



SOLID STATE CHEMISTRY

Editor

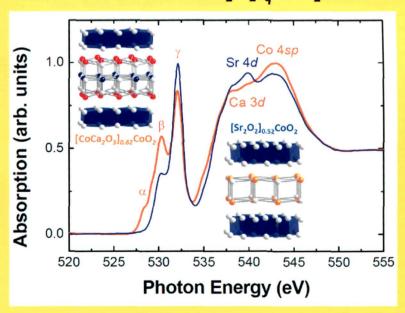
M.G. KANATZIDIS

Associate Editors

J. LI W. TREMEL S.J. CLARKE H.-C. ZUR LOYE

IN THIS ISSUE:

X-ray absorption spectroscopy study of parent misfit-layered cobalt oxide $[Sr_2O_2]_aCoO_2$



Ta-Lei Chou, Ting-Shan Chan, Jin-Ming Chen, Hisao Yamauchi and Maarit Karppinen

Available online at www.sciencedirect.com

SciVerse ScienceDirect



Volume 202, June 2013

JOURNAL OF SOLID STATE CHEMISTRY

CONTENTS

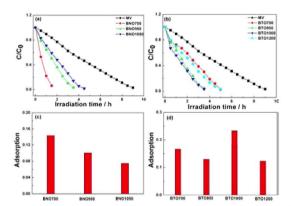
www.elsevier.com/locate/jssc

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

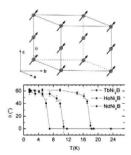
Preparation and visible-light photocatalytic properties of BiNbO₄ and BiTaO₄ by a citrate method

Hai-Fa Zhai, Ai-Dong Li, Ji-Zhou Kong, Xue-Fei Li, Jie Zhao, Bing-Lei Guo, Jiang Yin, Zhao-Sheng Li, Di Wu page 6



Photodegradation performance and adsorption ability of $BiNbO_4$ and $BiTaO_4$ powders, respectively. BNO700 with the best photocatalytic efficiency is ascribed to its large surface area and more positive conduction band level.

Magnetic structures in RNi₄B (R = Nd, Tb, Ho, Er) E. Alleno, C. Mazumdar page 15

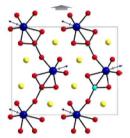


Simplified magnetic structure in NdNi₄B and full magnetic structure in RNi₄B (R = Tb, Ho). Variation with temperature of the easy magnetization axis direction (angle with c-axis) showing a spin re-orientation.

Regular Articles—Continued

Large scale synthesis, second-harmonic generation, and piezoelectric properties of a noncentrosymmetric vanadium phosphate, Li_2VPO_6

Eun Pyo Lee, Dong Woo Lee, Yoon-Ho Cho, T. Thao Tran, P. Shiv Halasyamani, Kang Min Ok *page 22*

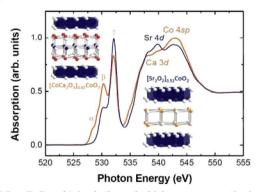


A net moment arising from the alignment of the distorted VO₆ octahedra is responsible for the SHG and piezoelectricity for the noncentrosymmetric vanadium phosphate, Li₂VPO₆.

X-ray absorption spectroscopy study of parent misfit-layered cobalt oxide [Sr₂O₂]₀CoO₂

Ta-Lei Chou, Ting-Shan Chan, Jin-Ming Chen, Hisao Yamauchi, Maarit Karppinen

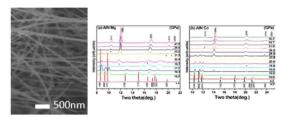
page 27



[Sr₂O₂]_{0.52}CoO₂ obtained through high-pressure synthesis is a parent of misfit-layered cobalt oxides, such as [CoCa₂O₃]_{0.62}CoO₂ or [$M_mA_2O_{2+m}$]_qCoO₂ in general. Our comprehensive X-ray absorption spectroscopy study shows that both [Sr₂O₂]_{0.52}CoO₂ and [CoCa₂O₃]_{0.62}CoO₂ possess mixed III/IV valence cobalt, but the average Co-valence is a little lower in the former. This is tentatively believed to be due to OH⁻ groups replacing part of O²⁻ ions in the [Sr₂O₂] layer block.

Pressure-induced structural phase transition in AlN:Mg and AlN:Co nanowires

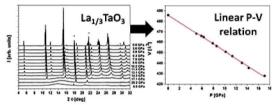
Yongsheng Xu, Hongyang Zhu, Chunli Ma, Pinwen Zhu, Ridong Cong, Xiaoxin Wu, Wei Gao, Qiliang Cui page 33



The high-pressure behaviors of AlN:Mg and AlN:Co nanowires have been investigated by *in situ* angle dispersive synchrotron X-ray diffraction.

Pressure-induced amorphization of La_{1/3}TaO₃

O. Noked, A. Melchior, R. Shuker, T. Livneh, R. Steininger, B.J. Kennedy, E. Sterer *page 38*

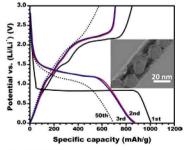


La_{1/3}Tao₃ exhibits linear pressure-volume relation until irreversible pressure induced amorphization at 18.5 Gpa.

Modification of carbon nanotubes by CuO-doped NiO nanocomposite foruse as an anode material for lithium-ion batteries

Syed Mustansar Abbas, Syed Tajammul Hussain, Saqib Ali, Nisar Ahmad, Nisar Ali, Saghir Abbas, Zulfiqar Ali

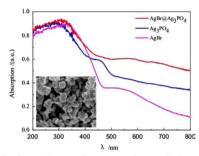
page 43



The porous CuNiO/CNT nanocomposite synthesized via a modified co-precipitation method in combination with subsequent-calcination was applied in the negative electrode materials for lithium-ion batteries and exhibited high electrochemical performance.

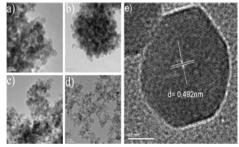
Novel visible-light AgBr/Ag₃PO₄ hybrids photocatalysts with surface plasma resonance effects

Yunfang Wang, Xiuli Li, Yawen Wang, Caimei Fan page 51



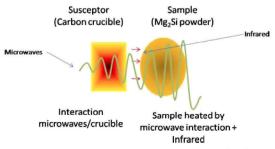
The optical absorption and structural morphology of the asprepared AgBr@Ag₃PO₄ photocatalyst using an anion-exchange precipitation method are conductive to the photocatalytic degradation of organics in water.

Effect of organic solvents on particle size of Mn₃O₄ nanoparticles synthesized by a solvothermal method Rui Song, Shouhua Feng, Hongjun Wang, Changmin Hou page 57



The comparison of the particle size of Mn_3O_4 nanoparticles synthesized using different solvents and HRTEM image of Mn_3O_4 individual nanoparticle revealed its single-crystal nature.

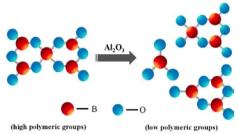
Microwaved assisted fast synthesis of n and p-doped Mg₂Si David Berthebaud, Franck Gascoin page 61



Schematic representation of microwave hybrid heating.

Relationship between $Eu^{3\,+}$ reduction and glass polymeric structure in Al_2O_3 -modified borate glasses under air atmosphere

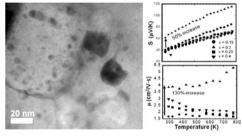
Qing Jiao, Xue Yu, Xuhui Xu, Dacheng Zhou, Jianbei Qiu page 65



A novel europium valence reduction phenomenon occurred in Al₂O₃ modified borate glasses, FTIR and Raman measurements revealed that high polymeric groups were destroyed to low polymery structures with Al₂O₃ addition.

Thermoelectric performance of nanostructured p-type $Zr_{0.5}Hf_{0.5}Co_{0.4}Rh_{0.6} Sb_{1-x}Sn_x$ half-Heusler alloys

Pramathesh Maji, Julien P.A. Makongo, Xiaoyuan Zhou, Hang Chi, Ctirad Uher, Pierre F.P. Poudeu page 70

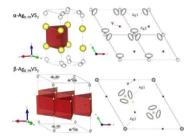


CoSb nanoinclusions embedded into a p-type $Zr_{0.5}Hf_{0.5}Co_{0.4}Rh_{0.6}$ $Sb_{1-x}Sn_x$ half-Heusler matrix simultaneously boost the thermopower and carrier mobility leading to a drastic enhancement of the power factor of the resulting bulk nanostructured materials.

Synthesis and characterization of two crystallographic forms of $Ag_{0.79}VS_2$

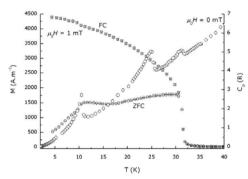
Mazhar N. Ali, Huiwen Ji, Daigorou Hirai, M.K. Fuccillo, R.J. Cava

page 77



Red = Vanadium, Gray = Silver, Yellow = Sulfur. Top left is α -Ag_{0.79}VS₂ in the 1s-InTaS₂ structure type. Top right: $2a \times 2b$ projection down the c-axis with displacement ellipsoids (50% probability) of atoms drawn to illustrate the split silver model. Bottom left is β -Ag_{0.79}VS₂ having the $a_o\sqrt{(3)}$ supercell. Bottom right: projection along the c-axis, displacement ellipsoids of atoms drawn.

On the synthesis, characterization and magnetic properties of two new phases discovered in the PbO-Fe₂O₃-P₂O₅ system Hassan El Hafid, Matias Velázquez, Olivier Pérez, Abdelaziz El Jazouli, Alain Pautrat, Rodolphe Decourt, Emmanuel Véron, Oudomsack Viraphong, Claude Delmas

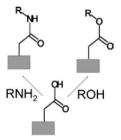


Three ferromagnetic-like phase transitions discovered in the new compound PbFe₃O(PO₄)₃ by specific heat and ZFC/FC magnetization measurements.

Synthesis and characterization of ester and amide derivatives of titanium(IV) carboxymethylphosphonate

Klára Melánová Ludvík Beneš, Miroslava Trchová, Jan Svoboda Vítězslav Zima

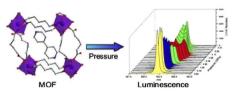
page 93



Ester and amide derivatives of layered titanium carboxymethylphosphonate were prepared by solvothermal treatment of amorphous solid with alkanol or alkylamine.

The influence of pressure on the photoluminescence properties of a terbium-adipate framework

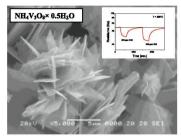
Elinor C. Spencer, Jing Zhao, Nancy L. Ross, Michael B. Andrews, Robert G. Surbella, Christopher L. Cahill *page 99*



The influence of pressure on the structure and photoluminescence emissions of a 3D terbium-adipate framework.

Behavior of sheet-like crystalline ammonium trivanadate hemihydrate (NH₄V₃O₈ × 0.5H₂O) as a novel ammonia sensing material

S.G. Leonardi, P. Primerano, N. Donato, G. Neri page 105

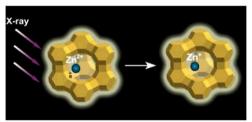


Sheet-like morphology of the synthesized trivanadate hemihydrate $(NH_4V_3O_8 \times 0.5H_2O)$. Inset: Its electrical response to different

ammonia concentrations in air.

Elucidation of the chemical environment for zinc species in an electron-rich zinc-incorporated zeolite

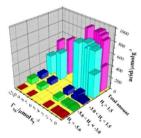
Jing-Feng Wang, Kai-Xue Wang, Jian-Qiang Wang, Lu Li, Yan-Mei Jiang, Xing-Xing Guo, Jie-Sheng Chen page 111



The chemical environment of the zinc species in an electorn-rich zeolite has been elucidated on the basis of X-ray absorption spectroscopy.

Dispersion states and acid properties of SiO₂-supported Nb2O5

Jie He, Qing-Jie Li, Yi-Ning Fan page 121

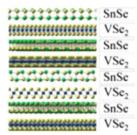


The acid amount and strength of Nb₂O₅/SiO₂ samples varied with the increase of Nb₂O₅ loading. The catalytic activities of the asprepared samples for the condensation and their acid properties were strongly affected by the dispersion states.

Synthesis, structure and electrical properties of a new tin vanadium selenide

Ryan Atkins, Sabrina Disch, Zachary Jones, Ines Haeusler, Corinna Grosse, Saskia F. Fischer, Wolfgang Neumann, Paul Zschack, David C. Johnson

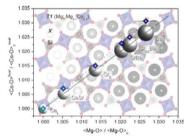
page 128



Turbostratically disordered (SnSe)_{1.15}VSe₂.

Next neighbors effect along the CaSrBa-åkermanite join: Long-range vs. short-range structural features

Michele Dondi, Matteo Ardit, Giuseppe Cruciani page 134

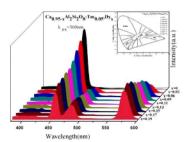


Average (MgO) vs. local (CoOlocal) tetrahedral bond distances in function of the average X cation radius in the (Ca,Sr,Ba)₂ $(Mg_{0.7}Co_{0.3})Si_2O_7$ join.

Single-phased CaAl₂Si₂O₈:Tm³⁺, Dy³⁺ white-light phosphors under ultraviolet excitation

Penghui Yang, Xue Yu, Xuhui Xu, Tingming Jiang, Hongling Yu, Dacheng Zhou, Zhengwen Yang, Zhiguo Song, Jianbei Qiu

page 143

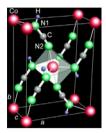


The results indicate the existence of energy transfer from ${\rm Tm}^{3+}$ to ${\rm Dy}^{3+}$. By tuning the concentration of ${\rm Dy}^{3+}$, single-phased white light can be realized.

The magnetic structure of $Co(NCNH)_2$ as determined by (spin-polarized) neutron diffraction

Philipp Jacobs, Andreas Houben, Anatoliy Senyshyn, Paul Müller, Richard Dronskowski

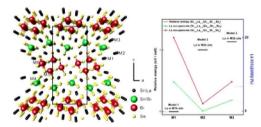
page 149



The magnetic ground state of $Co(NCNH)_2$ has been clarified by (spin-polarized) neutron diffraction data at low temperatures. Intensity changes below 4 K arise due to the onset of ferromagnetic ordering of the Co^{2+} spins parallel to the *c* axis, corroborated by various (magnetic) Rietveld refinements.

New quinternary selenides: Syntheses, characterizations, and electronic structure calculations

Ming-Yan Chung, Chi-Shen Lee page 154

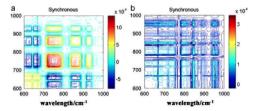


Quinternary selenides $Ae_{2.67}M_{0.33}Tt_{0.67}Pn_{2.33}Se_8$ (Ae, M, Tt, Pn = Sr/Ba, Y/La, Ge/Sn, Sb/Bi) were synthesized and their site preferences were characterized by single-crystal X-?ray diffraction and electronic structure calculation.

Two Keggin-type heteropolytung states with transition metal as a central atom: Crystal structure and magnetic study with 2D-IR correlation spectroscopy

Feng Chai, YiPing Chen, ZhuChai You, ZeMin Xia, SuZhi Ge, YanQiong Sun, BiHua Huang

page 161



The magnetic-dependent synchronous 2D correlation IR spectra of 1 (a), 2 (b) over 0–50 mT in the range of 600–1000 cm⁻¹, the obvious response indicate two Keggin polyanions skeleton susceptible to applied magnetic field.

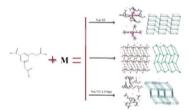
The "quiet Goldschmidt"—a mechanochemical, thermoanalytical, and spectroscopic study of selected steps of the aluminothermic reaction

R. Stößer, M. Feist, C. Willgeroth, F. Emmerling, M. Menzel, H. Reuther *page 173*



Six new coordination polymers constructed by 3-carboxyl-5-oxycarboxymethylpyridinio-1-carboxylate: Crystal structures, topologies, photoluminescent and magnetic properties

Hong-Yan Yuan, Min-Min Han, Xian-Rong Jiang, Zhan-Guo Jiang, Yun-Long Feng page 191

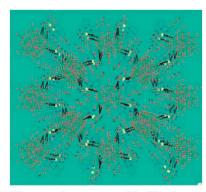


The structural differences show that the ligand, the metal center, and the reaction conditions have great influence on the structure of the final assembly.

A 3D POM-MOF composite based on Ni(II) ion and 2,2'-bipyridyl-3,3'-dicarboxylic acid: Crystal structure and proton conductivity

Meilin Wei, Xiaoxiang Wang, Jingjing Sun, Xianying Duan

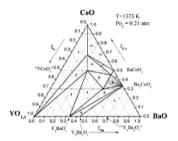
page 200



A POM–MOF composite constructed by Keggin-type polyanion, Ni $^{2+}$ and H₂bpdc shows good proton conductivities of $10^{-4}10^{-3}~\rm S~cm^{-1}$ at 100 °C under 3598% RH.

Phase equilibria, crystal structure and oxygen content of intermediate phases in the Y-Ba-Co-O system

A.S. Urusova, V.A. Cherepanov, T.V. Aksenova, L.Ya. Gavrilova, E.A. Kiselev *page 207*

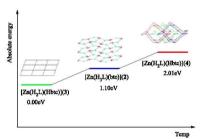


A projection of isobaric isothermal phase diagram of the Y-Ba-Co-O system to the metallic components triangle (T = 1373 K, $Po_2 = 0.21$ atm).

Synthesis and characterization of d^{10} metal complexes with mixed 1,3-di(1H-imidazol-4-yl)benzene and multicarboxylate ligands

Zhi-Hao Chen, Yue Zhao, Shui-Sheng Chen, Peng Wang, Wei-Yin Sun

page 215

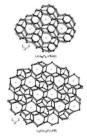


Seven new coordination polymers with multicarboxylate and rigid ditopic 4-imidazole containing ligands have been obtained and found to show different structures and topologies.

Ab initio investigations of the electronic structures and chemical bonding in LiCo₆P₄ and Li₂Co₁₂P₇

Samir F. Matar, Adel Al-Alam, Naïm Ouaini, Rainer Pöttgen

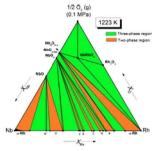
page 227



The cobalt-phosphorus networks in LiCo₆P₄ and Li₂Co₁₂P₇.

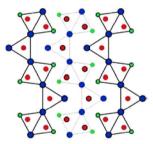
Phase chemistry of the system Nb-Rh-O

K.T. Jacob, Preeti Gupta, M. Vinay, Y. Waseda page 234



Isothermal section of ternary phase diagram for the system Nb–Rh–O at 1223 $\rm K.$

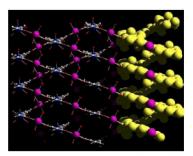
Ternary rare-earth ruthenium and iridium germanides $RE_3M_2Ge_3$ (RE=Y, Gd-Tm, Lu; M=Ru, Ir) Anton O. Oliynyk, Stanislav S. Stoyko, Arthur Mar page 241



 $RE_3M_2Ge_3$ (M = Ru, Ir) adopts the $Hf_3Ni_2Si_3$ -type structure containing slabs built up from Ge-centred trigonal prisms.

Structural variations and photoluminescent properties of a series of metal-organic frameworks constructed from 5-(4-carboxybenzoylamino)-isophthalic acid

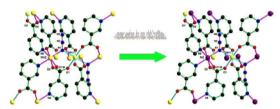
Wen Zhao, Li-Juan Zhang, Xiao-Li Zhao page 250



Solvothermal reactions of tricarboxylate ligand H_3L with Cd^{2+}/Ln^{3+} has yielded a series of new MOFs containing interesting structural motifs.

Novel heterometallic metal-azido complex synthesized by "one-step" reaction: synthetic strategy and magnetic properties

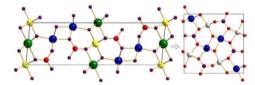
Yong-Kun Jiao, Xiu-Ping Li, Cui Zhao, Hai-Chao Wang, Min Xue, Jiong-Peng Zhao, Fu-Chen Liu page 257



A novel heterometallic 3D complex $[Ni_2Mn(N_3)_2(nic)_4 \cdot (H_2O)_2]_n$ (1) (nic = nicotinate) was synthesized by hydrothermal reaction. This complex exhibits interesting structural and magnetic properties

Crystal structures of two novel borate compounds $MgInBO_4$ and $MgIn_{7/8}D_{7/8}O_{29/8}$

H.K. Li, G.M. Cai, J.J. Fan, Z.P. Jin, T.T. Zhou, X.L. Chen page 262

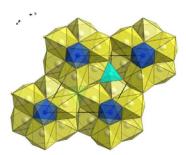


The structural transformation from the monoclinic $MgIn_{7/8}B_{7/8}$ $O_{29/8}$ $(P12_1/n1)$ to the orthorhombic $MgInBO_4$ (Pnma).

Ln₃FeGaQ₇: A new series of transition-metal rare-earth chalcogenides

Wenlong Yin, Wendong Wang, Lei Kang, Zheshuai Lin, Kai Feng, Youguo Shi, Wenyu Hao, Jiyong Yao, Yicheng Wu

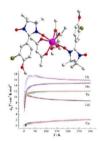
page 269



 Ln_3 FeGaQ $_7$ adopt a three-dimensional framework composed of LnQ_7 monocapped trigonal prisms with interesting ${}^1_\infty$ [FeS $_3$] $^{4-}$ chains and isolated GaQ $_4$ tetrahedra lying in two sets of channels in the framework.

Syntheses, crystal structures, magnetic and luminescence properties of five novel lanthanide complexes of nitronyl nitroxide radical

Ya-Li Wang, Yuan-Yuan Gao, Yue Ma, Qing-Lun Wang, Li-Cun Li, Dai-Zheng Liao page 276



Using a novel halogen phenyl-substituted nitronyl-nitroxide radical, we obtained and characterized five isostructural lanthanide mononuclear tri-spin compounds.

Role of dopants in LiF:Mg,Cu, LiF:Mg,P and LiF:Mg,Cu,P detectors

Kh. Mohammadi, A. Moussavi Zarandi, H. Afarideh, S. Shahmaleki

page 282

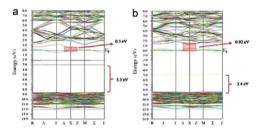
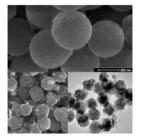


Figure (a) and (b) shows changes in electronic structure and band gap energy of LiF crystal due to presence of Mg and Cu, Mg and P ions respectively.

Carbonaceous spheres—an unusual template for solid metal oxide mesoscale spheres: Application to ZnO spheres Greta Patrinoiu, Jose Maria Calderón-Moreno, Daniela C.

Culita, Ruxandra Birjega, Ramona Ene, Oana Carp page 291

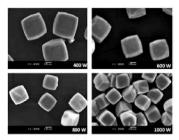


A novel and eco-friendly methodology for the synthesis of mesoscale solid ZnO spheres was developed. The protocol involves a double coating of the starch-derived carbonaceous spheres with successive layers of zinc-containing species by alternating a non-ultrasound and ultrasound-assisted deposition, followed by calcination treatments.

Synthesis and characterization of zinc borophosphates with ANA-zeotype framework by the microwave method

Yu Song, Ling Ding, Qingda An, Shangru Zhai, Xiaowei Song

page 300



Tailor-made ANA zeolites with varied size can be prepared by simply changing the reaction power.

Synthesis of flower-like Boehmite (γ -AlOOH) via a one-step ionic liquid-assisted hydrothermal route

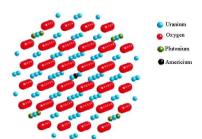
Zhe Tang, Jilei Liang, Xuehui Li, Jingfeng Li, Yunqi Liu, Chenguang Liu

page 305



The flower-like $\gamma\text{-AlOOH}$ architectures composed by nanosheets with narrow size distribution (1.6–2.2 $\mu m)$ and uniform pore size (6.92 nm) have been synthesized via a one-step ionic liquid-assisted hydrothermal route.

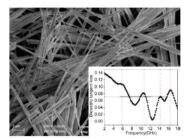
Americium characterization by X-ray fluorescence and absorption spectroscopy in plutonium uranium mixed oxide Claude Degueldre, Cedric Cozzo, Matthias Martin, Daniel Grolimund, Cyprian Mieszczynski page 315



Americium $L_{\rm III}$ XAFS spectra recorded for the irradiated MOX sub-sample in the rim zone for a 300 $\mu m \times$ 300 μm beam size area investigated over six scans of 4 h. The records remain constant during multi-scan. The analysis of the XAFS signal shows that Am is found as trivalent in the UO $_2$ matrix. This analytical work shall open the door of very challenging analysis (speciation of fission product and actinides) in irradiated nuclear fuels.

Multiple nonlinear dielectric resonance of ultra-long silver trimolybdate nanowires

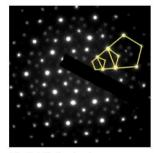
Guang-Sheng Wang, Bo Wen, Shuai He, Lin Guo and Mao-Sheng Cao page 320



The untralong silver trimolybdate nanowires were synthesized and the dielectric peoperties of the products were studied from 2 to 18 GHz. The as-established equivalent circuit model of the silver molybdate nanowires were employed to explain the nonlinear dielectric resonant behavior.

Rapid Communications

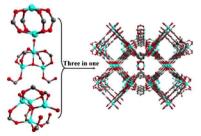
Icosahedral quasicrystalline $(Ti_{1.6}V_{0.4}Ni)_{100-x}Sc_x$ alloys: Synthesis, structure and their application in Ni-MH batteries Wen Hu, Jianhong Yi, Biju Zheng, Limin Wang page I



Quasicrystalline Ti–V–Ni–Sc hydrogen storage materials: Sc addition into Ti_{1.6}V_{0.4}Ni alloy forms the icosahedral phase (see picture). With optimal Sc dosage, the anodic cycling stability and self-discharge property are greatly enhanced.

A new zinc-1,3,5-benzenetricarboxylate framework integrated three distinct subunits (SBUs)

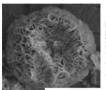
Yi-Ming Xie page 116

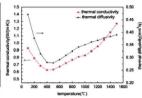


Presented here is a new zinc-1,3,5-benzenetricarboxylate framework integrated three distinct subunits (SBUs).

Synthesis of multi-hierarchical structured yttria-stabilized zirconia powders and their enhanced thermophysical properties

Fengmei Cao, Yanfeng Gao, Hongfei Chen, Xinling Liu, Xiaoping Tang, Hongjie Luo page 168





There are many tiny pores and grain boundaries in the multihierarchical structured yttria-stabilized zirconia (YSZ) powders, which greatly decrease the thermal conductivities of the YSZ powders.

Language services. Authors who require information about language editing and copyediting services pre- and post-submission please visit http://www.elsevier.com/locate/languagepolishing or our customer support site at http://epsupport.elsevier.com. Please note Elsevier neither endorses nor takes responsibility for any products, goods or services offered by outside vendors through our services or in any advertising. For more information please refer to our Terms & Conditions http://www.elsevier.com/termsandconditions

For a full and complete Guide for Authors, please go to: http://www.elsevier.com/locate/jssc

Journal of Solid State Chemistry has no page charges.