothermal method at 80–195 °C with a very short reaction time of 10 min. The as-prepared ZnIn₂S₄ sample can be used as visible light photocatalyst for degradation of organic dyes.

Large-scale controllable synthesis of dumbbell-like BiVO₄ photocatalysts with enhanced visible-light photocatalytic activity

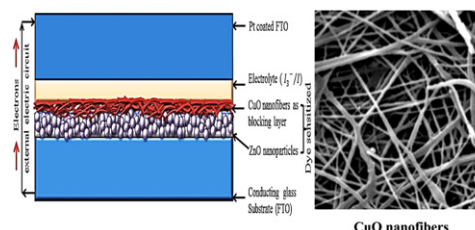
Yang Lu, Yong-Song Luo, De-Zhi Kong, De-Yang Zhang, Yong-Lei Jia and Xin-Wei Zhang
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The controllable synthesis of novel dumbbell-like BiVO₄ hierarchical nanostructures has been successfully obtained via a simple hydrothermal route; the as-prepared BiVO₄ hierarchical nanostructures demonstrated the superior visible-light-driven photocatalytic efficiency.

Synthesis and characterization of CuO nanofibers, and investigation for its suitability as blocking layer in ZnO NPs based dye sensitized solar cell and as photocatalyst in organic dye degradation

R. Sahay, J. Sundaramurthy, P. Suresh Kumar, V. Thavasi, S.G. Mhaisalkar and S. Ramakrishna
page 261

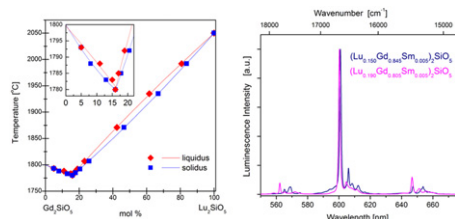


The study on the suitability of highly crystalline CuO nanofibers as the blocking layer in ZnO based DSSC was demonstrated and fabricated with possible energy applications.

Continued

Growth conditions, structure, Raman characterization and optical properties of Sm-doped $(\text{Lu}_x\text{Gd}_{1-x})_2\text{SiO}_5$ single crystals grown by the Czochralski method

Michał Głowacki, Grażyna Dominiak-Dzik, Witold Ryba-Romanowski, Radosław Lisiecki, Adam Strzęp, Tomasz Runka, Mirosław Drozdowski, Viktor Domukhovski, Ryszard Diduszko and Marek Berkowski
page 268

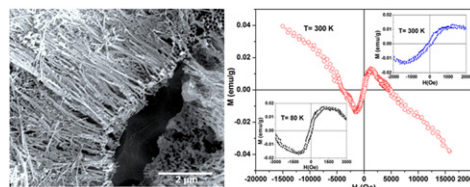


Single crystals of Sm^{3+} -doped $(\text{Lu}_x\text{Gd}_{1-x})_2\text{SiO}_5$ solid solutions have been grown by Czochralski method and characterized by various techniques. Crystal structure changes from $C2/c$ to $P2_1/c$ for composition with $0.15 < x < 0.17$. Change of crystal structure causes changes in emission spectra.

Rapid Communication

Origin of room temperature d^0 ferromagnetism and characteristic photoluminescence in pristine SnO_2 nanowires: A correlation

Gobinda Gopal Khan, S. Ghosh and Kalyan Mandal
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