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Regular Articles

Biomimetic synthesis of aragonite superstructures using hexamethylenetetramine

Long Chen, Fangzhi Huang, Shikuo Li, Yuhua Shen, Anjian Xie, Jian Pan, Yaping Zhang and Yan Cai





The well-defined aragonite hierarchical superstructures are formed using hexamethylenetetramine in aqueous solution.

Phase stability of some actinides with brannerite structure at high pressures

F.X. Zhang, M. Lang, Zhenxian Liu and R.C. Ewing *page 2834*



Actinide-bearing compounds with brannerite structure and their analog CeTi₂O₆ are not stable at high pressure. They were amorphized after ${\sim}20$ GPa and a minor pressure-induced phase transition or decomposition process was always observed before amorphization.

Regular Articles—Continued

The system Ce–Zn–B at 800 °C

Z. Malik, O. Sologub, G. Giester and P. Rogl page 2840



Existence of low temperature modification αCeZn_7 (Ce_{1-x}Zn_{5+2x}; $x \sim 0.33$) of Ce₂Zn₁₇ has been verified up to 750 °C that is attributed with the TbCu₇ type.

Synthesis, crystal structure and optical properties of the new lead fluoride borate—Pb₂BO₃F

Wenwu Zhao, Shilie Pan, Jian Han, Jiyong Yao, Yun Yang, Junjie Li, Min Zhang, Lian Han Zhang and Yin Hang

page 2849



The Pb atoms are in the five coordination environments bonded to three O atoms and two F atoms to make up the distortional PbO_3F_2 polyhedra. Every six PbO_3F_2 polyhedra are connected by one F(1) atom to form the symmetrical structure, and then the distortion of the PbO_3F_2 polyhedra is offset.

Thermal expansion in 3*d*-metal Prussian Blue Analogs—A survey study

Sourav Adak, Luke L. Daemen, Monika Hartl,

Darrick Williams, Jennifer Summerhill and Heinz Nakotte page 2854



The structure of Prussian Blue analogs (PBAs) consists of two types of metal centered octahedral units connected by cyanide ligand. Lattice and interstitial water molecules are present in these framework structures. All the PBAs of the M_3 [Co(CN)₆]₂ · nH₂O family show negative thermal expansion (NTE) behavior. The lattice parameters and magnitude of NTE correlates inversely with the Irving–Williams series of metal complex stability.

Layered double hydroxide/polyethylene terephthalate nanocomposites. Influence of the intercalated LDH anion and the type of polymerization heating method

M. Herrero, S. Martínez-Gallegos, F.M. Labajos and V. Rives

page 2862



Conventional and microwave heating routes were used to prepare PET–LDH (polyethylene terephthalate–layered double hydroxide) composites with 1–10 wt% LDH by *in situ* polymerization. To enhance the compatibility between PET and the LDH, terephthalate or dodecyl sulphate was previously intercalated into the LDH. The microwave process improves the dispersion and the thermal stability of nanocomposites due to the interaction of the microwave radiation and the dipolar properties of EG and the homogeneous heating.

Synthesis and characterization of the $La_{1-x}Sr_xFeO_{3-\delta}$ system and the fluorinated phases $La_{1-x}Sr_xFeO_{3-x}F_x$ Oliver Clemens, Melanie Kuhn and Robert Haberkorn *page 2870*



The crystal structures of the perovskites $La_{1-x}Sr_xFeO_{3-x}F_x$ for x=0.8 (a), 0.5 (b) and 0.1 (c).

Original electrochemical mechanisms of CaSnO₃ and CaSnSiO₅ as anode materials for Li-ion batteries M. Mouvane, M. Womes, J.C. Jumas, J. Olivier-Fourcade

and P.E. Lippens page 2877



¹¹⁹Sn Mössbauer spectra at the end of the first discharge of CaSnO₃ (dashed line) and CaSnSiO₅ (solid line) anodes for Li-ion batteries. Inset shows that relative amounts of Sn(0) based alloys formed during the first discharge are similar for CaSnO₃ and CaSnSiO₅ pristine materials.

Thick lanthanum zirconate buffer layers from water-based precursor solutions on Ni-5%W substrates

Vyshnavi Narayanan, Petra Lommens, Klaartje De Buysser, Ruben Hühne and Isabel Van Driessche *page 2887*



Thick LZO buffer layers from water-based precursor solutions were synthesized and their crystallinity, microstructure and buffer layer action were studied. The buffer layer action of the LZO layer was substantial to restrict the Ni penetration within 30 nm of a 140 nm thick film.

Synthesis, structural and electrical characterizations of $DySr_5Ni_{2,4}Cu_{0,6}O_{12-\delta}$

S. Hamdi, S. Ouni, H. Chaker, J. Rohlicek and R. Ben Hassen

page 2897



 $DySr_5Ni_{2.4}Cu_{0.6}O_{12-\delta}$ exhibits a semi-conducting behaviour over the whole temperature range 294–579 K with a conductivity maximum of 0.4 S cm⁻¹ at 510 K.

Synthetic approaches to borocarbonitrides, BC_xN (x = 1-2) Nitesh Kumar, Kalyan Raidongia, Abhishek K. Mishra, Umesh V. Waghmare, A. Sundaresan and C.N.R. Rao *page 2902*



Vapor phase synthesis of BC_xN (x = 1-2) by the reaction of BBr₃, ethylene and ammonia leads to the formation of pan-like structure.

A general solution-chemistry route to the synthesis $LiMPO_4$ (M = Mn, Fe, and Co) nanocrystals with [010] orientation for lithium ion batteries

Jing Su, Bing-Qing Wei, Jie-Peng Rong, Wen-Yan Yin, Zhi-Xia Ye, Xian-Qing Tian, Ling Ren, Min-Hua Cao and Chang-Wen Hu

page 2909



A general and efficient solvothermal strategy has been developed for the preparation of lithium transition metal phosphate microstructures under solvothermal conditions in the presence of PVP.

Preparation of Pt deposited nanotubular TiO₂ as cathodes for enhanced photoelectrochemical hydrogen production using seawater electrolytes

Wonsik Nam, Seichang Oh, Hyunku Joo and Jaekyung Yoon *page 2920*

On the basis of photoelectrochemical hydrogen production, 0.2 wt% Pt/TiO₂ was observed to exhibit the best performance among the various Pt/TIO₂ cathodes with natural seawater. In comparison of hydrogen evolution rate with various seawater electrolytes, 0.2 wt% Pt/TiO₂ was found to show the better performance as cathode with the concentrated seawater electrolytes obtained from membrane.

High temperature crystal structures and superionic properties of SrCl₂, SrBr₂, BaCl₂ and BaBr₂

Stephen Hull, Stefan T. Norberg, Istaq Ahmed, Sten G. Eriksson and Chris E. Mohn *page 2925*



Anomalous behaviour of the lattice expansion of SrCl₂ at temperatures of ~1000 K is associated with the gradual transition to a superionic phase, whilst SrBr₂ undergoes a first-order structural transition ($\beta \rightarrow \alpha$) to a fluorite-structured superionic phase at 920(3) K.

TiO₂ nanorods branched on fast-synthesized large clearance TiO₂ nanotube arrays for dye-sensitized solar cells Anzheng Hu, Haina Li, Zhiyong Jia and Zhengcai Xia page 2936



The schematic diagram of synthesis process for LTAs and BLTs is on the above and the corresponding FESEM images of obtained photoanodes samples are shown below.

Synthesis, structural characterization and magnetic properties of *RE*₂MgGe₂ (*RE*=rare-earth metal) Nian-Tzu Suen, Paul H. Tobash and Svilen Bobev *page 2941*



The structure of RE_2 MgGe₂ (RE = Y, Nd, Sm, Gd–Tm, Lu) can be best viewed as 2-dimensional slabs of Mg and Ge atoms (anionic sub-lattice), and layers of rare-earth metal atoms (cationic sublattice) between them. Within this description, one should consider the Ge–Ge dumbbells (formally Ge₂⁶⁻), interconnected with squareplanar Mg atom as forming flat [MgGe₂] layers (z=0), stacked along the *c*-axis with the layers at z=1/2, made of rare-earth metal cations (formally RE^{3+}).

Thermal and electronic charge transport in bulk nanostructured $Zr_{0.25}Hf_{0.75}NiSn$ composites with full-Heusler inclusions

Julien P.A. Makongo, Dinesh K. Misra, James R. Salvador, Nathan J. Takas, Guoyu Wang, Michael R. Shabetai, Aditya Pant, Pravin Paudel, Ctirad Uher, Kevin L. Stokes and Pierre F.P. Poudeu page 2948



Large reduction in the lattice thermal conductivity of bulk nanostructured half-Heusler/full-Heusler (Zr_{0.25}Hf₀₇₅NiSn/Zr_{0.25}Hf₀₇₅Ni₂Sn) composites, obtained by solid-state diffusion at 1073 K of elemental Ni into vacant sites of the half-Heusler structure, arising from the formation of regions of spinodally decomposed HH and FH phases with a spatial composition modulation of ~2 nm.

Topotactic synthesis of Co_3O_4 nanoboxes from $\text{Co}(\text{OH})_2$ nanoflakes

Li Tian, Kelong Huang, Younian Liu and Suqin Liu page 2961



The formation mechanism of Co_3O_4 nanoboxes can be expressed as epitaxial growth of Co_3O_4 nanocubes from β -Co(OH)₂ nanoflakes due to a topotactic transformation and hollowing process owing to Ostwald ripening.

Crystal structures of the novel hydrated borates Ba₂B₅O₉(OH), Sr₂B₅O₉(OH) and Li₂Sr₈B₂₂O₄₁(OH)₂ Colin McMillen, Carla Heyward, Henry Giesber and Joseph Kolis *page 2966*



Novel hydrated borate structures.

Synthesis, structure and conductivity of sulfate and phosphate doped SrCoO₃

C.A. Hancock, R.C.T. Slade, J.R. Varcoe and P.R. Slater page 2972



Phosphate/sulfate doping in $SrCoO_{3-y}$ leads to a structural change to a 3C-perovskite framework, with an accompanying large increase in conductivity.

Apatite metaprism twist angle (φ) as a tool for crystallochemical diagnosis

S.C. Lim, Tom Baikie, Stevin S. Pramana, Ron Smith and T.J. White

page 2978



 $[A^{II}]_{4}[A^{III}]_{6}(BO_{4})_{6}X_{2}$ apatites can flexibly accommodate numerous cationic, metalloid and anionic substitutions. Using a combination of new refinements and published structures, this paper reviews correlations between substituent type and framework adaptation through adjustment of the $A^{I}O_{6}$ metaprism twist angle, φ .

The ferroelectric phase of CdTiO₃: A powder neutron diffraction study

Brendan J. Kennedy, Qingdi Zhou and Maxim Avdeev page 2987



The structure of three phases of CdTiO₃ have been refined using high resolution powder neutron diffraction data. This involved the preparation of samples enriched in ¹¹⁴Cd. Cooling perovskite-type CdTiO₃ to 4 K results in a ferroelectric phase in *Pna*2₁.

Fabrication of monodispersed nickel flower-like architectures via a solvent-thermal process and analysis of their magnetic and electromagnetic properties

Jing Kong, Wei Liu, Fenglong Wang, Xinzhen Wang, Liqiang Luan, Jiurong Liu, Yuan Wang, Zijun Zhang, Masahiro Itoh and Ken-ichi Machida *page 2994*



Monodispersed Ni flower-like architectures composed of nanoflakes were synthesized through a facile solvent-thermal process. The Ni architectures exhibited a large coercivity and enhanced electromagnetic wave absorption in GHz.

Boron and nitrogen-codoped TiO₂ nanorods: Synthesis, characterization, and photoelectrochemical properties Xiaosong Zhou, Feng Peng, Hongjuan Wang and Hao Yu page 3002



Boron and nitrogen codoped TiO_2 nanorods (BNTRs) were synthesized using TiN. The BNTRs showed a higher photocatalytic activity and a bigger photocurrent than N–TiO₂ nanorods (NTRs) under visible light irradiation.

Micro- and nano-scale hollow TiO₂ fibers by coaxial electrospinning: Preparation and gas sensing Jin Zhang, Sun-Woo Choi and Sang Sub Kim *page 3008*



Microstructures of as-prepared and calcined hollow TiO_2 fibers prepared by the electrospinning technique with a coaxial needle. Dynamic response at various CO concentrations for the sensor fabricated with the hollow TiO_2 fibers.

Structural and catalytic properties of lanthanide (La, Eu, Gd) doped ceria

W.Y. Hernández, O.H. Laguna, M.A. Centeno and J.A. Odriozola





In this work, $Ce_{0.9}M_{0.1}O_{2-\delta}$ mixed oxides (M=La, Eu and Gd) were synthesized by coprecipitation. Independent of the dopant cation, the obtained solids maintain the F-type crystalline structure, characteristic of CeO₂ (fluorite structure) without phase segregation. The ceria lattice expands depending on the ionic radii of the dopant cation, as indicated by X-ray diffraction studies. This effect also agrees with the observed shift of the F_{2g} Raman vibrational mode. The presence of the dopant cations in the ceria lattice increases the concentration of structural oxygen vacancies and the reducibility of the redox pair Ce^{4+}/Ce^{3+} . All synthesized materials show higher catalytic activity for the CO oxidation reaction than that of bare CeO₂, being Eu-doped solid the one with the best catalytic performances despite of its lower surface area.

Influence of amine-grafted multi-walled carbon nanotubes on physical and rheological properties of PMMA-based nanocomposites

Ki-Seok Kim and Soo-Jin Park *page 3021*



This describes the increase of mechanical properties in NH-MWNTs-g-PMMA hybrid composites with different NH-MWNT contents.

Raman and structural characterization of LuAlO₃ Alberto Casu and Pier Carlo Ricci

page 3028



Raman active mode in LuAP crystal.

Continued

Adsorption of volatile organic compounds in porous metal–organic frameworks functionalized by polyoxometalates

Feng-Ji Ma, Shu-Xia Liu, Da-Dong Liang, Guo-Jian Ren, Feng Wei, Ya-Guang Chen and Zhong-Min Su *page 3034*



The adsorption behavior of volatile organic compounds in porous metal–organic frameworks functionalized by polyoxometalates has been systematically evaluated.

Structural and electronic evolution of Cr₂O₃ on compression to 55 GPa

Przemyslaw Dera, Barbara Lavina, Yue Meng and Vitali B. Prakapenka *page 3040*



New synchrotron single-crystal x-ray diffraction experiments to 55 GPa in Ne and He complemented by measurements of optical absorption spectra show no indication of the earlier reported monoclinic distortion at 15–30 GPa, but indicate evidence of two discontinuous transitions of electronic or magnetic nature, most likely associated with a change in the magnetic ordering and charge transfer. The compression mechanism established from single crystal refinements indicates much smaller distortion of the Cr^{3+} coordination environment than was previously assumed.

Synthesis of large surface area nano-sized BiVO₄ by an EDTA-modified hydrothermal process and its enhanced visible photocatalytic activity

Wanting Sun, Mingzheng Xie, Liqiang Jing, Yunbo Luan and Honggang Fu

page 3050



High visible active nano-sized $BiVO_4$ photocatalyst with large surface area is successfully synthesized, which is attributed to the chelating role of EDTA group inhibiting the growth of $BiVO_4$ crystallites.

Scalable synthesis and characterization of cobalt sodium tartrate nanowires with adjustable diameters

Lan Chen, Shaochun Tang, Sascha Vongehr, Kun Hu and Xiangkang Meng

page 3055



Cobalt sodium tartrate nanowires with smooth surfaces are synthesized hydrothermally. Their narrowly distributed diameters decrease with reaction time after initial two hours and are controllable from 80 to 250 nm.

The role of TiO_2 in the B_2O_3 -Na₂O-PbO-Al₂O₃ glass system

N.C.A. de Sousa, M.T. de Araujo, C. Jacinto, M.V.D. Vermelho, N.O. Dantas, C.C. Santos and I. Guedes *page 3062*





Behavior of the relative integrated intensity of the IR bands, Ar = A_4/A_3 , as TiO₂ content increases. A decrease of 45% of Ar indicates that the number of BO₄ groups is decreasing due to the BO₄ \rightarrow BO₃ back conversion.

ESR study on the visible photocatalytic mechanism of nitrogen-doped novel ${\rm TiO}_2$

Synergistic effect of two kinds of oxygen vacancies Jiwei Zhang, Zhensheng Jin, Caixia Feng, Laigui Yu, Jingwei Zhang and Zhijun Zhang *page 3066*



Synergistic action is realized between $(V_o^{\bullet})_{bulk}$ and $(V_o^{\bullet})_{surf}$ in the presence of active structures $(V_o^{\bullet})_{bulk}$ -NO-Ti and $(V_o^{\bullet\bullet})_{surf}$ -NO-Ti.

The first BETS radical cation salts with dicyanamide anion: Crystal growth, structure and conductivity study

N.D. Kushch, L.I. Buravov, A.N. Chekhlov, N.G.

Spitsina, P.P. Kushch, E.B. Yagubskii, E. Herdtweck and A. Kobayashi

page 3074



We studied electrochemical oxidation of BETS donor in the presence of simple and/or complex dicyanamides of transition metals (Ni, Fe, Mn) as electrolytes. New conducting salts α'' -BETS₂[N(CN)₂]·2H₂O and θ -BETS₂[N(CN)₂]·3.8H₂O have been synthesized and characterized.

Synthesis, crystal structure and magnetic properties of the open framework compound Co₃Te₂O₂(PO₄)₂(OH)₄ Iwan Zimmermann, Reinhard K. Kremer and Mats Johnsson

page 3080



The new compound $Co_3Te_2O_2(PO_4)_2(OH)_4$ has been synthesized using hydrothermal techniques. It crystallizes in the monoclinic space group C2/m. Building blocks are $[Co(1)O_6]$, $[TeO_3(OH)_2]$, $[PO_4]$ and $[Co(2)O_2(OH)_4]$. The magnetic susceptibility shows two antiferromagnetic transitions at 21 K and 4 K, respectively.

Oriented $SrFe_{12}O_{19}$ thin films prepared by chemical solution deposition

Josef Buršík, Ivo Drbohlav, Zdeněk Frait, Karel Knížek, Radomír Kužel and Karel Kouřil

page 3085



XRD and AFM patterns of $SrFe_{12}O_{19}$ thin film epitaxially grown on $SrTiO_3(111)$ single crystal using seeding layer templating.

Synthesis and characterization of Pd-poly(N-vinyl-2pyrrolidone)/KIT-5 nanocomposite as a polymer–inorganic hybrid catalyst for the Suzuki–Miyaura cross-coupling reaction

Roozbeh Javad Kalbasi and Neda Mosaddegh page 3095



Pd-poly(N-vinyl-2-pyrrolidone)/KIT-5 was prepared as an organic–inorganic hybrid catalyst for the Suzuki–Miyaura reaction. The stability of the catalyst was excellent and could be reused 8 times in the Suzuki–Miyaura reaction.

Sorption and desorption properties of a CaH₂/MgB₂/CaF₂ reactive hydride composite as potential hydrogen storage material

K. Suarez Alcantara, U. Boesenberg, O. Zavorotynska, J. Bellosta von Colbe, K. Taube, M. Baricco, T. Klassen and M. Dornheim

page 3104



PCI of $3CaH_2 + 4MgB_2 + CaF_2$ reactive hydride composite at 325 °C and 350 °C. Open marks: dehydrogenation, closed marks: hydrogenation.

Evidence of a transition to reorientational disorder in the cubic alkali-metal dodecahydro-*closo***-dodecaborates** Nina Verdal, Hui Wu, Terrence J. Udovic, Vitalie Stavila,

Wei Zhou and John J. Rush page 3110



 $Cs_2B_{12}H_{12}$ undergoes an order–disorder phase transition near 529 K. Similar transitions are observed for $K_2B_{12}H_{12}$ and $Rb_2B_{12}H_{12}.$

Synthesis, structure and physical properties of reduced barium titanate Ba₂Ti₁₃O₂₂

Kunimitsu Kataoka, Norihito Kijima, Hiroshi Hayakawa, Akira Iyo, Ken-ichi Ohshima and Junji Akimoto page 3117



Temperature dependence of the electrical conductivity of Ba₂. Ti₁₃O₂₂. A plot of ln σ versus T^{-1} is shown by open circles, and a plot of ln σ versus $T^{-1/4}$ is shown by open triangles.

Two multi-dimensional frameworks constructed from zinc coordination polymers with pyridine carboxylic acids

Yuanyuan Guo, Pengtao Ma, Jingping Wang and Jingyang Niu

page 3121



Two new transition metal coordination polymers, namely, $[Zn_2(H_2O)L_1(MOO_4)]_n$ (1), $[Zn_4(PO_4)_2L_2(H_2O)]_n$ (2) $(H_2L_1=2,2'-bipyridine-6,6'-dicarboxylic acid, <math>H_2L_2=2,2'-bipyridine-4,4'-dicarboxylic acid)$ have been hydrothermally synthesized. 1 represents a 2-D sheet structure while 2 represents 3-D network.

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Journal of Solid State Chemistry has no page charges.

Low-temperature structural phase transition in synthetic libethenite Cu₂PO₄OH

Alexei A. Belik, Panče Naumov, Jungeun Kim and Shunsuke Tsuda

page 3128



Fragments of experimental synchrotron X-ray powder diffraction patterns of Cu₂PO₄OH between 100 and 280 K. Arrows show additional reflections that appear below 160 K in the monoclinic $P2_1/n$ phase.