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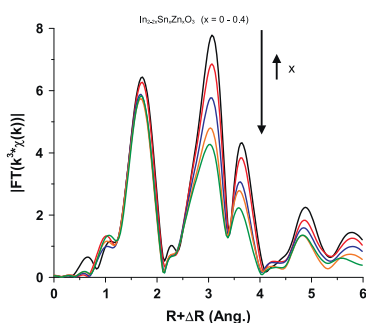
Regular Articles

Probing the local structure of crystalline ZITO:

$\text{In}_{2-2x}\text{Sn}_x\text{Zn}_x\text{O}_3$ ($x \leq 0.4$)

Cathleen A. Hoel, Jean-François Gaillard and Kenneth R. Poeppelmeier

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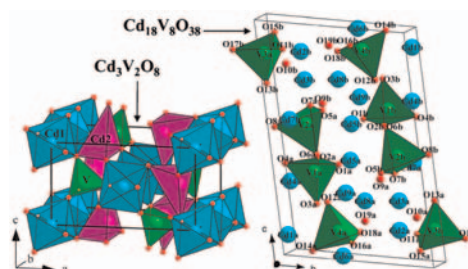
The local structure of Zn and Sn cosubstituted In_2O_3 was determined by X-ray absorption spectroscopy, which was consistent with random substitutions of In by Zn and Sn into bixbyite In_2O_3 .

Regular Articles—Continued

Structural study of the $\text{NaCdVO}_4\text{--Cd}_3\text{V}_2\text{O}_8$ and $\text{CdO--V}_2\text{O}_5$ sections of the ternary system $\text{Na}_2\text{O--CdO--V}_2\text{O}_5$

Hamdi Ben Yahia, Etienne Gaudin, Cédric Feral-Martin and Jacques Darriet

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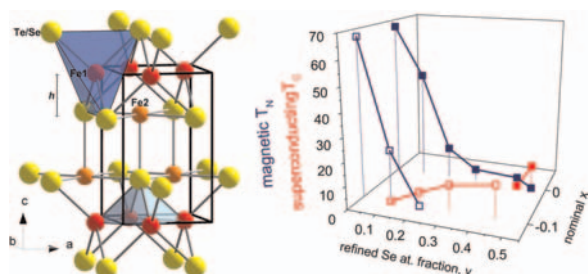
The binary compounds $\text{Cd}_3\text{V}_2\text{O}_8$ and $\text{Cd}_{18}\text{V}_8\text{O}_{38}$ have been successfully synthesized by solid state reaction route and the crystal structures were determined from single-crystal X-ray diffraction data.

Effect of Fe excess on structural, magnetic and superconducting properties of single-crystalline

$\text{Fe}_{1+x}\text{Te}_{1-y}\text{Se}_y$

R. Viennois, E. Giannini, D. van der Marel and R. Černý

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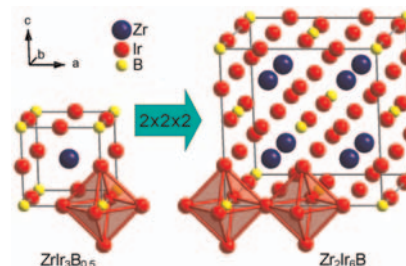


Single crystals of $\text{Fe}_{1+x}\text{Te}_{1-y}\text{Se}_y$ have been grown with a controlled Fe off-stoichiometry and Se doping and the crystal structure has been refined for various compositions, thus proving the effect of both Fe excess and Se-substitutions on the structural properties. Either antiferromagnetic or superconducting ground state is driven by doping and related structural modifications. An improved 3-D phase diagram is proposed.

$\text{Zr}_2\text{Ir}_6\text{B}$ with an eightfold superstructure of the cubic perovskite-like boride $\text{ZrIr}_3\text{B}_{0.5}$: Synthesis, crystal structure and bonding analysis

Martin Hermus and Boniface P.T. Fokwa

Page 784

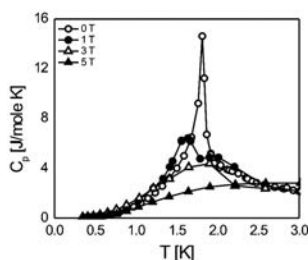


$\text{Zr}_2\text{Ir}_6\text{B}$ crystallizes with an eightfold superstructure of the already reported simple cubic perovskite ZrIr_3B_x . According to the result of tight-binding electronic structure calculations, Ir–B and Ir–Zr interactions are mainly responsible for its structural stability, and the Ir–Ir bonding within the empty Ir_6 clusters is two times stronger than that in the BIr_6 octahedra.

Magnetic and thermodynamic properties of NdT_2Ge_2 ($T = \text{Pd, Ag}$) compounds

Ł. Gondek, B. Penc, D. Kaczorowski, S. Baran, A. Hoser, S. Gerischer and A. Szytuła

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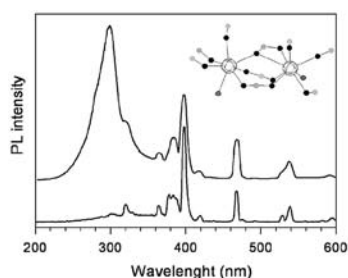


Low-temperature specific heat of NdAg_2Ge_2 under external magnetic fields. The λ -like anomaly originates from onset of magnetic ordering below 1.80 K. Shifting the anomaly position towards the lower temperatures, when raising the magnetic field, hints at antiferromagnetic behaviors.

Interactions between Eu^{3+} ions in inorganic-organic hybrid materials

Fabienne Pellé, Patrick Aschehoug, Suzy Surlé, Franck Millange, Christian Serre and Gérard Férey

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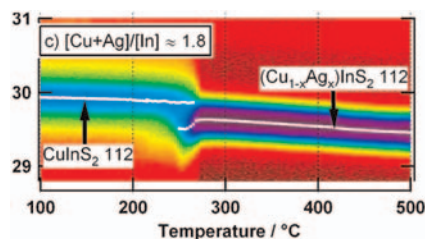


Excitation spectra monitoring the $^5\text{D}_0 \rightarrow ^7\text{F}_2$ transition with a dimer structure.

Recrystallization of Cu-poor CuInS_2 assisted by metallic Cu or Ag

Humberto Rodriguez-Alvarez, Roland Mainz, Bjoern Marsen and Hans-Werner Schock

Page 803

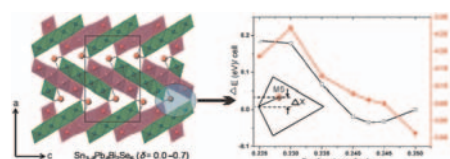


In-situ monitoring by means of energy-dispersive X-ray diffraction of the thin-film recrystallization of Cu-poor CuInS_2 assisted by metallic Ag.

Experimental and theoretical studies of $\text{Sn}_{3-\delta}\text{Pb}_\delta\text{Bi}_2\text{Se}_6$ ($\delta = 0.0-0.7$)

Kuei-Bo Chen and Chi-Shen Lee

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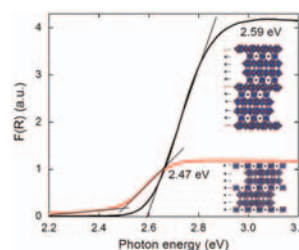


New ternary and quaternary chalcogenides, $\text{Sn}_{3-\delta}\text{Pb}_\delta\text{Bi}_2\text{Se}_6$ ($\delta = 0.0-0.7$), were synthesized and their structures are related to that of $\text{Pb}_3\text{Bi}_2\text{S}_6$ with an atomic position near the cell-twinning plane. Band structure calculations confirmed that the structure is stabilized when the position of the $M5$ site is farther from the cell-twinning plane. All compounds are n-type semiconductors with small band gaps.

Syntheses, optical properties and electronic structures of copper(I) tantalates: $\text{Cu}_5\text{Ta}_{11}\text{O}_{30}$ and $\text{Cu}_3\text{Ta}_7\text{O}_{19}$

Olena Palasyuk, Andriy Palasyuk and Paul A. Maggard

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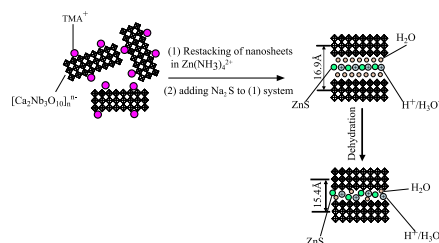


The copper(I) tantalates, $\text{Cu}_5\text{Ta}_{11}\text{O}_{30}$ and $\text{Cu}_3\text{Ta}_7\text{O}_{19}$, were synthesized by high-temperature solid-state reactions and by a new CuCl flux method, respectively. Their structures consist of single and double layers of TaO_7 pentagonal bipyramids separated by isolated TaO_6 octahedra and Cu atoms. UV-vis spectra show visible-light bandgap sizes of $\sim 2.5-2.6$ eV, which LMTO calculations show arise primarily from indirect transitions between the filled $\text{Cu } 3d^{10}$ and the empty $\text{Ta } 5d^0$ orbitals in the TaO_7 pentagonal bipyramids.

Structural and optical properties of ZnS/niobate composites synthesized by exfoliation/self-assembly processing

Yufeng Chen, Songhua Zhou, Xiaojing Yang and Yi Ou-Yang

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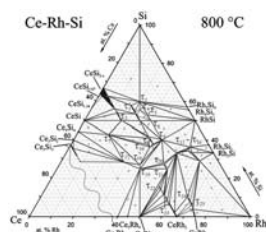


ZnS/niobate composites were first synthesized by exfoliation/self-assembly processing. The composites were characterized by X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), X-ray photoelectron spectroscopy (XPS), scanning electron microscope (SEM) and energy dispersive spectrometer (EDS), IR spectrum, UV-vis spectrum, and photoluminescence spectrum. The photoluminescence spectrum of the ZnS/niobate composite shows blue shift attributed to quantum sizes effects.

The ternary system cerium–rhodium–silicon

Alexey Lipatov, Alexander Gribanov, Andriy Grytsiv, Sergey Safronov, Peter Rogl, Julia Rousnyak, Yurii Seropegin and Gerald Giester

Page 829

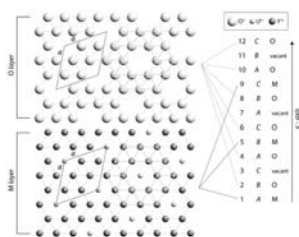


Phase relations in the ternary system Ce–Rh–Si have been established for the isothermal section at 800 °C based on X-ray powder and single-crystal diffraction, metallography, SEM and EMPA techniques on about 80 alloys. 25 ternary compounds were observed.

Order-to-disorder phase transformation in ion irradiated uranium-bearing delta-phase oxides $RE_6U_1O_{12}$ ($RE = Y, Gd, Ho, Yb, \text{ and } Lu$)

M. Tang, K.S. Holliday, C. Jiang, J.A. Valdez, B.P. Uberuaga, P.O. Dickerson, R.M. Dickerson, Y. Wang, K.R. Czerwinski and K.E. Sickafus

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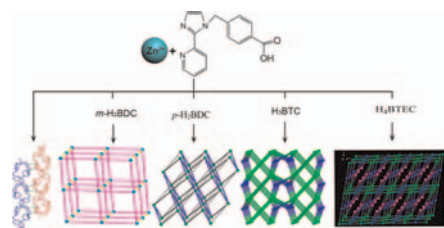


The different order-to-disorder (*O–D*) phase transformation tendencies in irradiated uranium-bearing δ -phase $RE_6U_1O_{12}$ compounds ($Y_6U_1O_{12}$, $Gd_6U_1O_{12}$, $Ho_6U_1O_{12}$, $Yb_6U_1O_{12}$, and $Lu_6U_1O_{12}$) are revealed by grazing incidence X-ray diffraction and transmission electron microscopy measurements, and theoretical simulations of the *O–D* transformation energies, performed using DFT, also support our experimental results.

Auxiliary aromatic-acid effect on the structures of a series of Zn^{II} coordination polymers: Syntheses, crystal structures, and photoluminescence properties

Yan-Hong Xu, Ya-Qian Lan, Kui-Zhan Shao, Zhong-Min Su and Yi Liao

Page 849

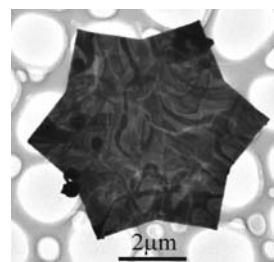


Five novel Zn^{II} -organic architectures have been hydrothermally synthesized through varying auxiliary aromatic-acid ligands and characterized by X-ray diffraction, the photoluminescence properties of compounds 1–5 were studied.

Formation of gold and silver nanostructures within polyvinylpyrrolidone (PVP) gel

Caixia Kan, Changshun Wang, Jiejun Zhu and Hongchen Li

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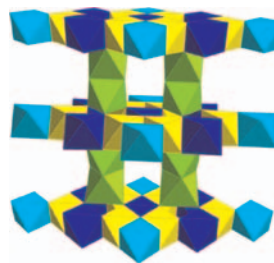


If a temperature difference was introduced to the gel of $Au^{3+}(H_2O)$ -PVP, large sized Au nanoplates with new and well-defined star shape were observed.

Verwey-type transition within the $Pb_3Rh_{7-x}Mn_xO_{15}$ solid solution

Alvin J. Gatimu, Hiroshi Mizoguchi, Arthur W. Sleight and M.A. Subramanian

Page 866

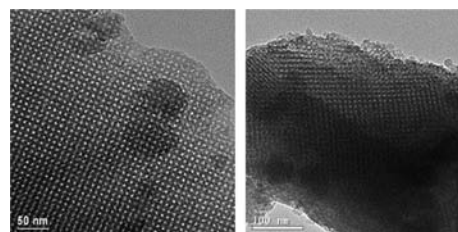


A complete solid solution is formed between isostructural $Pb_3Mn_7O_{15}$ and $Pb_3Rh_7O_{15}$. The effect of Mn substitution for Rh on the previously discovered Verwey-type transition in $Pb_3Rh_7O_{15}$ is described.

Hybrid materials of SBA-16 functionalized by rare earth (Eu^{3+} , Tb^{3+}) complexes of modified β -diketone (TTA and DBM): Covalently bonding assembly and photophysical properties

Yajuan Li, Bing Yan and Ying Li

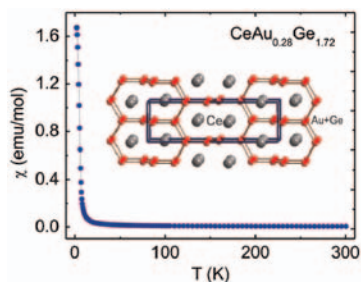
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Novel organic–inorganic mesoporous luminescent hybrids containing RE^{3+} complex covalently attached to the β -diketone-functionalized ordered mesoporous SBA-16, which were designated as $bpy-RE-TTA-S16$ and $bpy-RE-DBM-S16$, were obtained by sol-gel process.

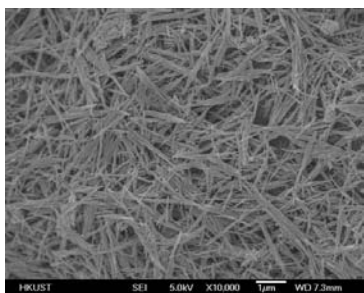
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Ferromagnetic ordering in ThSi₂ type CeAu_{0.28}Ge_{1.72}
 C. Peter Sebastian and Mercuri G. Kanatzidis
 Page 878



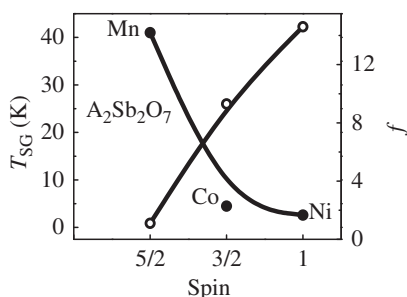
CeAu_{0.28}Ge_{1.72} crystallizes in the ThSi₂ structure type in the tetragonal space group *I*₄₁/*amd* and orders ferromagnetically at ~8 K.

Morphological and structural evolution of α-MnO₂ nanorods synthesized via an aqueous route through MnO₄⁻/Mn²⁺ reaction
 Xiaobo Fu, Jiyun Feng, Huan Wang and Ka Ming Ng
 Page 883



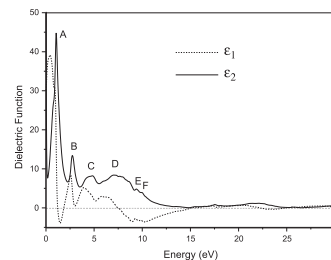
α-MnO₂ nanorods were synthesized via an aqueous route through MnO₄⁻/Mn²⁺ reaction under mild conditions.

Spin glass transitions in the absence of chemical disorder for the pyrochlores A₂Sb₂O₇ (A = Mn, Co, Ni)
 H.D. Zhou, C.R. Wiebe, J.A. Janik, B. Vogt, A. Harter, N.S. Dalal and J.S. Gardner
 Page 890



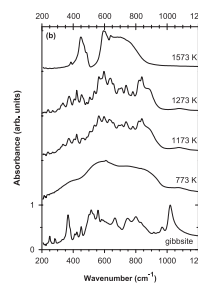
A comparison of the spin glass ordering temperature, *T*_{SG}, and the frustration index *f* as a function of the spin for the pyrochlore series A₂Sb₂O₇. In the limit of low spin, the frustration index increases by an order of magnitude.

Structural phase transition and 5*f*-electrons localization of PuSe explored by *ab initio* calculations
 Shouxin Cui, Wenxia Feng, Haiquan Hu, Zizheng Gong and Hong Liu
 Page 895



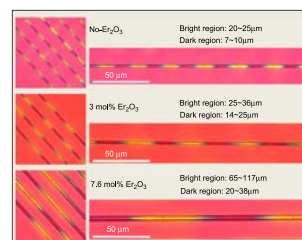
5*f*-electrons are more localized by the analysis of the density of states (SOC). The origin spectra peaks was interpreted based on electronic structures.

Experimental and *ab initio* infrared study of χ-, κ- and α-aluminas formed from gibbsite
 L. Favaro, A. Boumaza, P. Roy, J. Lédion, G. Sattonnay, J.B. Brubach, A.M. Huntz and R. Tétot
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Infrared spectra of the sequence Gibbsite → χ → κ → α-Al₂O₃ obtained from 24 h calcinations of Gibbsite at 773 K, 1173 K, 1273 K and 1573 K. All intensity maxima are normalized at 1.

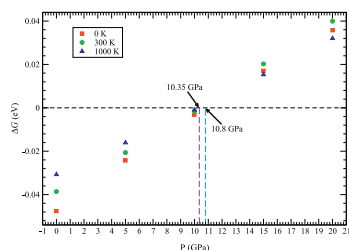
Origin of periodic domain structure in Er³⁺-doped β'-(Sm,Gd)₂(MoO₄)₃ crystal lines patterned by laser irradiations in glasses
 Futoshi Suzuki, Tsuyoshi Honma and Takayuki Komatsu
 Page 909



This figure shows the polarized optical photographs (top view) for the lines patterned by laser irradiations with the power of *P* = 1.3 W and the scanning speed of *S* = 5 μm/s in *x*Er₂O₃-(18.25-*x*)Gd₂O₃-3Sm₂O₃-63.75MoO₃-15B₂O₃ (mol%) glasses. This figure indicates that the periodicity of domain structures in β'-(Sm,Gd)₂(MoO₄)₃ crystal lines, i.e., the lengths of bright (high refractive index) and dark (low refractive index) color regions, changes depending on the amount of Er₂O₃ addition. It is demonstrated that the origin of the periodicity of domain structures is due to spontaneous strains in ferroelastic β'-(Sm,Gd)₂(MoO₄)₃ crystals.

Pressure induced structural phase transition of OsB₂: First-principles calculations

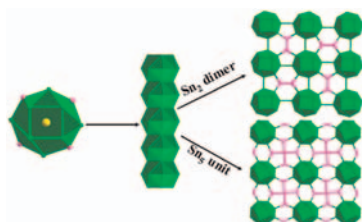
Fengzhu Ren, Yuanxu Wang and V.C. Lo
Page 915



Pressure induced structural phase transition from the orthorhombic structure to the hexagonal one for OsB₂ takes place under 10.8 GPa (0 K), 10.35 GPa (300, 1000 K) by the first-principles predictions.

Yb₅Ni₄Sn₁₀ and Yb₇Ni₄Sn₁₃: New polar intermetallics with 3D framework structures

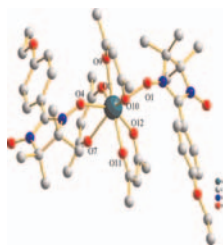
Xiao-Wu Lei, Zhong-Ming Sun, Long-Hua Li, Guo-Hua Zhong, Chun-Li Hu and Jiang-Gao Mao
Page 920



Two new ytterbium nickel stannides, namely, Yb₅Ni₄Sn₁₀ and Yb₇Ni₄Sn₁₃, have been synthesized and structurally characterized by single-crystal X-ray diffraction studies. Both their structures feature three-dimensional (3D) frameworks based on three different types of one-dimensional (1D) channels, which are situated by all the Yb atoms. Electronic structure calculations based on density functional theory (DFT) indicate that both compounds are metallic, which are in accordance with the results from temperature-dependent resistivity and magnetic susceptibility measurements.

Two tri-spin complexes based on gadolinium and nitronyl nitroxide radicals: Structure and ferromagnetic interactions

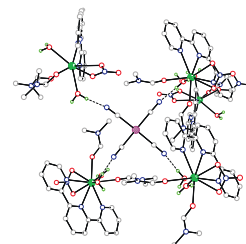
Na Zhou, Yue Ma, Chao Wang, Gong-Feng Xu, Jinkui Tang, Shi-Ping Yan and Dai-Zheng Liao
Page 927



Two tri-spin complexes based on gadolinium-radical have been synthesized and characterized, the magnetic studies show that in the two complexes the Gd-radical interaction is ferromagnetic and the radical-radical interaction is antiferromagnetic. An analogous complex containing the diamagnetic Lu^{III} ions has also been synthesized to further demonstrate the nature of the magnetic coupling between radicals.

Synthesis, structures, and photoluminescence properties of novel lanthanide tetracyanoplatinates lacking Pt-Pt interactions

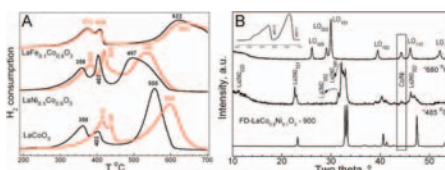
Milorad Stojanovic, Nicholas J. Robinson, Xi Chen, Philip A. Smith and Richard E. Sykora
Page 933



The synthesis of an isostructural series of lanthanide tetracyanoplatinates incorporating 2,2':6',2''-terpyridine are presented. Solid-state absorption and luminescence properties are discussed for the Eu³⁺ and La³⁺ compounds.

Crystal structure, microstructure and reducibility of LaNi_xCo_{1-x}O₃ and LaFe_xCo_{1-x}O₃ Perovskites (0 < x ≤ 0.5)

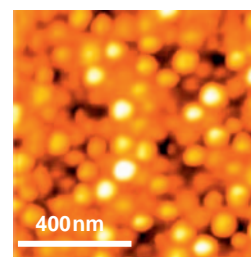
S. Ivanova, A. Senyshyn, E. Zhecheva, K. Tenchev, R. Stoyanova and H. Fues
Page 940



LaCo_{1-x}Ni_xO₃ and LaCo_{1-x}Fe_xO₃ with rhombohedrally distorted perovskite structure were obtained in the temperature range of 600–900 °C by thermal decomposition of freeze-dried La-Co/Ni(Fe)-citrate and by the Pechini method. The complete reduction of LaCo_{1-x}Ni_xO₃ with H₂ proceeds to Co/Ni-metal and La₂O₃, while the interaction of LaCo_{1-x}Fe_xO₃ with H₂ is not complete up to 700 °C. For LaCo_{1-x}Fe_xO₃, the reaction proceeds by preferential oxidation of Co³⁺ to Co²⁺ without affecting Fe³⁺ ions.

Magnetic properties of the Fe^{II} spin crossover complex in emulsion polymerization of trifluoroethylmethacrylate using poly(vinyl alcohol)

Atsushi Suzuki, Motoi Iguchi, Takeo Oku and Motoyasu Fujiwara
Page 951



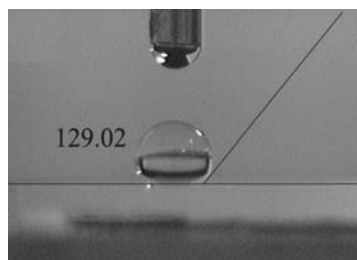
AFM surface image of the emulsion particles with the spin crossover complex.

Continued

Synthesis of hydrophobic zinc borate nanoflakes and its effect on flame retardant properties of polyethylene

Shengli Li, Beihong Long, Zichen Wang, Yumei Tian, Yunhui Zheng and Qian Zhang

Page 957

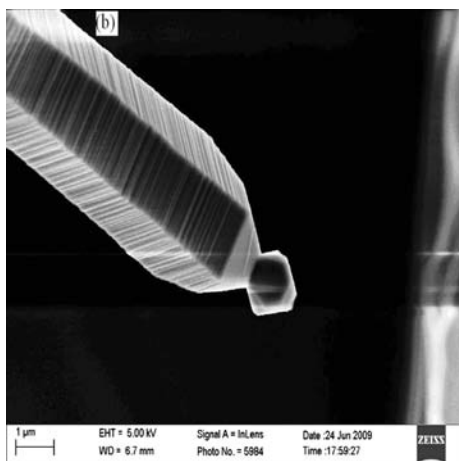


The contact angle of hydrophobic zinc borate nanoflakes is 129.02° with added 2.0 wt% of oleic acid.

Morphological development and oxidation mechanisms of aluminum nitride whiskers

Xin-mei Hou, Chang-sheng Yue, Ankit Kumar Singh, Mei Zhang and Kuo-Chih Chou

Page 963

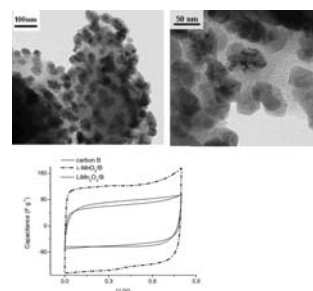


Hexagonal aluminum nitride (AlN) whiskers have been synthesized at 1873 K under a flowing nitrogen atmosphere. The synthesized whiskers are long straight filaments with diameters between 1 and 5 μm and length in the cm range.

Carbon/ λ -MnO₂ composites for supercapacitor electrodes

A. Malak-Polaczyk, C. Matei-Ghimbeu, C. Vix-Guterl and E. Frackowiak

Page 969



Comparison of capacitance characteristics for initial carbon and synthesised composites for CB in 1 mol L⁻¹ Na₂SO₄ solution.

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