

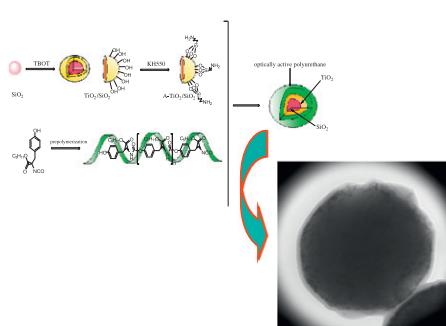
## CONTENTS

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**Regular Articles**
**Preparation, characterization, and infrared emissivity property of optically active polyurethane/TiO<sub>2</sub>/SiO<sub>2</sub> multilayered microspheres**

Yong Yang, Yuming Zhou, Jianhua Ge, Yongjuan Wang and Yunxia Zhu

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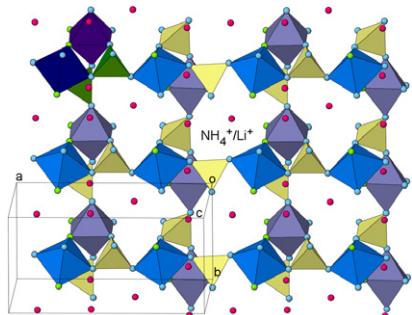


Optically active polyurethane/titania/silica (LPU/TiO<sub>2</sub>/SiO<sub>2</sub>) multilayered core-shell composite microspheres were prepared by the combination of titania deposition on the surface of silica spheres and subsequent polymer grafting.

**Mild hydrothermal synthesis, crystal structure, thermal behaviour, spectroscopic and magnetic properties of (NH<sub>4</sub>)<sub>0.80</sub>Li<sub>0.20</sub>[Fe(AsO<sub>4</sub>)F]**

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

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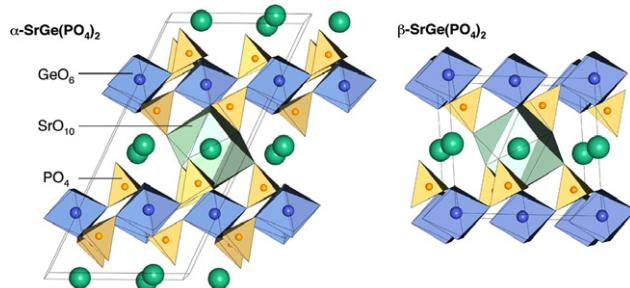


Three-dimensional structure of (NH<sub>4</sub>)<sub>0.80</sub>Li<sub>0.20</sub>[Fe(AsO<sub>4</sub>)F], a fluoroarsenate containing lithium and ammonium in the structural cavities.

**Regular Articles—Continued**
***M*<sup>II</sup>Ge(PO<sub>4</sub>)<sub>2</sub> (*M*=Ca, Sr, Ba): Crystal structure, phase transitions and thermal expansion**

Karin Popa, Gilles Wallez, Damien Bregiroux and Pascal Loiseau

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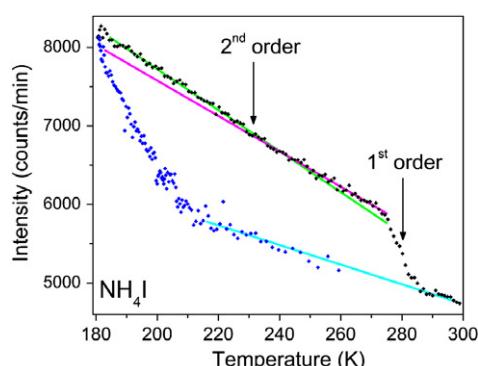


The superstructure of SrGe(PO<sub>4</sub>)<sub>2</sub> at room temperature () results from the off-centering of cation Sr<sup>II</sup>.

**Detection of dynamical transitions in hydrogenous materials using transmission measurements with very cold neutrons**

Nina Verdal, Terrence J. Udovic, John R.D. Copley and John J. Rush

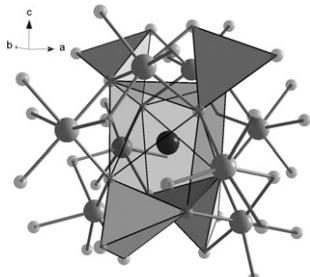
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The transmission of very long wavelength neutrons is a highly sensitive probe of dynamical transitions in hydrogenous materials.

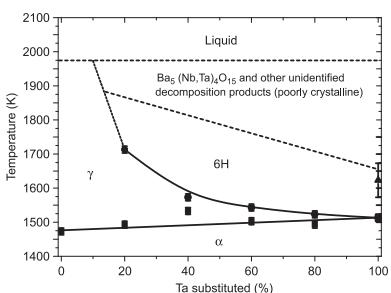
*Continued*

**New phases in the system  $\text{LiMnVO}_4$ – $\text{Mn}_3(\text{VO}_4)_2$**   
 Oliver Clemens, Robert Haberkorn and  
 Horst Philipp Beck  
 page 2640



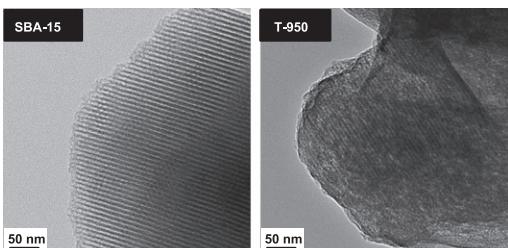
The unusual coordination of Mn in the form of a stella quadrangula with the surrounding vanadate groups.

**Phase diagram, chemical stability and physical properties of the solid-solution  $\text{Ba}_4\text{Nb}_{2-x}\text{Ta}_x\text{O}_9$**   
 Matthew T. Dunstan, Peter D. Sounthon, Cameron J. Kepert, James Hester, Justin A. Kimpton and Chris D. Ling  
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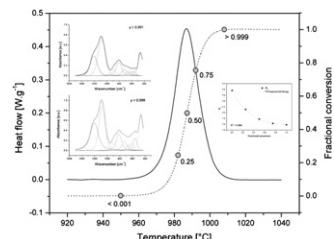
Thermodynamic phase diagram of  $\text{Ba}_4\text{Nb}_{2-x}\text{Ta}_x\text{O}_9$ .

**Preparation and characterization of ordered porous carbons for increasing hydrogen storage behaviors**  
 Seul-Yi Lee and Soo-Jin Park  
 page 2655



It is described that the considerable long-range ordering and the presence of mono-dimensional aligned channels between the two aligned nanorods of the porous framework from the SBA-15 was retained in the T-950 sample during the carbonization process.

**Mid-infrared spectroscopic study of crystallization of cubic spinel phase from metakaolin**  
 Petr Ptáček, František Šoukal, Tomáš Opravil, Magdaléna Nosková, Jaromír Havlica and Jiří Brandstetr  
 page 2661

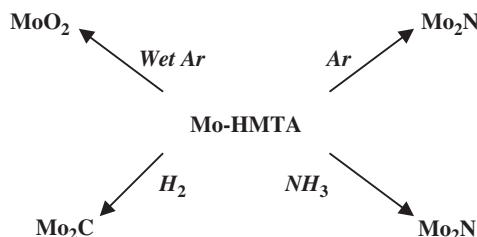


The thermal conversion of metakaolinite into spinel phase was investigated by mid-infrared spectroscopy to found relationship between bands features and fractional conversion.

**Decomposition of molybdate–hexamethylenetetramine complex: One single source route for different catalytic materials**

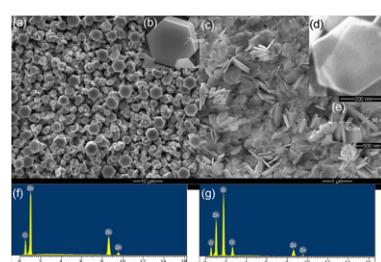
Sandra Chouzier, Tivadar Czeri, Magalie Roy-Auberger, Christophe Pichon, Christophe Geantet, Michel Vrinat and Pavel Afanasiev

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Depending on the conditions, decomposition of molybdate–HMTA complex yields highly dispersed molybdenum nitride, carbide or oxide.

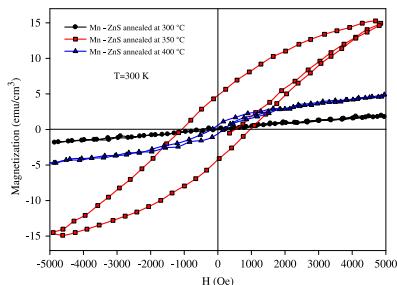
**Growth and characterization of Cl-doped ZnO hexagonal nanodisks**  
 Ramin Yousefi, A.K. Zak and M.R. Mahmoudian  
 page 2678



Cl-doped ZnO nanodisks and undoped ZnO microdisks have been grown using a thermal evaporation method.

## The influence of diffusion temperature on the structural, optical and magnetic properties of manganese-doped zinc oxysulfide thin films

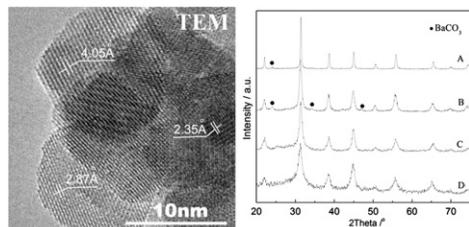
İ. Polat, S. Aksu, M. Altunbaş, S. Yılmaz and E. Bacaksız  
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*M–H* variation of Mn diffusion-doped Zn(O,S) thin films measured at 300 K.

## Grain size modulation on BaTiO<sub>3</sub> nanoparticles synthesized at room temperature

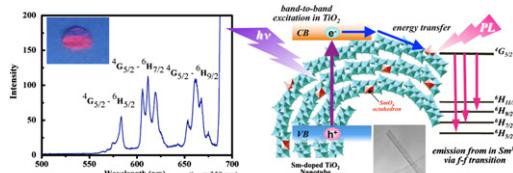
Jian Quan Qi, Li Sun, Xi Wei Qi, Yu Wang and Helen Lai Wah Chan  
page 2690



This paper offers a direct facile approach to BaTiO<sub>3</sub> nanoparticles at room temperature with a large quantity. The grain size can be modulated purposefully.

## Photoluminescence of samarium-doped TiO<sub>2</sub> nanotubes

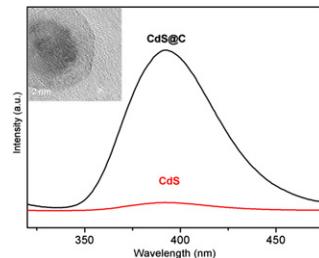
Dong Jin Park, Tohru Sekino, Satoshi Tsukuda, Asuka Hayashi, Takafumi Kusunose and Shun-Ichiro Tanaka  
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Samarium-doped TiO<sub>2</sub> nanotubes (TNTs) having a nanotubular structure were synthesized by soft chemical route. It was revealed that the energy associated by the band-to-band excitation of TNT matrix transferred to the doped Sm<sup>3+</sup> ions in the lattice, resulting in emission of strong and visible red fluorescence.

## An improved pyrolysis route to synthesize carbon-coated CdS quantum dots with fluorescence enhancement effect

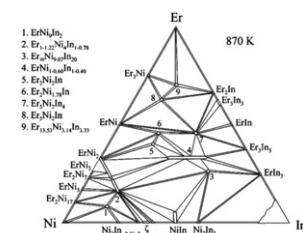
Kejie Zhang and Xiaoheng Liu  
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We demonstrated a facile approach to synthesize well-dispersed carbon-coated CdS quantum dots. The as-prepared nanoparticles presented remarkable fluorescence enhancement effect.

## Ternary system Er–Ni–In at *T* = 870 K

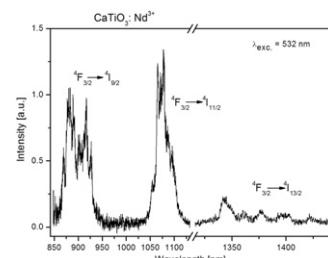
M. Dzevenko, Yu. Tyvanchuk, L. Bratash, V. Zaremba, L. Havela and Ya. Kalychak  
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Phase relations in the ternary system Er–Ni–In have been established for the isothermal section at *T* = 870 K based on X-ray phase and EDX-analyses. Nine ternary compounds were observed.

## Spectroscopic properties of Nd<sup>3+</sup> ions in nano-perovskite CaTiO<sub>3</sub>

K. Lemański, A. Gągor, M. Kurnatowska, R. Pązik and P.J. Dereń  
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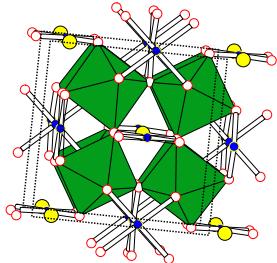
The 300 K emission spectrum of CaTiO<sub>3</sub>: 1% Nd<sup>3+</sup> annealed at 700 °C and measured at 300 K on InGaAs detector.

*Continued*

## Synthesis and microstructural TEM investigation of $\text{CaCu}_3\text{Ru}_4\text{O}_{12}$ ceramic and thin film

Virginie Brizé, Cécile Autret-Lambert, Jérôme Wolfman, Monique Gervais and François Gervais

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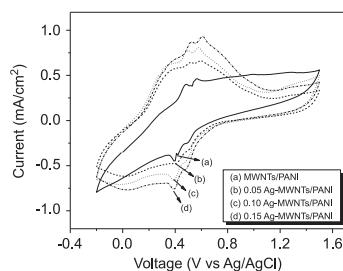


Structure of  $\text{CaCu}_3\text{Ru}_4\text{O}_{12}$  showing the  $\text{RuO}_6$  octahedra and the square planar environment for  $\text{Cu}^{2+}$ .

## Influence of silver-decorated multi-walled carbon nanotubes on electrochemical performance of polyaniline-based electrodes

Ki-Seok Kim and Soo-Jin Park

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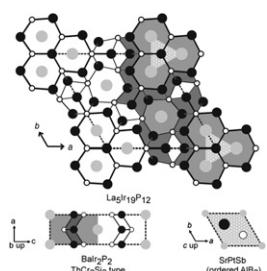


The current density of MWNTs/PANI increased with increasing the Ag concentration due to the bridge effect of Ag nanoparticles incorporated between MWNTs and PANI.

## Metal-rich phosphides $RE_5\text{Ir}_{19}\text{P}_{12}$ with $\text{Sc}_5\text{Co}_{19}\text{P}_{12}$ type structure

Ulrike Pfannenschmidt, Ute Ch. Rodewald, Rolf-Dieter Hoffmann and Rainer Pöttgen

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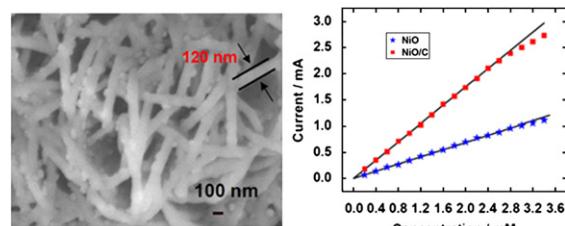


The intergrowth structure  $\text{La}_5\text{Ir}_{19}\text{P}_{12}$ .

## Preparation of nickel oxide and carbon nanosheet array and its application in glucose sensing

Xin Li, Anzheng Hu, Jian Jiang, Ruimin Ding, Jinping Liu and Xintang Huang

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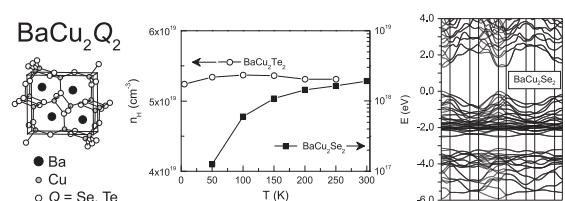


The thickness of nanosheets is about 90–120 nm. They are decorated with small particles. In glucose sensing, NiO and carbon composite exhibits higher response current than pure NiO.

## Transport and optical properties of heavily hole-doped semiconductors $\text{BaCu}_2\text{Se}_2$ and $\text{BaCu}_2\text{Te}_2$

Michael A. McGuire, Andrew F. May, David J. Singh, Mao-Hua Du and Gerald E. Jellison

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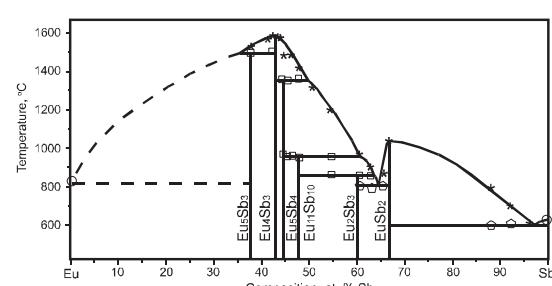


Combined experimental and theoretical study of orthorhombic  $\text{BaCu}_2\text{Se}_2$  and  $\text{BaCu}_2\text{Te}_2$  to assess potential for photovoltaic and thermoelectric applications.

## Phase equilibrium and intermediate phases in the Eu–Sb system

M.N. Abdusalyamova and I.G. Vasilyeva

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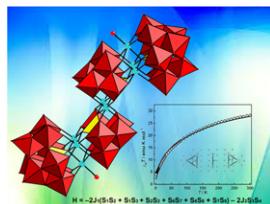


The high-temperature range of the  $T$ – $x$  phase diagram for the Eu–Sb system.

**Synthesis, structure and magnetism of a S-shaped multi-iron substituted arsenotungstate containing a trivacant Keggin  $[B-\alpha\text{-As}^{\text{V}}\text{W}_9\text{O}_{34}]^{9-}$  and a hexavacant Keggin  $[\alpha\text{-As}^{\text{V}}\text{W}_6\text{O}_{26}]^{11-}$  fragments**

Junwei Zhao, Qiuxia Han, Dongying Shi, Lijuan Chen, Pengtao Ma, Jingping Wang and Jingyang Niu

page 2756

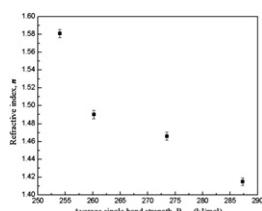


S-shaped multi-iron substituted arsenotungstate consisting of two asymmetric sandwich-type subunits has been hydrothermally synthesized and structurally characterized. Its magnetic properties have been investigated.

**Role of oxygen on the optical properties of borate glass doped with  $\text{ZnO}$**

Manal Abdel-Baki and Fouad El-Diasty

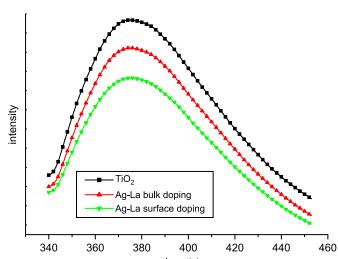
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$\text{O}1s$ , Yamashita-Kurosawa's parameter and average single bond strength of charge overlapping between electronic shells are used to explain enhanced oxide ion  $2p$  electron density, which increases refractive index of glasses.

**Microstructures and photocatalytic properties of  $\text{Ag}^+$  and  $\text{La}^{3+}$  surface codoped  $\text{TiO}_2$  films prepared by sol-gel method**

Nan Zhao, Ming-ming Yao, Fang Li and Fei-peng Lou  
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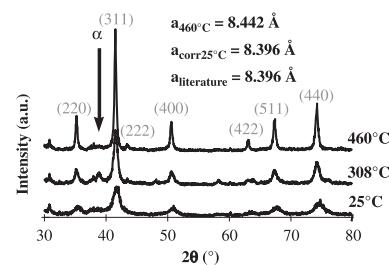


The PL intensity of  $\text{Ag}^+$  and  $\text{La}^{3+}$  surface codoped  $\text{TiO}_2$  was the lowest among all samples, indicating the recombination of electron and hole was effectively prohibited compared with pure  $\text{TiO}_2$ ,  $\text{Ag}^+$  and  $\text{La}^{3+}$  bulk codoped  $\text{TiO}_2$ .

**Oxygen stoichiometry control of nanometric oxide compounds: The case of titanium ferrites**

N. Millot and P. Perriat

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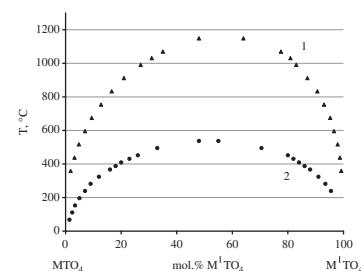


XRD patterns of  $\text{Fe}_{3(1-\delta)}\text{O}_4$  nanometric powders obtained *in situ* during a reducing treatment. The stoichiometric compound was obtained by a thermal annealing at  $460\text{ }^\circ\text{C}$  under  $p\text{O}_2 = 3 \times 10^{-26}\text{ Pa}$  ( $\Phi_{\text{DRX}} = 100\text{ nm}$ ). In inset, data of the experimental lattice parameter compared to the theoretical one.  $\alpha$  represents the rhomboedrical phase which precipitates during this thermal treatment, then disappeared.

**Analysis of solid solutions stability in scheelite-type molybdates and tungstates**

V.D. Zhuravlev, O.G. Reznitskikh, Yu.A. Velikodnyi, T.A. Patrusheva and O.V. Sivtsova

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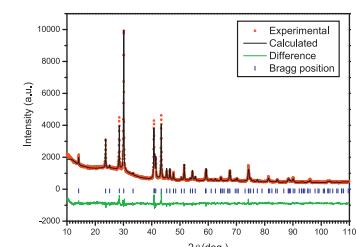


Calculated boundaries of solid solutions in  $\text{BaWO}_4\text{-CaWO}_4$  (1) and  $\text{PbMoO}_4\text{-CaMoO}_4$  (2) systems.

**Superstructure and stacking faults in hydrothermal-grown  $\text{KBe}_2\text{BO}_3\text{F}_2$  crystals**

Jinqui Yu, Lijuan Liu, Shifeng Jin, Haitao Zhou, Xiaoling He, Changlong Zhang, Weining Zhou, Xiaoyang Wang, Xiaolong Chen and Chuangtian Chen

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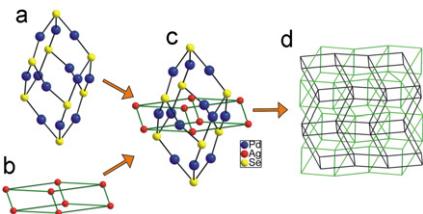


A new structure of the  $\bar{R}\bar{3}c$  space group with cell parameters of  $a = 4.422(1)\text{ \AA}$  and  $c = 37.524(3)\text{ \AA}$  was obtained from hydrothermal-grown  $\text{KBe}_2\text{BO}_3\text{F}_2$  crystals by powder XRD and Rietveld refinement.

*Continued*

## Crystal and electronic structure study of AgPd<sub>3</sub>Se

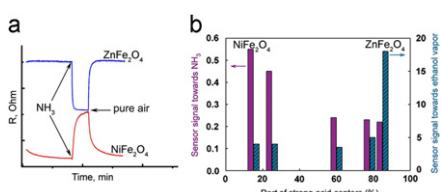
F. Laufek, A. Vymazalová, D.A. Chareev, A.V. Kristavchuk, Q. Lin, J. Drahokoupil and T.M. Vasilchikova  
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(a) Prolate rhombohedron formed by Pd and Se atoms, (b) oblate rhombohedron formed by Ag atoms and (c) their interpenetration at unit cell level. (d) 3D network of prolate and oblate rhombohedra.

## Nanocrystalline ferrites Ni<sub>x</sub>Zn<sub>1-x</sub>Fe<sub>2</sub>O<sub>4</sub>: Influence of cation distribution on acidic and gas sensing properties

A.P. Kazin, M.N. Rumyantseva, V.E. Prusakov, I.P. Suzdalev and A.M. Gaskov  
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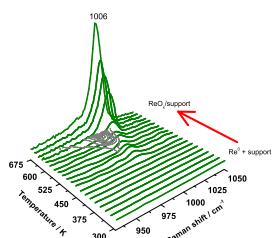


(a) *n*- and *p*-types change in electrical resistance and (b) sensor signal of Ni<sub>x</sub>Zn<sub>1-x</sub>Fe<sub>2</sub>O<sub>4</sub> towards NH<sub>3</sub> and ethanol vapor *vs.* the part of strong acid sites.

## Supported oxorhenate catalysts prepared by thermal spreading of metal Re<sup>0</sup> for methanol conversion to methylal

Xavier Sécordel, Anthony Yoboué, Sylvain Cristol, Christine Lancelot, Mickaël Capron, Jean-François Paul and Elise Berrier

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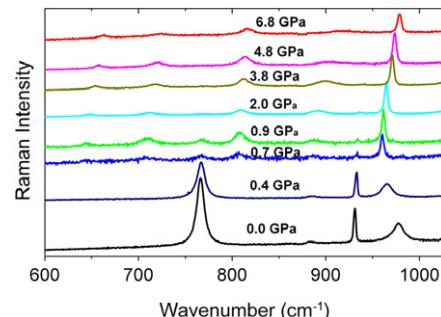


Evolution of the 900–1000 cm<sup>-1</sup> region of the Raman spectrum of a mixture of metal rhenium with anatase TiO<sub>2</sub> K03 upon heating in pure O<sub>2</sub>.

## Pressure-induced phase transitions in multiferroic

RbFe(MoO<sub>4</sub>)<sub>2</sub>—Raman scattering study

M. Mączka, M. Ptak, C. Luz-Lima, P.T.C. Freire, W. Paraguassu, S. Guerini and J. Hanuza  
page 2812

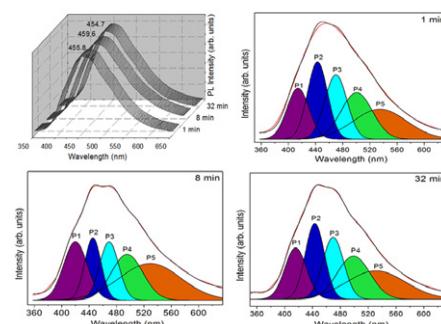


Raman spectra of RbFe(MoO<sub>4</sub>)<sub>2</sub> crystal in the high wavenumber region recorded at different pressures during compression experiment.

## Formation of $\beta$ -nickel hydroxide plate-like structures under mild conditions and their optical properties

A.P. de Moura, R.C. Lima, E.C. Paris, M.S. Li, J.A. Varela and E. Longo

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Nanostructural  $\beta$ -Ni(OH)<sub>2</sub> crystalline powders were prepared by rapid microwave-hydrothermal method for 1, 8 and 32 min. The hexagonal-shaped nanoplates obtained presented PL emission in the blue-green region and each decomposed component represents a different type of electronic transition, which can be linked to the structural arrangement or surface defects.

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