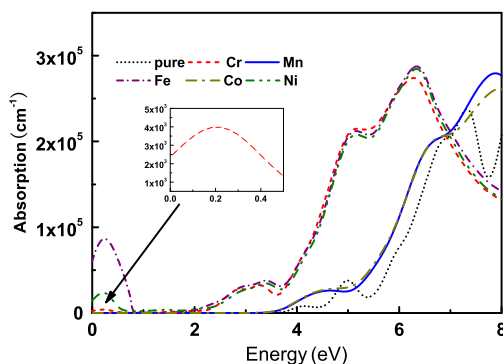


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## Regular Articles

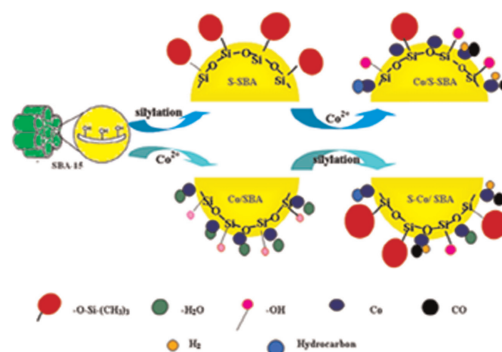
**Infrared, visible and ultraviolet absorptions of transition metal doped ZnS crystals with spin-polarized bands**  
J.H. Zhang, J.W. Ding, J.X. Cao and Y.L. Zhang  
page 477



Absorption coefficients of  $w$ - $TM_xZn_{1-x}S$  crystals ( $TM = Cr^{2+}$ ,  $Mn^{2+}$ ,  $Fe^{2+}$ ,  $Co^{2+}$  and  $Ni^{2+}$ ) at  $x = 0.028$ . The results may be helpful for the design and applications of  $TM:ZnS$  devices, especially for the new high efficiency solar-cell prototype, UV detector and UV LEDs.

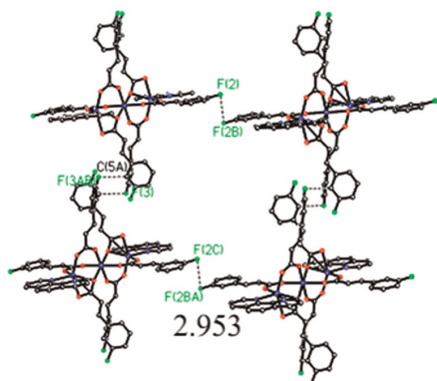
## Regular Articles—Continued

**Silylated Co/SBA-15 catalysts for Fischer–Tropsch synthesis**  
Lihong Jia, Litao Jia, Debao Li, Bo Hou, Jungang Wang and Yuhuan Sun  
page 488



The silylation of an SBA-15 before cobalt impregnation enhanced the reducibility of cobalt oxides on an SBA-15-supported cobalt catalyst and consequently increased the catalytic activity for Fischer–Tropsch synthesis.

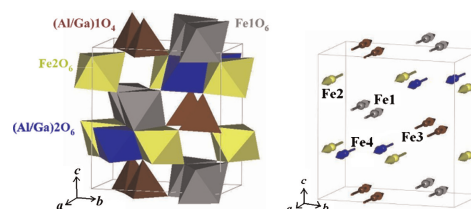
**The C–F...F–C short contacts in the metal complexes of fluoro-phenyl-acrylic acids**  
Gui-lei Liu, Cai-Ming Liu and Hui Li  
page 481



The short distance between F...F (2.953 Å) was found in the complex of  $[Mn_3(L1)_6(L2)_2] \cdot H_2O \cdot CH_3CN$  ( $L1 = (E)$ -3-(3-fluorophenyl)-acrylic acid,  $L2 = 1,10$ -phenanthroline).

**Structure and magnetic properties of the  $Al_{1-x}Ga_xFeO_3$  family of oxides: A combined experimental and theoretical study**

Rana Saha, Ajmala Shireen, A.K. Bera, Sharmila N. Shirodkar, Y. Sundarayya, Nandakumar Kalarikkal, S.M. Yusuf, Umesh V. Waghmare, A. Sundaresan and C.N.R. Rao  
page 494

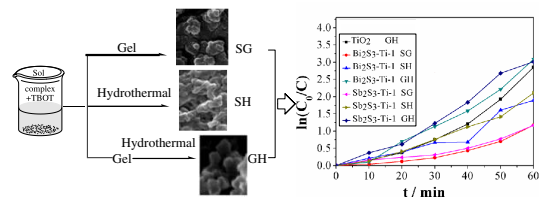


We have studied both experimentally and theoretically the important role of disorder at the cation site on magnetic and related properties of the  $Al_{1-x}Ga_xFeO_3$  family of oxides crystallizing in a non-centrosymmetric space group.

Continued

## Preparation and photocatalytic activity of $\text{Sb}_2\text{S}_3/\text{Bi}_2\text{S}_3$ doped $\text{TiO}_2$ from complex precursor via gel-hydrothermal treatment

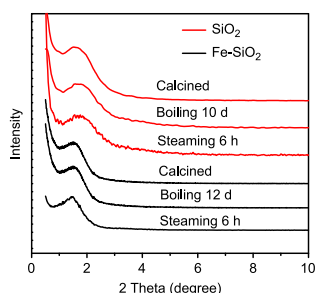
Yan Huang, Gang Xie, Sanping Chen and Shengli Gao  
page 502



$\text{Sb}_2\text{S}_3/\text{Bi}_2\text{S}_3$  doped  $\text{TiO}_2$  were prepared using  $[M(\text{S}_2\text{COEt})_3]$  ( $M = \text{Sb}, \text{Bi}$ ;  $\text{S}_2\text{COEt} = \text{pyrrolidine-1-dithiocarbamate}$ ) as precursors via gel-hydrothermal techniques.  $\text{M}_2\text{S}_3$  doped  $\text{TiO}_2$  performs better photocatalytic activity for photodegradation reaction of 4-nitrophenol.

## High-temperature synthesis of highly hydrothermal stable mesoporous silica and $\text{Fe-SiO}_2$ using ionic liquid as a template

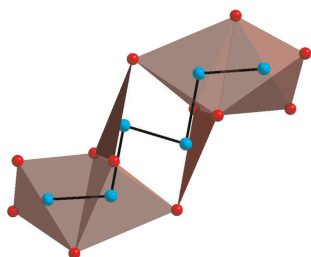
Hong Liu, Mengyang Wang, Hongjiu Hu, Yuguang Liang, Yong Wang, Weiran Cao and Xiaohong Wang  
page 509



Worm-like mesoporous silica and  $\text{Fe-SiO}_2$  with high hydrothermal stability have been synthesized using ionic liquid 1-hexadecane-3-methylimidazolium bromide as a template under the assistance of NaF at high temperature.

## Synthesis, crystal and electronic structure, and physical properties of the new lanthanum copper telluride $\text{La}_3\text{Cu}_5\text{Te}_7$

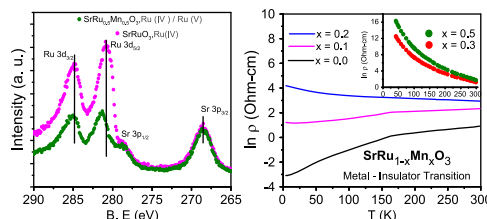
Mariya Zelinska, Abdeljalil Assoud and Holger Kleinke  
page 516



Oligomeric unit comprising interconnected  $\text{CuTe}_3$  pyramids and  $\text{CuTe}_4$  tetrahedra.

## Valence and origin of metal-insulator transition in Mn doped $\text{SrRuO}_3$ studied by electrical transport, X-ray photoelectron spectroscopy and LSDA + $U$ calculation

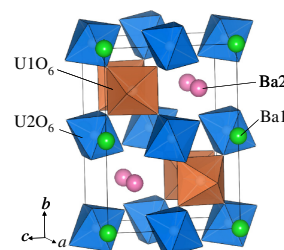
Ranjan K. Sahu, Sudhir K. Pandey and L.C. Pathak  
page 523



XPS data and electrical transport data show that doping of Mn in metallic  $\text{SrRuO}_3$  induces mixed ionic pair  $\text{Ru(IV)/Ru(V)} \leftrightarrow \text{Mn(III)/Mn(IV)}$  and the system undergoes a transition from metal to insulator at the critical Mn doping level,  $x \sim 0.2$ . The origin for the metal-insulator transition has been discussed.

## Magnetic properties of barium uranate $\text{Ba}_2\text{U}_2\text{O}_7$

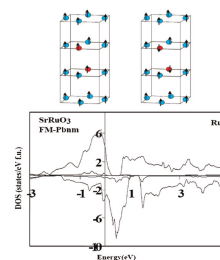
Akio Nakamura, Yoshihiro Doi and Yukio Hinatsu  
page 531



Magnetic susceptibility, magnetization, and specific heat measurements reveal that  $\text{Ba}_2\text{U}_2\text{O}_7$  undergoes a canted antiferromagnetic ordering at 19 K. In addition, another magnetic anomaly is observed at 58 K, which may be due to one-dimensional magnetic correlations of the U ions.

## Ferromagnetism and antiferromagnetism coexistence in $\text{SrRu}_{1-x}\text{Mn}_x\text{O}_3$ : Density functional calculation

H. Hadipour, S. Fallahi and M. Akhavan  
page 536

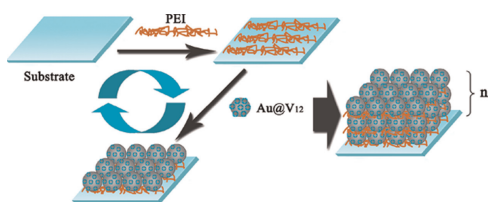


The antiparallel alignment between the Mn and Ru ions are consistent with the competition between ferromagnetism and antiferromagnetism with the formation of a spin glass phase. We have calculated the electronic structure of  $\text{SrRu}_{1-x}\text{Mn}_x\text{O}_3$  using the full potential linearized augmented plane wave method by LSDA and LSDA +  $U$  in the range of both low and high Mn-doping for parallel and antiparallel alignments of Ru and Mn moments. In the low Mn-doped polycrystalline samples with tetragonal structure, the AFM hybridization between Mn and the Ru host lattice strongly favors alignment of the Ru moments, and provides an explanation for retaining of high Curie temperature of  $\text{SrRuO}_3$  with Mn substitution.

## One-step synthesis and stabilization of gold nanoparticles and multilayer film assembly

Ya-Yan Bao, Li-Hua Bi and Li-Xin Wu

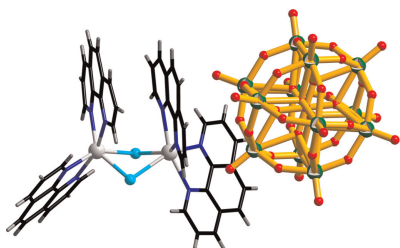
page 546



The wheel-shaped  $V^V-V^{IV}$  mixed-valence tungstovanadate  $[P_8W_{48}O_{184}\{V_4V^{IV}O_{12}(H_2O)_2\}_2]^{32-}$  (V12) stabilized Au nanoparticles (Au@V12 NPs) have been synthesized and characterized. The multilayer films containing Au@V12 NPs were fabricated and their electrocatalytic properties were studied.

## Two new hybrid compounds assembled from Keggin-type polyoxometalates and transition metal coordination complexes

Yan Wang, Bo Zou, Li-Na Xiao, Ning Jin, Yu Peng, Feng-Qing Wu, Hong Ding, Tie-Gang Wang, Zhong-Min Gao, Da-Fang Zheng, Xiao-Bing Cui and Ji-Qing Xu  
page 557

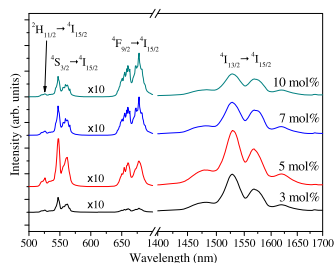


Two new hybrid compounds based on different Keggin-type polyoxometalates have been hydrothermally synthesized and characterized by IR, UV-Vis, XPS, XRD, elemental analysis and single crystal X-ray diffraction analysis.

## Visible and infrared luminescence properties of $Er^{3+}$ -doped $Y_2Ti_2O_7$ nanocrystals

Chu-Chi Ting, Yi-Shan Chiu, Chia-Wei Chang and Liang-Chih Chuang

page 563

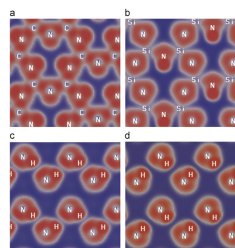


Emission fluorescence spectra of the  $Er^{3+}$  (3, 5, 7, or 10 mol%)-doped  $Y_2Ti_2O_7$  nanocrystals annealed at 800 °C for 1 h under 980 nm pumping. The  $Er^{3+}$ -doped  $Y_2Ti_2O_7$  nanocrystals absorbing 980 nm photons can produce the upconversion (526, 547, and 660 nm;  $^2H_{11/2} \rightarrow ^4I_{15/2}$ ,  $^4S_{3/2} \rightarrow ^4I_{15/2}$ , and  $^4F_{9/2} \rightarrow ^4I_{15/2}$ , respectively) and Stokes (1528 nm;  $^4I_{13/2} \rightarrow ^4I_{15/2}$ ) photoluminescence.

## Low-compressibility and hard material carbon nitride imide $C_2N_2(NH)$ : First principles calculations

Hai-Yan Yan, Qun Wei, Bao-bing Zheng and Ping Guo

page 572

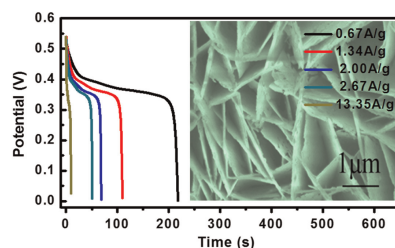


Contours of electronic localization function (ELF) of  $C_2N_2(NH)$  on the: (0 0 1) plane (a), (1 0 0) plane (b), an ELF of  $Si_2N_2(NH)$  on the: (0 0 1) plane (c) and (1 0 0) plane (d).

## Direct synthesis of porous NiO nanowall arrays on conductive substrates for supercapacitor application

Jianhui Zhu, Jian Jiang, Jingping Liu, Ruimin Ding, Hao Ding, Yamin Feng, Guangming Wei and Xintang Huang

page 578

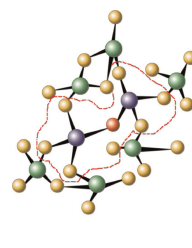


Porous NiO nanowall arrays (NWAs) grown on alloy substrate have been made using nullaginite as precursor and studied as supercapacitor electrodes. Porous nanowalls interconnected with each other resulting in the formation of extended-network architectures and exhibited excellent capacitor properties. NiO NWAs electrode delivered a capacitance of 270 F/g (0.67 A/g); even at high current density, the electrode could still deliver a high capacitance up to 236 F/g (13.35 A/g). Besides, it exhibited excellent cycle lifetime with ~93% capacitance kept after 4000 cycles. These remarkable results made it possible for mass production of NiO NWAs and future thin-film microelectronic applications.

## Evidence of network demixing in $GeS_2$ - $Ga_2S_3$ chalcogenide glasses: A phase transformation study

Changgui Lin, Laurent Calvez, Haizheng Tao, Mathieu Allix, Alain Moréac, Xianghua Zhang and Xiujian Zhao

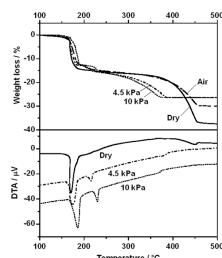
page 584



**Synopsis:** network demixing in  $GeS_2$ - $Ga_2S_3$  chalcogenide glasses.

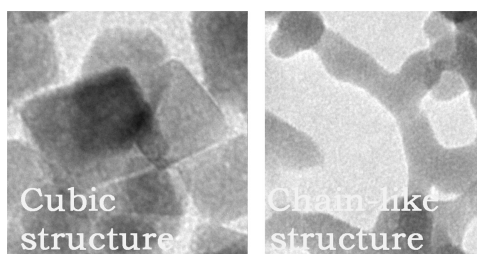
Continued

**Effect of water vapor on the thermal decomposition process of zinc hydroxide chloride and crystal growth of zinc oxide**  
Takahiro Kozawa, Ayumu Onda, Kazumichi Yanagisawa, Akira Kishi and Yasuaki Masuda  
*page 589*



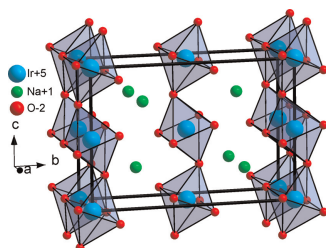
Thermal decomposition process of zinc hydroxide chloride (ZHC),  $\text{Zn}_5(\text{OH})_8\text{Cl}_2 \cdot \text{H}_2\text{O}$ , has been investigated by novel thermal analyses with three different water vapor partial pressures. In the water vapor atmosphere, the formation of ZnO was completed at lower temperatures than in dry.

**Effects of surfactants on morphology in synthesis of  $\alpha\text{-Mn}_2\text{O}_3$  nanostructures**  
D. Ramarajan and P. Sivagurunathan  
*page 597*



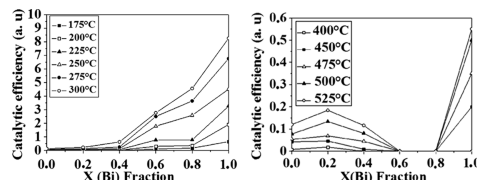
Cubic and chain-like nanostructure of  $\alpha\text{-Mn}_2\text{O}_3$  has been synthesized by air oxidation of manganese chloride as precursor, hexamine, and mercaptosuccinic acid as wetting agent, respectively.

**$\text{NaIrO}_3$ —A pentavalent post-perovskite**  
M. Bremholm, S.E. Dutton, P.W. Stephens and R.J. Cava  
*page 601*



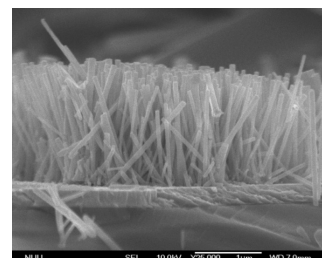
Sodium iridium(V) oxide,  $\text{NaIrO}_3$ , synthesized by a high pressure solid state method and recovered to ambient conditions is found to crystallize as the post-perovskite structure and is the first example of a pentavalent  $\text{ABO}_3$  post-perovskite.

**Structural, microstructural and surface properties of a specific  $\text{CeO}_2\text{-Bi}_2\text{O}_3$  multiphase system obtained at 600 °C**  
Lamia Bourja, Bahcine Bakiz, Abdeljalil Benlhachemi, Mohamed Ezahri, Sylvie Villain, Olivier Crosnier, Claude Favotto and Jean-Raymond Gavarri  
*page 608*



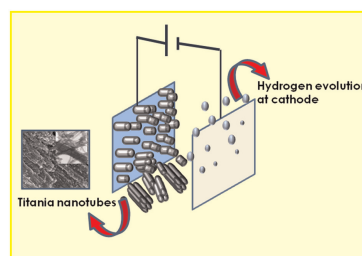
**Catalytic efficiencies of  $\text{CeO}_2\text{-Bi}_2\text{O}_3$  system:** catalytic actions on methane (on the left) or carbon monoxide (on the right) of  $(1-x)\text{CeO}_2-x/2 \text{ Bi}_2\text{O}_3$  samples, as a function of the fraction  $x$ , and for fixed temperatures: on the vertical axis, the intensities of  $\text{CO}_2$  FTIR absorption bands are reported. Strong efficiency of bismuth rich samples for CO conversion.

**Optimization of processing parameters on the controlled growth of ZnO nanorod arrays for the performance improvement of solid-state dye-sensitized solar cells**  
Yi-Mu Lee and Hsi-Wen Yang  
*page 615*



The ZnO nanorod arrays demonstrate well-alignment, high aspect ratio ( $L/D \sim 21$ ) and excellent optical transmittance by low-temperature chemical bath deposition (CBD).

**Rapid breakdown anodization technique for the synthesis of high aspect ratio and high surface area anatase  $\text{TiO}_2$  nanotube powders**  
Rajini P. Antony, Tom Mathews, Arup Dasgupta, S. Dash, A.K. Tyagi and Baldev Raj  
*page 624*

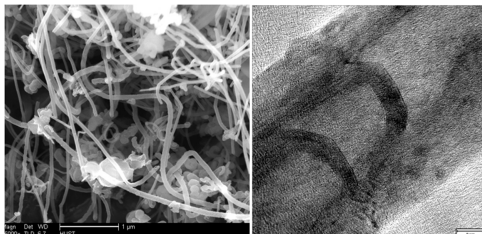




### Catalytic synthesis of bamboo-like multiwall BN nanotubes via SHS-annealing process

L.P. Zhang, Y.L. Gu, J.L. Wang, G.W. Zhao, Q.L. Qian, J. Li, X.Y. Pan and Z.H. Zhang

page 633

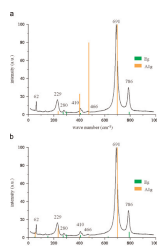


A novel and effective annealing porous precursor route to bulk synthesis of bamboo-like multiwall BN nanotubes. Four growth models of VLS growth mechanism for these nanotubes are proposed.

### Crystal chemistry peculiarities of $\text{Cs}_2\text{Te}_4\text{O}_{12}$

David Hamani, Andrei Mirgorodsky, Olivier Masson, Thérèse Merle-Méjean, Maggy Colas, Mikhael Smirnov and Philippe Thomas

page 637

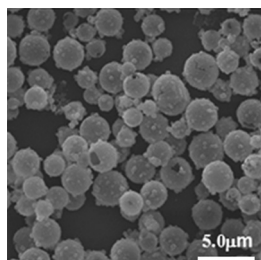


Two versions of the BPM estimations of the Raman intensity for the  $\text{Cs}_2\text{Te}_4\text{O}_{12}$  lattice vibrations: (a) without including effects of the Cs-O bonds and (b) including the above mentioned effects. Experimentally observed peaks are characterized by their frequency positions.

### Photochemical preparation of CdS hollow microspheres at room temperature and their use in visible-light photocatalysis

Yuying Huang, Fengqiang Sun, Tianxing Wu, Qingsong Wu, Zhong Huang, Heng Su and Zihe Zhang

page 644

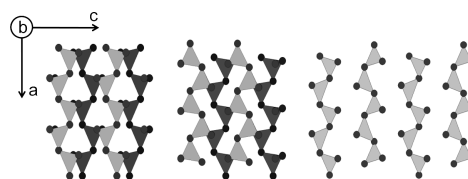


Taking polystyrene spheres dispersed in a precursor solution as templates, CdS hollow microspheres composed of nanoparticles were successfully prepared via a new photochemical route at room temperature.

### Crystallographic and magnetic characterisation of the brownmillerite $\text{Sr}_2\text{Co}_2\text{O}_5$

Eirin Sullivan, Joke Hadermann and Colin Greaves

page 649

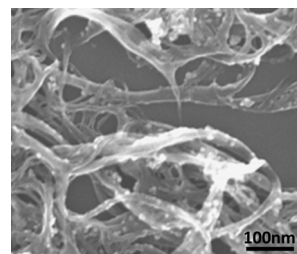


Possible ordering of the tetrahedral chains in  $\text{Sr}_2\text{Co}_2\text{O}_5$ .

### Study of the surface chemistry and morphology of single walled carbon nanotube-magnetite composites

F. Marquez-Linares, O.N.C. Uwakweh, N. Lopez, E. Chavez, R. Polanco, C. Morant, J.M. Sanz, E. Elizalde, C. Neira, S. Nieto and R. Roque-Malherbe

page 655

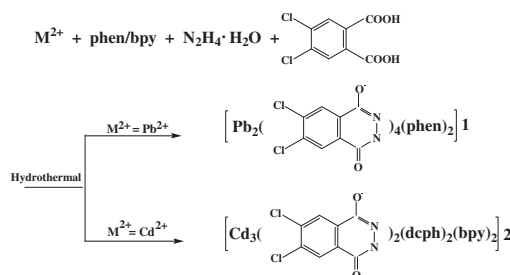


A large amount of Lewis acid sites were found in the highly dispersed magnetite which is supported on the SWCNT outer surface.

### New 4,5-dichlorophthalhydrazide-bridged chained coordination polymers

Juan Jin, Ming-Jun Jia, Yu Peng, Jie-Hui Yu, Yu-Chang Wang and Ji-Qing Xu

page 667



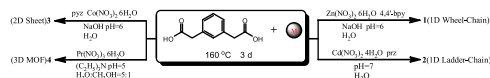
By applying the *in situ* acylation reaction between 4,5-dichlorophthalic acid and  $\text{N}_2\text{H}_4 \cdot \text{H}_2\text{O}$ , two 4,5-dichlorophthalhydrazide-bridged chained coordination compounds  $[\text{Pb}_2(\text{DCPTH})_4(\text{phen})_2]$  and  $[\text{Cd}_3(\text{DCPTH})_2(\text{dcp})_2(\text{bpy})_2]$  (4,5-dichlorophthalhydrazide = DCPH, and dcp = 4,5-dichlorophthalate) were hydrothermally synthesized.

Continued

## Synthesis, structures, luminescent and magnetic properties of four coordination polymers with the flexible 1,3-phenylenediacetate ligands

Jin-Zhong Gu, Dong-Yu Lv, Zhu-Qing Gao, Jian-Zhao Liu, Wei Dou and Yu Tang

page 675

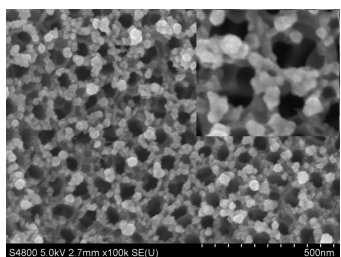


Four new coordination polymers with 1,3-phenylenediacetate ligands have been hydrothermally synthesized and characterized. Complexes **1** and **2** display strong blue fluorescent emission at room temperature. Magnetic susceptibility measurements of **3** and **4** exhibit antiferromagnetic interactions between the nearest metal centers.

## Fabrication and photocatalytic activity of high-efficiency visible-light-responsive photocatalyst ZnTe/TiO<sub>2</sub> nanotube arrays

Yutang Liu, Xilin Zhang, Ronghua Liu, Renbin Yang, Chengbin Liu and Qingyun Cai

page 684

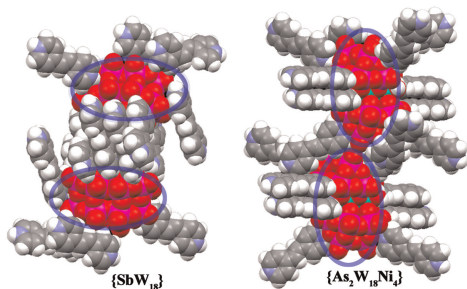


Surface-view SEM images of ZnTe/TiO<sub>2</sub> NT prepared under  $-2.0$  V, and the inset is the corresponding enlarged drawings.

## Assemblies based on the directing effect of non-classical W<sub>18</sub> anionic clusters and the rod-like trans-1,2-di-(4-pyridyl)-ethylen (bpe)

Zhangang Han, Yanna Wang, Xuejun Song, Jiao Huang and Xueliang Zhai

page 690

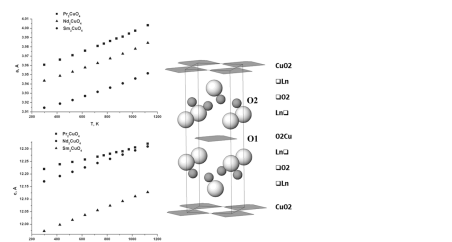


Two polyoxometalate-based supramolecular assemblies built upon W<sub>18</sub> clusters and the rigid organic trans-1,2-di-(4-pyridyl)-ethylen (bpe) have been synthesized and characterized.

## High-temperature crystal structure and transport properties of the layered cuprates Ln<sub>2</sub>CuO<sub>4</sub>, Ln = Pr, Nd and Sm

M.S. Kaluzhskikh, S.M. Kazakov, G.N. Mazo, S.Ya. Istomin, E.V. Antipov, A.A. Gippius, Yu. Fedotov, S.I. Bredikhin, Yi Liu, G. Svensson and Z. Shen

page 698

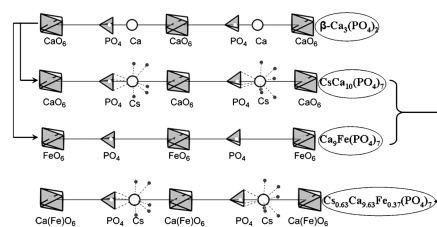


Anomalous anisotropic thermal expansion behavior was observed for Pr<sub>2</sub>CuO<sub>4</sub> in comparison with Ln<sub>2</sub>CuO<sub>4</sub>, Ln = Pr and Nd having tetragonal T'-structure with thermal expansion coefficients (TEC) along *a*- and *c*-axis changing from TEC(*a*)/TEC(*c*)  $\approx$  1.37 (Pr) to 0.89 (Nd) and 0.72 (Sm). It was found that the trace diffusion coefficient (*D<sub>T</sub>*) of oxygen in Pr<sub>2</sub>CuO<sub>4</sub> determined by secondary ion mass spectrometry (SIMS) varies in the range  $7.2 \times 10^{-13}$  cm<sup>2</sup>/s (973 K) and  $3.8 \times 10^{-10}$  cm<sup>2</sup>/s (1173 K) which are in between those observed for the manganese and cobalt-based perovskites.

## Synthesis and characterization of phosphates in molten systems Cs<sub>2</sub>O–P<sub>2</sub>O<sub>5</sub>–CaO–M<sup>III</sup>O<sub>3</sub> (M<sup>III</sup>—Al, Fe, Cr)

Igor V. Zatovsky, Nataliya Yu. Strutynska, Vyacheslav N. Baumer, Nikolay S. Slobodyanik, Ivan V. Ogorodnyk and Oleg V. Shishkin

page 705

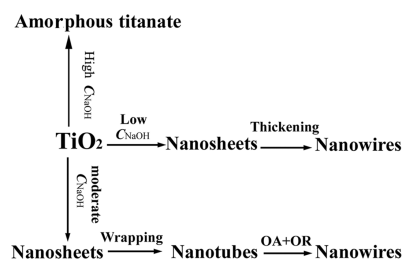


Structural relationships between  $\beta$ -Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> and synthesized compounds is shown in terms of aliovalent substitution of calcium atoms, which reside on three-fold axis, by other metals in  $\beta$ -Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> framework.

## Formation of titanate nanostructures under different NaOH concentration and their application in wastewater treatment

Jiquan Huang, Yongge Cao, Zhonghua Deng and Hao Tong

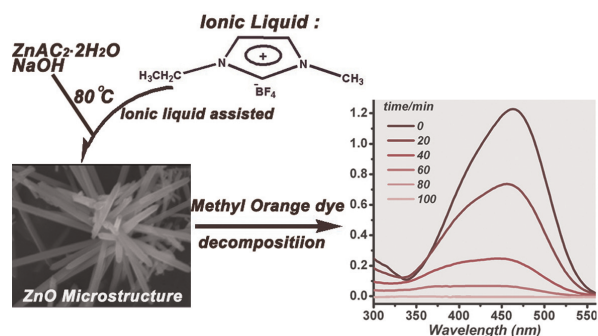
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The morphologies of the titanates depend deeply on the concentration of NaOH. With increasing NaOH concentration, three different formation mechanisms were proposed. The application of these titanate nanostructures in the wastewater treatment was studied.

# Microbundles of zinc oxide nanorods: Assembly in ionic liquid [EMIM]<sup>+</sup>[BF<sub>4</sub>]<sup>-</sup>, photoluminescence and photocatalytic properties

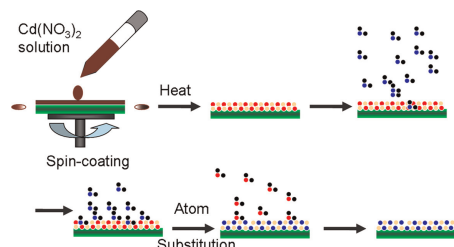
Li Wang, Shen-Zhi Xu, Hui-Jun Li, Li-Xian Chang, Zhi-Su, Ming-Hua Zeng, Li-Na Wang and Yi-Neng Huang  
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Easy formation of microbundles of ZnO nanorods were accomplished in low temperature with [EMIM]<sup>+</sup>[BF<sub>4</sub>]<sup>-</sup> (1-ethyl-3-methylimidazolium tetrafluoroborate) ionic liquid, which exhibit significant green-yellow photoluminescence property and high photodegradation of Methyl Orange dye.

## Rapid Communication

CdS thin films on LiNbO<sub>3</sub> (1 0 4) and silicon (1 1 1) substrates prepared through an atom substitution method  
Haiming Qin, Yue Zhao, Hong Liu, Zheng Gao, Jiyang Wang, Duo Liu, Yuanhua Sang, Bin Yao and Robert I. Boughton  
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Elemental O in CdO is substituted by elemental S from the atmosphere in the apparatus, which is designated as an atom substitution process. This novel method involving an atom substitution reaction between the CdO precursor thin film and its environment can provide a new low cost approach to the preparation of chalcogenide or other compound thin films.

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