

SYMPOSIUM DD

Solid-State Chemistry of Inorganic Materials IV

December 2 – 6, 2002

Chairs

Martha Greenblatt	Rutgers Univ
M. Stanley Whittingham	SUNY-Binghamton
Miguel A. Alario-Franco	Univ of Complutense
Gregory S. Rohrer	Carnegie Mellon Univ

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* Invited paper

SESSION DD1: METAL-TO-INSULATOR TRANSITION - I

Chairs: M. Stanley Whittingham and Peter K. Davies
Monday Morning, December 2, 2002
Back Bay C (Sheraton)

8:45 AM *DD1.1

SOFT X-RAY EMISSION AND RESONANT INELASTIC X-RAY SCATTERING STUDIES OF ELECTRONIC STRUCTURE IN METAL OXIDES. Kevin E. Smith, Cormac McGuinness, James E. Downes, Cristian B. Stagarescu, Philip J. Ryan, Dongfeng Fu, Department of Physics, Boston University; Steven D. Hulbert, National Synchrotron Light Source, Brookhaven National Laboratory; J.M. Honig, Department of Chemistry, Purdue University; Russel Egdell, Inorganic Chemistry Laboratory, Oxford University.

9:15 AM DD1.2

A Cr(IV) BASED 1212-TYPE CUPRATE. Rocio Ruiz-Bustos, Myriam H. Aguirre, E. Moran, M.A. Alario-Franco, Laboratorio de Quimica del Estado Solido, Facultad de Quimica, Universidad Complutense, Madrid, SPAIN; J.L. Martinez, ICMM, CSIC, Canto Blanco, Madrid, SPAIN.

9:30 AM DD1.3

STUDIES OF THE ELECTRONIC PROPERTIES OF BaV₁₀O₁₅: CRYSTALLOGRAPHIC PHASE TRANSITION, ELECTRICAL TRANSPORT AND MAGNETIC PROPERTIES. Craig Bridges, John E. Greedan, McMaster University, Brockhouse Institute for Materials Research and Department of Chemistry, Hamilton, ON, CANADA.

9:45 AM BREAK

10:15 AM *DD1.4

VERNIER STRUCTURES IN NOWOTNY CHIMNEY LADDER PHASES AND γ -BRASS DERIVATIVES. Stephen Lee, Bernd Harbrecht, Jianhua Lin, Roald Hoffmann, Mikhail Shatruk, Daniel Fredrickson, Lan-Feng Yuan and Joshua Teal Schmidt, Departments of Chemistry, Cornell University, NY; Univ. of Marburg, GERMANY; Peking University, CHINA.

10:45 AM DD1.5

SOLVING THE STRUCTURE OF THE PHASES IN THE Al-Mg-Si ALLOY SYSTEM WITH THE HELP OF AB INITIO MODELLING. Anders Froseth, NTNU, Dept of Physics, Trondheim, NORWAY; Peter Derlet, Paul Scherrer Institute, Villigen PSI, SWITZERLAND; Sigmund Andersen and Calin Marioara, SINTEF Materials Technology, Trondheim, NORWAY.

11:00 AM DD1.6

RULES FOR UNDERSTANDING AND DESIGNING NOVEL MOLECULE-BASED RARE-EARTH MAGNETIC COMPOUNDS. Lindsay E. Roy, Timothy Hughbanks, Texas A&M University, Department of Chemistry, College Station, TX.

11:15 AM DD1.7

STABILITY AND HARDNESS OF COVALENT COMPOUNDS. John Gilman, UCLA, Dept of Materials Science and Engineering, Los Angeles, CA.

11:30 AM DD1.8

HYDROSTATIC PRESSURE INDUCED STRUCTURAL TRANSITIONS IN MANGANITES WITH ORBITAL ORDERING. Michael Kaplan, Simmons College, Depts of Chemistry and Physics, Boston, MA; George Zimmerman, Boston University, Dept of Physics, Boston, MA.

11:45 AM DD1.9

ORBITAL ORDERING TRANSITION IN La₄Ru₂O₁₀. Peter Khalifah, Rongying Jin, Solid State Division, Oak Ridge National Laboratory; David Mandrus, Solid State Division, Oak Ridge National Laboratory and Dept. of Physics, University of Tennessee; Raymond Osborn, Materials Science Division, Argonne National Laboratory; Qingzhen Huang, NIST Center for Neutron Research and Dept. of Materials and Nuclear Engineering, University of Maryland; Henny Zandbergen, National Center for High Resolution Electron Microscopy, Technical University of Delft; Ying Liu, Department of Physics, The Pennsylvania State University; Robert J. Cava, Dept. of Chemistry and Princeton Materials Institute, Princeton University.

SESSION DD2: METAL-TO-INSULATOR TRANSITION - II

Chairs: John E. Greedan and Stephen Lee
Monday Afternoon, December 2, 2002
Back Bay C (Sheraton)

1:30 PM *DD2.1

MANGANITES AND COBALTITES: SIMILARITIES AND DIFFERENCES. D. Khomskii, Laboratory of Solid State Physics, Groningen University, Groningen, THE NETHERLANDS.

2:00 PM DD2.2

STRUCTURAL AND MAGNETIC CONSEQUENCES OF CONTROLLED OXYGEN DEFICIENCY IN LAYERED MANGANITES AND COBALTATES. J.F. Mitchell, J. Burley, H. Zheng, S. Short, Materials Science Division, Argonne National Laboratory, Argonne, IL; P.G. Radaelli, ISIS Facility, Rutherford Appleton Laboratory, Chilton, UNITED KINGDOM.

2:15 PM DD2.3

NUCLEAR AND MAGNETIC STRUCTURES OF K₂NiF₄-TYPE IRON(III) OXIDES AND OXIDE HALIDES. Andrew L. Hector, Alexander I. MacDonald, Daniel J. Price and Mark T. Weller, Department of Chemistry, University of Southampton, UNITED KINGDOM.

2:30 PM DD2.4

MAGNETORESISTANCE IN PEROVSKITE RUTHENATES. Alexander Mamchik, I-Wei Chen, Univ of Pennsylvania, Dept of Materials Science and Engineering, Philadelphia, PA.

2:45 PM BREAK

3:15 PM *DD2.5

MAGNETIC MATERIALS WITH TRANSITION METALS: ANALYSIS AND DESIGN USING THEORETICAL TOOLS. Eliseo Ruiz^a, Cedric Desplanches^a, Antonio Rodriguez-Fortea^a, Santiago Alvarez^a; ^aDepartament de Quimica Inorganica and Centre de Recerca en Quimica Terica (CERQT), Universitat de Barcelona, Barcelona, SPAIN.

3:45 PM DD2.6

PREPARATION, ELECTRICAL PROPERTIES AND MICROSTRUCTURE CHARACTERIZATION OF MAGNETO-RESISTIVE (La,Ca)MnO₃ THIN FILMS. Laurent Dusoulier, Benedicte Vertruyen, Jean-Francois Fagnard, Jacques Delwiche, Andre Rulmont, Philippe Vanderbenden, Marcel Ausloos and Rudi Cloots University of Liege, SUPRAS, Liege, BELGIUM.

4:00 PM DD2.7

DEVELOPMENT AND APPLICATION OF A NEW INTERATOMIC POTENTIAL FOR THE MODELLING OF LIGAND FIELD EFFECTS. Scott M. Woodley, C. Richard, A. Catlow, Royal Institution of Great Britain, London, UNITED KINGDOM; Peter D. Battle, Oxford Uni, Inorganic Chemistry Lab, Oxford, UNITED KINGDOM; Julian D. Gale, Imperial College, Dept of Chemistry, London, UNITED KINGDOM.

4:15 PM DD2.8

A DRASTIC INFLUENCE OF POINT DEFECTS ON PHASE STABILITY IN MnO_2 . Dane Morgan, Dinesh Balachandran, G. Ceder, MIT, Materials Science and Engineering, Cambridge, MA; A. van de Walle, Northwestern, Materials Science and Engineering, Evanston, IL.

4:30 PM DD2.9

SINGLE CRYSTAL DIFFRACTION STUDY OF COMMENSURATE-TO-INCOMMENSURATE PHASE TRANSITION IN CHARGE ORDERED $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ BY ELECTRON NANODIFFRACTION. Jing Tao, J.M. Zuo, Univ. of Illinois at Urbana-Champaign, Dept. of Materials Science and Engineering and Materials Research Laboratory, Urbana, IL.

4:45 PM DD2.10

STRUCTURE-PROPERTY RELATIONSHIPS OF $\text{La}_n\text{MIn}_3n + 2(n = 1, 2, \infty; M = \text{Rh, Ir})$ and $\text{Ce}_n\text{MIn}_3n + 2(n = 1, 2, \infty; M = \text{Rh, Ir})$. Robin T. Macaluso and Julia Y. Chan, Dept. of Chemistry, Louisiana State University, Baton Rouge, LA; John L. Sarrao, Condensed Matter & Thermal Physics Group, Los Alamos National Laboratory, Los Alamos, NM.

SESSION DD3: POROUS MATERIALS

Chair: Miguel A. Alario-Franco
Tuesday Morning, December 3, 2002
Back Bay C (Sheraton)

8:30 AM *DD3.1

NANOPOROUS NICKEL PHOSPHATES; PROPERTIES AND POTENTIAL APPLICATIONS. Anthony K. Cheetham, Materials Research Laboratory, University of California, Santa Barbara, CA.

9:00 AM DD3.2

INORGANIC-INORGANIC MESOPOROUS AND COMPOSITES MATERIALS BASED ON MINERAL LIQUID CRYSTALS. Jean-Christophe P. Gabriel[†], Franck Camerel, Patrick Batail, Sciences Moleculaires aux Interfaces, Nantes, FRANCE. [†]Present address: Nanomix, Inc., Emeryville, CA.

9:15 AM DD3.3

CATIONIC, NEUTRAL AND ANIONIC MICROPOROUS MATERIALS BASED ON Ge, Sn AND Pb. Scott R.J. Oliver, State University of New York at Binghamton, Department of Chemistry, Binghamton, NY.

9:30 AM DD3.4

SYNTHESIS AND CHARACTERIZATION OF NEW MATERIALS BASED ON LOWER GROUP 14 ELEMENTS: BING-5,6,9,10. Dat T. Tran, Peter Y. Zavilij, Scott R.J. Oliver, State University of New York at Binghamton, Dept of Chemistry, Binghamton, NY.

9:45 AM BREAK**10:15 AM *DD3.5**

PERIODIC NANOSCALE SEMICONDUCTORS THROUGH SURFACTANT-DRIVEN SELF-ORGANIZATION OF SOLUBLE ZINTL CLUSTERS. Sarah Tolbert, Andrew Riley, Dong Sun, Ashley Cadby, University of California, Los Angeles, Department of Chemistry and Biochemistry, Los Angeles, CA.

10:45 AM DD3.6

OPEN FRAMEWORK AND MICROPOROUS TRANSITION METAL SILICATES. Allan J. Jacobson, Xiqu Wang, Lumei Liu, J. Huang, Department of Chemistry, University of Houston, Houston, TX.

11:00 AM DD3.7

WATER INSERTION IN HYDROPHOBIC POROUS OXIDES. D. Carrière, S. Sidis, K. Lahlil, M. Moreau, P. Barboux, J.-P. Boilot, CNRS UMR 7643C, Ecole Polytechnique, Laboratoire de Physique de la Matière Condensée, Ecole Polytechnique, Palaiseau, FRANCE.

11:15 AM DD3.8

THE MANIPULATION OF SILICA MESOCELLULAR FOAM PARTICLE MORPHOLOGY: APPLICATIONS IN FINE CHEMICAL SYNTHESIS. Thomas M. Lancaster, Jackie Y. Ying, Massachusetts Institute of Technology, Department of Chemical Engineering, Cambridge, MA.

11:30 AM DD3.9

SYNTHESIS AND CHARACTERIZATION OF NEW IRON AND ZINC PHOSPHATE MATERIALS WITH OPEN FRAMEWORK. Yanning Song, Peter Y. Zavilij, M. Stanley Whittingham, State University of New York at Binghamton, Dept of Chemistry, Binghamton, NY.

SESSION DD4: DIELECTRIC MATERIALS

Chairs: Colin Greaves and Susan M. Kauzlarich
Tuesday Afternoon, December 3, 2002
Back Bay C (Sheraton)

1:30 PM *DD4.1

NEW EXAMPLES OF CATION ORDER IN MIXED-METAL PEROVSKITES. Peter K. Davies, Dept Materials Science & Engineering, University of Pennsylvania, Philadelphia, PA.

2:00 PM DD4.2

DISPLACIVE DISORDER IN BISMUTH ZINC NIOBATES. Igor Levin, Tammy Amos, Terrell Vanderah, NIST, MSEL, Gaithersburg, MD; Juan Nino, Clive Randall, Michael Lanagan, Penn State Univ, CDS, MRL, University Park, PA.

2:15 PM DD4.3

CATION ORDERING, DOMAIN GROWTH AND ZINC LOSS IN THE MICROWAVE DIELECTRIC OXIDE $\text{Ba}_3\text{ZnTa}_2\text{O}_9$ DURING PROCESSING USING REAL-TIME X-RAY AND NEUTRON POWDER DIFFRACTION. M. Bieringer, S.M. Moussa, M.J. Rosseinsky, University of Liverpool, Department of Chemistry, Liverpool, UNITED KINGDOM; R.M. Ibberson, ISIS Facility, Didcot, UNITED KINGDOM; A.N. Fitch, ESRF, Grenoble, FRANCE.

2:30 PM DD4.4

SYNTHESIS AND SINTERING OF (K,Na)NbO₃ BASED CERAMICS. Barbara Malič, Darja Jenko, Janez Bernard, Jena Cilenšek, Marija Kosec, Jožef Stefan Institute, Ljubljana, SLOVENIA.

2:45 PM BREAK**3:15 PM DD4.5**

PHASE EQUILIBRIA, CRYSTAL CHEMISTRY, AND DIELECTRIC BEHAVIOR IN COMPLEX OXIDES. T.A. Vanderah, R.S. Roth, W. Febo, V. Miller, I. Levin, W. Wong-Ng, NIST, Ceramics Division, Gaithersburg, MD; S.M. Bell, TRAK Ceramics, Inc., Hagerstown, MD.

3:30 PM DD4.6

EXTRINSIC CONTRIBUTIONS TO THE DIELECTRIC RESPONSE IN $\text{PbSc}_{1/2}\text{Nb}_{1/2}\text{O}_3$ FROM FIRST PRINCIPLES. Eric Cockayne, Ceramics Division, NIST, Gaithersburg, MD; Umesh Waghmare, Theoretical Sciences Unit, JNCASR, Bangalore, INDIA; Serguei Prosdandeev, Physics Department, Rostov State Univ., Rostov-on-Don, RUSSIA; Benjamin P. Burton, Ceramics Division, NIST, Gaithersburg, MD.

3:45 PM DD4.7

STRUCTURE AND PHASE TRANSITIONS IN AURIVILLIUS PHASE FERROELECTRICS. Philip Lightfoot, Charles Hervoches, Alan Snedden, University of St. Andrews, School of Chemistry, St. Andrews, UNITED KINGDOM.

4:00 PM DD4.8

HOW TO DESIGN INTERACTION BETWEEN π AND d ELECTRONS IN CONDUCTING AND MAGNETIC HYBRID ORGANIC-INORGANIC MOLECULAR MATERIALS. Lahcene Ouahab, Laboratoire de Chimie du Solide et Inorganique Moleculaire, UMR 6511 CNRS - Universite de Rennes 1, Rennes, FRANCE.

4:15 PM DD4.9

SYNTHESIS AND CHARACTERISATION OF B-SITE DOPED COPPER-TANTALATES. Bernd Renner, Stefan Ebbinghaus, Armin Reller, Universität Augsburg, Lehrstuhl für Festkörperchemie, Augsburg, GERMANY; David Schrupp, Universität Augsburg, Lehrstuhl für Experimentalphysik II, Augsburg, GERMANY; Hans-Albrecht Krug von Nidda, Monika Heinrich, Peter Lunkenheimer, Michael Schetter, Universität Augsburg, Lehrstuhl für Experimentalphysik V, Augsburg, GERMANY.

4:30 PM DD4.10

SITE MIXING INVESTIGATIONS IN THREE-LAYER FERROELECTRIC AURIVILLIUS CERAMICS. M.S. Haluska, S.T. Mixture, New York State College of Ceramics at Alfred University, Alfred, NY.

4:45 PM DD4.11

FERROELECTRIC NANOCOMPOSITE WITH HIGH DIELECTRIC CONSTANT. Mai T.N. Pham, B.A. Boukamp, H.J.M. Bouwmeester, University of Twente, Faculty of Chemical Technology, Enschede, THE NETHERLANDS.

SESSION DD5: POSTER SESSION
NANOMATERIALS
Chair: Gregory S. Rohrer
Tuesday Evening, December 3, 2002
8:00 PM
Exhibition Hall D (Hynes)

DD5.1

A NEW MECHANISM FOR THE CATALYTIC GROWTH OF CARBON FIBERS AND METAL DUSTING PHENOMENON. Zuotao Zeng, and Ken Natesan, Argonne National Laboratory, Energy Technology Division, Argonne, IL.

DD5.2

CARBON NANOTUBE SIDEWALLS AND END CAPS AS TARGET SITES FOR CHEMICAL MODIFICATION: CHEMICAL CONTROL OVER NANOTUBE PROPERTIES. Sarbajit Banerjee, Stanislaus S. Wong, Department of Chemistry, SUNY at Stony Brook, Stony Brook, NY, Materials and Chemical Sciences Department, Brookhaven National Laboratory, Upton, NY.

DD5.3

PREFERENTIALLY ORIENTED FILM OF MONOCLINIC TITANIUM DIOXIDE DERIVED FROM NEGATIVELY CHARGED TETRATITANATE NANOSHEETS. Wataru Sugimoto, Osamu Terabayashi, Yasushi Murakami, Yoshio Takasu, Shinshu Univ, Dept Fine Materials Engineering, Nagano, JAPAN.

DD5.4

IN-SITU STUDY ON THE NUCLEATION AND GROWTH OF CERIUM OXIDE NANOPARTICLES AT ROOM TEMPERATURE. Feng Zhang, Qiang Jin, Jonathan E. Spanier, Richard D. Robinson, Irving P. Herman, Siu-Wai Chan, Columbia University, Department of Applied Physics and Applied Mathematics, and Materials Research Science and Engineering Center, New York, NY.

DD5.5

LATTICE EXPANSION OF CERIUM OXIDE NANOPARTICLES. Feng Zhang, Jonathan E. Spanier, Richard D. Robinson, Irving P. Herman and Siu-Wai Chan.

DD5.6

COBALT NANOCRYSTAL GROWTH: SIZE, SHAPE AND STRUCTURE CONTROL. Victor F. Puentes, A. Paul Alivisatos, Chemistry Dept, UC Berkeley, Berkeley, CA; Can Erdonmez, Materials Science Department, UC Berkeley, Berkeley, CA; Daniela Zanchet, Laboratório Nacional de Luz Síncrotron, Campinas, BRAZIL.

DD5.7

SYNTHESIS BY THE OXIDANT PEROXO METHOD (OPM) AND DYNAMIC CHARACTERIZATION *IN SITU* BY HRTEM OF THE CRYSTALLIZATION OF NANOSIZED LEAD TITANATE. Emerson R. Camargo, Edson R. Leite, UFSCar-Federal University of Sao Carlos, Dept of Chemistry, LIEC, Sao Carlos, SP, BRAZIL.

DD5.8

SYNTHESIS OF MONODISPERSE FERRITE NANOPARTICLES: XANES (K-EDGE) DETERMINATION OF CATION OXIDATION STATE AND DISTRIBUTION. Pete Bonitatebus, Mike Larsen, Yan Gao, GE Global Research Center, PSCT Emerging Technologies, Niskayuna, NY.

DD5.9

SYNTHESIS AND CHARACTERIZATION OF DISCRETE PHASE-PURE Mn AND Fe PHOSPHIDE NANOPARTICLES WITH NARROW POLYDISPERSITIES. Susanthri C. Perera, Stephanie L. Brock, Department of Chemistry, Wayne State University, Detroit, MI.

DD5.10

SOLVENT EFFECTS ON THE Au DISTRIBUTION ON Pt-Au/C CATALYSTS PREPARED BY SURFACE REDOX REACTIONS. P. Del Angel, J.M. Dominguez, J.A. Montoya, Instituto Mexicano del Petroleo, Ingenieria Molecular, MEXICO; M.J. Yacaman, P. Santiago, The University of Texas at Austin, Dept. of Chemical Engineering, Austin, TX.

DD5.11

NOVEL SYNTHESIS OF METAL OXIDE TUBULAR STRUCTURES AND NANOFIBERS USING POLYLACTIDE TEMPLATE. Samuel Lutta, Peter Y. Zavalij, M. Stanley Whittingham, State University of New York at Binghamton, Institute for Materials Research and Dept of Chemistry, Binghamton, NY.

DD5.12

SYNTHESIS BY SOFT CHEMISTRY ROUTES AND

CHARACTERIZATION OF Sr₂Bi_{1.4}Ca_{0.6}O₆ NANOPARTICLES. Isaela Villalpando, Claudia C. Luhrs, Departamento de Quimica, CUCEI, Universidad de Guadalajara, Jalisco, MEXICO.

DD5.13

A NOVEL NANOPARTICLE/LAMELLA OXIDE HYBRID: TiO₂-PILLARED MoO₃. Seung-Min Paek, Hyun Jung, Jin-Ho Choy, Seoul National University, Seoul, KOREA.

DD5.14

STRUCTURE AND ELECTRONIC PROPERTIES OF THE DIBORIDE NANOTUBES. Leonid A. Chernozatonskii, A.R. Sabirov, Dept of Material Research, Institute of Biochemical Physics, Moscow, RUSSIA.

DD5.15

REDOX CHEMISTRY APPROACH TO THE SPONTANEOUS FORMATION OF NANOTUBE/NANOPARTICLE HYBRID STRUCTURE. Hee Cheul Choi, Moonsub Shim, Sarunya Bangsaruntip, Hongjie Dai, Stanford Univ, Dept of Chemistry, Stanford, CA.

DD5.16

STRUCTURE, MAGNETIZATION AND MOSSBAUER STUDY OF NANOSTRUCTURED Ni_{0.5}Zn_{0.5}Fe₂O₄ FERRITE POWDERS. Shihui Ge, Zongtao Zhang, Y.D. Zhang, Mingzhong Wu, Inframat Corporation; D.P. Yang, College of the Holy Cross.

DD5.17

TEMPERATURE-DEPENDENT MAGNETIC PROPERTIES OF SiO₂-COATED Ni₇₅Fe₂₅ NANOPARTICLES. Mingzhong Wu, Inframat Corporation, Farmington, CT; University of Connecticut, Department of Physics and Institute of Materials Science, Storrs, CT; Y.D. Zhang, S. Hui, Shihui Ge, Inframat Corporation, Farmington, CT; M.J. Yacaman, University of Texas, Department of Chemical Engineering, Austin, TX.

DD5.18

OBSERVATION OF NANO-SCALE CLUSTERS IN Nd-Fe-Al GLASSY HARD MAGNETS BY HIGH RESOLUTION TRANSMISSION ELECTRON MICROSCOPY. N. Lupu and H. Chiriac, National Institute of R&D for Technical Physics, Lasi, ROMANIA.

DD5.19

EPITAXIAL GROWTH OF MAGNETIC NICKEL NANODOTS BY PULSED LASER DEPOSITION. Honghui Zhou, D. Kumar, A. Kvit, Ashutosh Tiwari and J. Narayan, NSF Center for Advanced Materials and Smart Structures, Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC.

DD5.20

SYNTHESIS AND CHARACTERIZATION OF STRUCTURE CONTROLLED NANO-COBALT PARTICLES. Shiqiang (Rob) Hui^a, Y.D. Zhang^a, Mingzhong Wu^{a,b}, Dajing Yan, W.A. Hines^b, and T.T. Chen^b; ^aInframat Corporation, Willington, CT; ^bDept. of Physics and Institute of Materials Science, University of Connecticut, Storrs, CT.

SESSION DD6: POSTER SESSION
SYNTHESIS OF MATERIALS
Chair: Gregory S. Rohrer
Tuesday Evening, December 3, 2002
8:00 PM
Exhibition Hall D (Hynes)

DD6.1

MICROSCALE TITANIA MORPHOLOGIES GROWN WITHIN SWOLLEN PDMS. Arthur Doble, Scott R.J. Oliver and Daniel P. Brennan, State University of New York at Binghamton, Department of Chemistry, Binghamton, NY.

DD6.2

PREPARATION OF NEW BISMUTH OXIDES BY HYDROTHERMAL REACTION (111). N. Kumada, T. Takei and N. Kinomura, Faculty of Engineering, Yamanashi University, Kofu, JAPAN.

DD6.3

PREPARATION OF CRYSTALLIZED Ba_{1-x}Sr_xMoO₄ FILMS BY ELECTROCHEMICAL METHOD AT ROOM TEMPERATURE. Daojiang Gao, Dingquan Xiao, Jian Bi, Wen Zhang, Ping Yu, Dunmin Lin, Dept of Materials Science, Sichuan Univ, Chengdu, P.R. CHINA.

DD6.4

RAPID SYNTHESIS AND CONCURRENT CONSOLIDATION OF TERNARY COMPOUND Ti_3SiC_2 FROM DIFFERENT POWDER MIXTURES. ZhengMing Sun, Hitoshi Hashimoto, Toshihiko Abe, National Institute of Advanced Industrial Science and Technology (AIST Tohoku), Sendai, JAPAN.

DD6.5

SYNTHETIC PATHWAYS TO NEW ION-EXCHANGEABLE MIXED-ANION LAYERED COMPOUNDS. Gabriel Caruntu, Nasser Naura, Jason W. Baisch, Leonard Spinu and John B. Wiley, Advanced Materials Research Institute and Chemistry Department, University of New Orleans, New Orleans, LA.

DD6.6

Abstract Withdrawn

DD6.7

SYNTHESIS AND CHARACTERIZATION OF $BaFe_{11.6-2x}M_xTi_xO_{19}$. G. Mendoza-Suarez, A.F. Fernandez, Cinvestav-Salttillo, Saltillo, MEXICO; O.E. Ayala-Valenzuela, CIMAV, Chihuahua, Chi., MEXICO.

DD6.8

HYDROTHERMAL SYNTHESIS OF A MICROPOROUS ORGANIC-INORGANIC HYBRID FRAMEWORK $NH_4FeO(C_8H_4O_4)_x[C_8H_4O_4(NH_4)_2]$. Tabatha Whitfield, Xiqu Wang, Allan J. Jacobson, Department of Chemistry, University of Houston, Houston, TX.

DD6.9

VARIANT OF THE FLUX SYNTHESIS METHOD AND CRYSTAL STRUCTURE OF THE NEW COMPOUND Sm-Mn-Ge-O BY SEM-TEM. Erick Juarez-Arellano, Ivonne Rosales, Gabriel Gamboa-Espinosa, Armando Lara, Lauro Bucio, Eligio Orozco, UNAM, Instituto de Fisica, Departamento de Estado Solido, MEXICO.

DD6.10

ANION INTERCALATION AND ANION EXCHANGE IN BISMUTH COMPOUNDS. Masamichi Tsuji, Tokyo Institute of Technology, Research Center for Carbon Recycling and Energy, Tokyo, JAPAN; Makoto Yamaguchi, Institute of Research and Innovation, Chiba, JAPAN; Satoshi Murao, National Institute of Advanced Industrial Science and Technology, Institute for Geo-resources and Environment, Tsukuba, JAPAN.

DD6.11

CONVERSION OF CALCIUM PHOSPHATES TO HYDROXYLAPATITE. Alexander Veresov, Olga Simitsina, Yuri Kolenko, Moscow State University, Dept of Materials Science, Moscow, RUSSIA; Valery Putlayev, Yuri Tretyakov, Moscow State University, Dept of Chemistry, Moscow, RUSSIA.

DD6.12

TOWARDS AN ARSENIC ANALOG OF HITTORF'S PHOSPHORUS: MIXED PNICTOGEN CHAINS IN $Cu_2P_{1-x}As_xI_2$ $x < 0.5$. Buddhimathie Jayasekera, Jennifer A. Aitken, Mary Jane Heeg, and Stephanie L. Brock, Department of Chemistry, Wayne State University, Detroit, MI.

DD6.13

SYNTHESIS OF SEVERAL TUNGSTEN (VI) COMPLEX PEROVSKITES, $Ba(B^{III}_{0.67}B^{VI}_{0.33})O_3$, BY THE POLYMERIC PRECURSORS METHOD. Antonio F. Fuentes, Guillermo Mendoza-Suarez, J.I. Escalante-García, CINVESTAV-IPN Unidad Saltillo, Saltillo, Coahuila, MEXICO; Ulises Amador, Dept. de Química Inorgánica y Materiales, Facultad de Ciencias Experimentales y Técnicas, Universidad San Pablo CEU, Boadilla del Monte, Madrid, SPAIN.

DD6.14

CUBIC MESOSTRUCTURED SEMICONDUCTORS IN SINGLE-CRYSTAL FORM. Pantelis N. Trikalitis and Mercouri G. Kanatzidis, Department of Chemistry, Michigan State University, East Lansing, MI.

DD6.15

STRUCTURE OF Na-4-MICA AS AFFECTED BY EXCHANGE WITH VARIOUS CATIONS. Man Park, Jin-Ho Choy, School of Chemistry and Molecular Engineering, Seoul National University, KOREA; Dong Hoon Lee, Sang Su Kim, Choi Jyung, Department of Agricultural Chemistry, Kyungpook National University, KOREA; Sridhar Komarneni, Materials Research Laboratory, The Pennsylvania State University, PA.

DD6.16

PHOTOCHEMICAL REACTIVITY OF $Sr_2(Ta_xNb_{1-x})_2O_7$ ($0.8 < x < 1$) AS A FUNCTION OF COMPOSITION. Jennifer L. Giocondi, Ariana M. Zimbouski, Shahrzad Samadzadeh, Gregory S. Rohrer, Carnegie Mellon University, Dept of Materials Science and Engineering, Pittsburgh, PA.

DD6.17

SYNTHESIS OF Silylated α -ZIRCONIUM PHOSPHATE AND ITS THERMAL BEHAVIOR. Takahiro Takeji, Emi Aaraya, Nobuhiro Kumada, Nobukazu Kinomura, Yamanashi Univ, Center for Crystal Science and Technology, Faculty of Engineering, Yamanashi, JAPAN; Hirokazu Nakayama, Mitsutomo Tshako, Kobe Pharmaceutical Univ, Kobe, JAPAN.

DD6.18

HETEROGENEOUS DESIGN: CONCENTRATION FIELDS DETERMINATION WITH THE UNIQUE CRYSTALLIZATION SCHEMES AND MICROSTRUCTURES. Vasily Lutsyk, Vera Vorob'eva, Anna Zelenaya, Buryat Scientific Center, Physical Problems Dept, Ulan-Ude, RUSSIA; Julia Arzhitova, Buryat Univ, Dept of Physics, Ulan-Ude, RUSSIA.

DD6.19

A SERIES OF NEW LOW-DIMENSIONAL TIN OXALATES AND PHOSPHATES: BING-1,2,3,4,7,8. Tolulope O.Salami, Peter Y. Zavalij and Scott R.J. Oliver, State University of New York at Binghamton, Dept of Chemistry, Binghamton, NY.

DD6.20

CLATHRATED STATE OF OXYGENIC RADICALS O^- AND O_2^- IN NANO-POROUS CRYSTAL $12CaO \cdot 7Al_2O_3$ STUDIED BY CW AND PULSED EPR. Satoru Matsuishi^{a,b}, Katsuro Hayashi^b, Masahiro Hirano^b and Hideo Hosono^{a,b}, ^aMaterials and Structures Laboratory, Tokyo Institute of Technology, JAPAN; ^bHosono Transparent Electro-Active Materials Project, ERATO, JST, JAPAN.

DD6.21

SYNTHESIS OF Ru-Sr-Zr OXIDE ELECTRICAL CONDUCTOR FROM PRECURSOR SOLUTION. Tadashi Ishigaki, Keishi Nishio, Takashi Nakajima, and Toshio Tsuchiya, Department of Materials Science and Technology, Tokyo University of Science, Chiba, JAPAN.

DD6.22

THE TERNARY SYSTEM $Li_2O - Sb_2O_5 - CuO$. María A. Castellanos R., M. Sonia Trujillo T., Depto de Q. Analítica, Facultad de Química, UNAM, México D.F., MEXICO.

DD6.23

NEW METHOD OF PREPARATION OF SUPERIONIC $BaSnF_4$. Georges Dénès, A. Muntasar and Tony Retrif, Concordia University, Dept of Chemistry and Biochemistry, Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, Laboratories for Inorganic Materials, Montreal, Québec, CANADA.

DD6.24

SYNTHESIS OF METAL-DOPED CRYPTOMELANE NANOMATERIALS USING CROSS-LINKING REAGENTS. Jia Liu^a, Jun Cai^b, Xiongfei Shen^a, Steven L. Suib^{a,b,c}, Mark Aindow^{a,d}, ^aInstitute of Materials Science, ^bDepartment of Chemistry, ^cDepartment of Chemical Engineering, ^dDepartment of Metallurgy and Materials Engineering, University of Connecticut, Storrs, CT.

DD6.25

PREPARATION AND PROPERTIES OF Li-Mn-O-F COMPOUNDS. Hanxing Liu, Yale University, Department of Electrical Engineering, Wuhan University of Technology, State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan, P.R. CHINA; Junlei Xia, Shixi Zhao, Chen Hua, Shixi Ouyang, Wuhan University of Technology, State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan, Hubei, P.R. CHINA.

DD6.26

Na^+/H^+ TOPOTACTIC EXCHANGE ON $Na_6Nb_6W_4O_{30}$ WITH TTB-LIKE STRUCTURE: THE SERIES $H_xNa_{6-x}Nb_6W_4O_{30}$. Flaviano Garcia-Alvarado, Alois Kuhn and Carlos Repáraz, Universidad San Pablo-CEU, Departamento de Químicas, Boadilla del Monte, Madrid, SPAIN.

DD6.27

DESIGN OF NEW OXIDE CERAMIC MATERIALS AND NANOCOMPOSITES WITH MIXED CONDUCTIVITY BY USING MECHANICAL ACTIVATION ROUTE. Vladimir V. Zyrianov, N.F. Uvarov, V.G. Kostrovskii, Inst. of Solid State Chem. and

Mechanochemistry, Novosibirsk, RUSSIA; Vladislav A. Sadykov, T.G. Kuznetsova, V.A. Rogov, E.B. Burgina, V.I. Zaikovskii, V.V. Kriventsov, D.I. Kochubei, G.S. Litvak, Boreskov Inst. Catalysis, Novosibirsk, RUSSIA; Stylianos Neophytides, Inst. of Chem. Eng. & High Temperature Proc., Patras, GREECE.

DD6.28

ULTRATHIN, PROTECTIVE COATINGS OF POLY(O-PHENYLENEDIAMINE) AT NANOSTRUCTURED METAL OXIDE ELECTRODES: MAKING MnO₂ STABLE IN ACID ELECTROLYTES. Jeffrey Long, Christopher Rhodes, Amanda Young, Debra Rolison, Naval Research Laboratory, Washington, DC.

DD6.29

SUPERPROTONIC PHASE TRANSITION OF C₆H₅SO₄: A MOLECULAR DYNAMICS SIMULATION STUDY WITH NEW MSXX FORCE FIELD. Calum Chisholm, Lan Yang, Sossina M. Haile, Dept of Materials Science, California Institute of Technology, Pasadena, CA; Yun Hee Jang, William A. Goddard III, Materials and Process Simulation Center, California Institute of Technology, Pasadena, CA.

DD6.30

PREPARATION AND CHARACTERIZATION OF Pb₂SnF₆, THE FIRST LEAD(II)-TIN(II) FLUORIDE THAT IS A SUPER-STRUCTURE OF α -PbF₂. Raimondo Calandrino, Anthony Collin, Georges Denes, Morgane Logiou, and M. Cecilia Madamba, Concordia University, Department of Chemistry and Biochemistry, Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, Laboratories for Inorganic Materials, Montreal, Quebec, CANADA.

SESSION DD7: FILMS AND CATALYTIC MATERIALS

Chairs: Allan J. Jacobson and Terrell A. Vanderah
Wednesday Morning, December 4, 2002
Back Bay C (Sheraton)

8:30 AM *DD7.1

EPITAXIAL STABILISATION IN THIN FILMS OF OXIDES. Andrey R. Kaul, Oleg Yu. Gorbenko, Igor E. Graboy, Mikhail A. Novojilov, Alexei A. Bosak, Anton A. Kamenev and Sergey V. Samoilenkov, Moscow State University, Department of Chemistry, Moscow, RUSSIA.

9:00 AM DD7.2

THIN FILM SYNTHESIS OF HEXAGONAL RARE-EARTH MANGANESE OXIDES. Balasubramanian Kavaipatti, Antoine Berret, and Paul A. Salvador, Carnegie Mellon University, Department of Materials Science and Engineering, Pittsburgh, PA.

9:15 AM DD7.3

HIGH QUALITY ERBIUM-DOPED BISMUTH-BASED OXIDE FILM FOR PLANER WAVEGUIDE AMPLIFIER PREPARED BY SPUTTERING. Susumu Suzuki, Yuki Kondo, Tatsuo Nagashima, Setsuro Ito, Research Center, Asahi Glass Co., Ltd., Yokohama, JAPAN.

9:30 AM DD7.4

THIN FILMS OF TITANIUM DIOXIDE PREPARED BY CHEMICAL ROUTES USING NOVEL PRECURSORS. K. Shalini, Materials Research Centre; S. Chandrasekaran, Department of Organic Chemistry; S.A. Shivashankar, Materials Research Centre, Indian Institute of Science, Bangalore, INDIA.

9:45 AM BREAK

10:15 AM *DD7.5

DESIGNING NEW PHOTOCATALYSTS AND TRANSPARENT CONDUCTORS: ELECTRONIC STRUCTURE STUDIES OF COMPLEX SEMICONDUCTING METAL OXIDES. Patrick M. Woodward, Hiroshi Mizoguchi, and Hank W. Eng, Ohio State University, Dept. of Chemistry, Columbus, OH.

10:45 AM DD7.6

ORIENTATION DEPENDENCE OF THE PHOTOCHEMICAL REACTIVITY OF Sr₂Nb₂O₇ AND BaTi₄O₇. Jennifer L. Giocondi, Ariana M. Zimbouski, Shahrzad Samadzadeh, Gregory S. Rohrer, Carnegie Mellon University, Dept of Materials Science and Engineering, Pittsburgh, PA.

11:00 AM DD7.7

THE CATALYTIC AND REACTIVE ACTIVITY OF SILICON/SILICA NANOSTRUCTURES PREPARED FROM METAL/METAL OXIDES AT HIGH TEMPERATURES. James Gole and Amanda Jacob, School of Physics, and Brian D. Shinall, Alexei V.

Iretskii, and Mark G. White, School of Chemical Engineering, Georgia Institute of Technology, Atlanta, GA; Ann S. Erickson, Department of Chemistry, Department of Physics, Reed College, Portland, OR.

11:15 AM DD7.8

MIXED-ANIONS (O, S, F) RARE EARTH-BASED COMPOUNDS: DESIGN AND OPTICAL PROPERTIES. Damien Pauwels, Alain Demourgues, Alain Tressaud, Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB-CNRS), Pessac, FRANCE.

11:30 AM DD7.9

OPTICAL AND TRANSPORT PROPERTIES OF P-TYPE BaCuXF (X=S, Se). H. Yanagi, J. Tate, Department of Physics, Oregon State University, Corvallis, OR; S-M. Park, C-H. Park and D.A. Keszler Department Chemistry, Oregon State University, Corvallis, OR.

11:45 AM DD7.10

ON THE NATURE AND STRUCTURE OF NEW MoVTeO AND MoVTeNbO CRYSTALLINE PHASES. E. Garcia-Gonzalez, J.M. Gonzalez-Calbet, Dpto Quimica Inorgánica, Facultad de Químicas, Universidad Complutense de Madrid, SPAIN; J.M. Lopez-Nieto, P. Botella, B. Solsona, Inst Tecnología Química, UPV-CSIC, Valencia, SPAIN.

SESSION DD8: CMR MATERIALS

Chairs: Daniel I. Khomskii and Kevin E. Smith
Wednesday Afternoon, December 4, 2002
Back Bay C (Sheraton)

1:30 PM *DD8.1

NON-STOICHIOMETRY, STRUCTURE AND MAGNETIC PROPERTIES OF LAYERED MANGANESE OXIDES. Lisa Gillie, Helen Palmer, Colin Greaves, School of Chemical Sciences, University of Birmingham, Birmingham, UNITED KINGDOM; Joke Hadermann, Gustaaf Van Tendeloo, EMAT, RUCA, Antwerp, BELGIUM.

2:00 PM DD8.2

INVESTIGATION OF ORDERED SINGLE PHASE Sr₂FeMoO₆ AND ITS SOLID SOLUTION WITH LaFeO₃. M.R. Suhomel, P.K. Davies, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA.

2:15 PM DD8.3

LARGE EFFECTS OF A-SITE AVERAGE CATION SIZE ON THE PROPERTIES OF THE DOUBLE PEROVSKITES, Ba_{2-x}Sr_xMnReO₆: A d⁵-d¹ SYSTEM. Guerman Popov, Martha Greenblatt, Department of Chemistry and Chemical Biology; Mark Croft, Department of Physics and Astronomy, Rutgers, the State University of New Jersey, Piscataway, NJ.

2:30 PM DD8.4

DISORDERLY CONDUCT IN Bi₂Ln₂Ti₃O₁₂ AURIVILLIUS PHASES (Ln = La, Pr, Nd, Sm). N.C. Hyatt, Department of Engineering Materials, The University of Sheffield, Sheffield, UNITED KINGDOM; J.A. Hriljac, School of Chemical Sciences, The University of Birmingham, Birmingham, UNITED KINGDOM.

2:45 PM BREAK

3:15 PM *DD8.5

TOWARDS AN UNDERSTANDING OF THE COLLOSAL MAGNETORESISTANCE BEHAVIOR IN A₁₄MnPn₁₁ COMPOUNDS. Susan M. Kauzlarich, Department of Chemistry, University of California, Davis, Davis, CA.

3:45 PM DD8.6

DESIGNING CRYSTAL STRUCTURES FROM ATOMS UP. Enkhe Dashjav, Holger Kleinke, Dept. of Chemistry, University of Waterloo, Waterloo, Ontario, CANADA.

4:00 PM DD8.7

Abstract Withdrawn

4:15 PM DD8.8

NEUTRON DIFFRACTION STUDY OF ALaMnMoO₆ (A=Ba, Sr) DOUBLE PEROVSKITES. M.V. Lobanov, M. Greenblatt, Rutgers University, Piscataway, NJ; E.N. Caspi, J.D. Jorgensen, Argonne National Laboratory, Argonne, IL.

4:30 PM DD8.9

VACANCY-DOPED Nd_{1-x}TiO₃. MAGNETIC AND TRANSPORT PROPERTIES AT THE METAL-INSULATOR TRANSITIONS. Athena Sefa-Sefat, John E. Greedan, McMaster Univ, Chemistry Dept, Hamilton, Ontario, CANADA.

4:45 PM DD8.10

STRUCTURAL AND PHYSICAL PROPERTY TRENDS OF THE HYPERSTOICHIOMETRIC RUDDLEDEN-POPPER SYSTEM, $\text{La}_2\text{Ni}_{(1-x)}\text{Co}_x\text{O}_{4+d}$ ($0 \leq x \leq 1$). Gisele Amow, Pamela Whitfield, Isobel Davidson, Institute for Chemical Process and Environmental Technology, National Research Council, Ottawa, Ontario, CANADA; Stephen Skinner, Centre for Ion Conducting Membranes, Department of Materials, Imperial College of Science, Technology & Medicine, London, UNITED KINGDOM.

SESSION DD9: NANOMATERIALS
Chairs: Martha Greenblatt and Angus Paul Wilkinson
Thursday Morning, December 5, 2002
Back Bay C (Sheraton)

8:30 AM *DD9.1

INORGANIC NANORODS: SYNTHESIS, PROPERTIES, APPLICATIONS. Paul Alivisatos, Univ of California-Berkeley, Dept of Chemistry and Lawrence Berkeley National Lab, Berkeley, CA.

9:00 AM DD9.2

SOLUTION-PHASE APPROACHES TO CHALCOGEN AND CHALCOGENIDE NANOWIRES. Byron Gates, Brian Mayers and Younan Xia, University of Washington, Department of Chemistry, Seattle, WA.

9:15 AM DD9.3

ELECTRONIC ORIGIN OF SINGLE WALL CARBON NANOTUBE ACTUATION. Miklos Kertesz, Guangyu Sun, Jenő Kurti, Georgetown University, Department of Chemistry, Washington, DC; Ray H. Baughman, Department of Chemistry and NanoTech Institute, University of Texas at Dallas, Richardson, TX.

9:30 AM DD9.4

NUCLEATION AND GROWTH OF GALLIUM OXIDE TUBES, NANOPAINTBRUSHES AND NANOWIRES FROM MOLTEN GALLIUM. Shashank Sharma, Mahendra K. Sunkara, University of Louisville, Department of Chemical Engineering, Louisville, KY.

9:45 AM BREAK**10:15 AM *DD9.5**

FUNCTIONAL NANOWIRES. Peidong Yang, Department of Chemistry, University of California, Berkeley, CA.

10:45 AM DD9.6

ENERGETICS OF ZIRCONIA NANOCRYSTALS. Michael Pitcher and Alexandra Navrotsky, University of California, Davis, CA.

11:00 AM DD9.7

USING THREE DIMENSIONS IN NANOSTRUCTURED, MESOPOROUS Au-TiO_2 FOR SMALL-MOLECULE OXIDATION. Jeremy Pietron^a, Rhonda M. Stroud^b, and Debra R. Rolison^a; Surface Chemistry Branch, ^aCode 6170 and Surface Modification Branch, ^bCode 6370 Naval Research Laboratory, Washington, DC.

11:15 AM DD9.8

LYOTROPIC LIQUID CRYSTAL MEDIATED SYNTHESIS OF BISMUTH AND BISMUTH ALLOY NANOPARTICLES THAT EXHIBIT QUANTUM CONFINEMENT. T.M. Dellinger and P.V. Braun, Dept. of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL.

11:30 AM DD9.9

CHALCOGENIDE-BASED AEROGELS: A NEW CLASS OF NANOSTRUCTURED SEMICONDUCTORS DEMONSTRATING HIGH POROSITY. Jaya L. Mohanan, Shimanti Dasgupta, Heather Perrone, Janusz Brniak, Stephanie L. Brock, Wayne State Univ, Dept of Chemistry, Detroit, MI.

SESSION DD10: THERMOELECTRIC MATERIALS
Chairs: Mercuri G. Kanatzidis and C. Austen Angell
Thursday Afternoon, December 5, 2002
Back Bay C (Sheraton)

1:30 PM *DD10.1

SOLVING NEIGHBORING ELEMENT PROBLEMS IN TYPE-I CLATHRATES AND OTHER COMPLEX MATERIALS USING RESONANT DIFFRACTION. Angus P. Wilkinson, Georgia Institute of Technology, School of Chemistry and Biochemistry, Atlanta, GA; Yuegang Zhang, Peter L. Lee, SRI CAT, Advanced Photon Source, Argonne National Laboratory, IL; George S. Nolas, University of South Florida, Department of Physics, Tampa, FL.

2:00 PM DD10.2

MAGNETIC STRUCTURE AND EXCHANGE INTERACTIONS IN THE $\text{Eu}_4\text{Ga}_8\text{Ge}_{16}$. Henrik Birkedal, J. Daniel Bryan, Galen D. Stucky, Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA; Mogens Christensen, Bo B. Iversen, Department of Chemistry, University of Aarhus, Aarhus, DENMARK.

2:15 PM DD10.3

IMPROVEMENT OF THERMOELECTRIC PROPERTY OF OXIDE CERAMICS BY NANO-STRUCTURAL CONTROL. Masanobu Awano, Yoshinobu Fujishiro, Synergy Materials Research Center, AIST, Nagoya, JAPAN; Osamu Shiono, Shingo Katayama, Synergy Ceramics Lab, FCRA, Nagoya, JAPAN.

2:30 PM DD10.4

ENHANCED THERMOELECTRIC PROPERTIES OF $(\text{Ca}_2\text{CoO}_{3-\delta})_{0.62}\text{CoO}_2$ POLYCRYSTALLINE BULK BY CONTROL OF MICROSTRUCTURE AND OXYGEN CONTENT. M. Sano, S. Horii, K. Otzsch, J. Shimoyama and K. Kishio, Univ. of Tokyo, Dept. of Superconductivity, Tokyo, JAPAN; I. Matsubara, M. Shikano, R. Funahashi, National Institute of Advanced Industrial Science and Technology, Kansai, Osaka, JAPAN.

2:45 PM BREAK**3:15 PM DD10.5**

SYNTHESIS OF $[\text{Ca}_2(\text{Co}_{1-x}\text{Cu}_x)_2\text{O}_4]_z\text{CoO}_2$ SINGLE CRYSTALS AND THEIR INTRINSIC PROPERTIES. M. Suzuki, M. Sano, K. Fujie, K. Otzsch, S. Horii, J. Shimoyama and K. Kishio, Dept. of Superconductivity, Univ. of Tokyo, Tokyo, JAPAN.

3:30 PM *DD10.6

NEGATIVE THERMAL EXPANSION IN OXIDES. Arthur Sleight, Oregon State University, Dept of Chemistry, Corvallis, OR.

4:00 PM DD10.7

SELECTIVE PREPARATION OF NICKEL SILICIDES AND NICKEL GERMANIDES FROM MULTILAYER REACTANTS. Jacob M. Jensen, Sochetra Ly, David C. Johnson, University of Oregon, Dept of Chemistry and Materials Science Institute, Eugene, OR.

SESSION DD11: POSTER SESSION
DIELECTRICS, CATALYSTS, PHOSPHORS, FILMS,
PROPERTIES

Chair: Miguel A. Alario-Franco
Thursday Evening, December 5, 2002
8:00 PM
Exhibition Hall D (Hynes)

DD11.1

NOVEL STRUCTURAL BEHAVIOR OF THE STRONTIUM ALUMINATE DOPED WITH EUROPIUM. W.S. Shi, K. Nishikubo, C.N. Xu, National Institute of Advanced Industrial Science and Technology (AIST), Kyushu, Tosu, Saga, JAPAN; H. Yamada, C.N. Xu, PRESTO, Japan Science and Technology Corporation (JST), Kawaguchi, JAPAN.

DD11.2

PREPARATION OF STRONTIUM TITANATE THIN FILMS BY ELECTROCHEMICAL METHOD AT LOW TEMPERATURE. Jian Bi, Dingquan Xiao, Daojiang Gao, Ping Yu, Wen Zhang, Dunmin Lin, Sichuan Univ, Dept of Materials Science, Chengdu, P.R. CHINA.

DD11.3

$\text{BaNi}_2\text{V}_2\text{O}_8$: A TWO-DIMENSIONAL HONEYCOMB ANTIFERROMAGNET. N. Rogado, R.J. Cava, Princeton Univ, Dept of Chemistry and Princeton Materials Institute, Princeton, NJ; Q. Huang, J.W. Lynn, National Institute of Science and Technology, NIST Center for Neutron Research, Gaithersburg, MD; A.P. Ramirez, Los Alamos National Lab, Dept of Thermal Physics, Los Alamos, NM; D. Huse, Princeton Univ, Dept of Physics, Princeton, NJ.

DD11.4

STEP MOTIONS AT $\text{NaCl}(001)$ SURFACE AT ELEVATED TEMPERATURES STUDIED WITH ATOMIC FORCE MICROSCOPY. Hitoshi Shindo, Takashi Hiyama, Chuo Univ, Dept of Applied Chemistry, Tokyo, JAPAN.

DD11.5

FRICTIONAL FORCE MICROSCOPIC DETECTION OF ANISOTROPY AND ASYMMETRY AT $(10\bar{1}4)$ SURFACE OF $\text{CaLCITE}(\text{CaCO}_3)$. Musun Kwak, Hitoshi Shindo, Chuo Univ, Dept of Science and Engineering, Tokyo, JAPAN.

DD11.6

CONTROLLED SYNTHESIS OF BARIUM, STRONTIUM AND TITANIUM PRECURSORS FOR THE PRODUCTION OF BARIUM AND STRONTIUM TITANATE THIN FILMS BY MOCVD – TECHNIQUE. Denis V. Sevastyanov, Vladimir G. Sevastyanov, Nikolai T. Kuznetsov, Institute of General and Inorganic Chemistry, Moscow, RUSSIA; Elizaveta P. Simonenko, Moscow State Academy of Fine Chemical Technology, Moscow, RUSSIA; Tim Kemmitt, Industrial Research Ltd, Lower Hutt, NEW ZEALAND; Boris I. Petrov, Institute of Metalloorganic Chemistry, Nizhni Novgorod, RUSSIA.

DD11.7

HIGH FREQUENCY MOLECULAR REORIENTATION AND ION MOBILITY IN POROUS FAU TYPE ALUMINOSILICATE HOSTS. David C. Doetschman, Randy C. Mehlenbacher, Binghamton University, Dept. of Chemistry, Binghamton, NY; David W. Dwyer, Science Applications International Corporation, P.A. & E., Arlington, VA.

DD11.8

VIBRATIONAL SPECTROSCOPY AND MASNMR OF A MIXED (${}^7\text{Li}^+$, ${}^2\text{H}^+$) FORM CRYPTOMELANE-TYPE MANGANIC ACID. Masamichi Tsuji, Tokyo Institute of Technology, Research Center for Carbon Recycling and Energy, Tokyo, JAPAN; Younkee Paik, Clare P. Grey, State University of New York at Stony Brook, Stony Brook, NY; Satoshi Murao, National Institute of Advanced Industrial Science and Technology, Institute for Geo-resources and Environment, Tsukuba, JAPAN.

DD11.9

STRUCTURE AND PROPERTIES OF NEW LI-BASED ORDERED PEROVSKITES. Albina Y. Borisevich and Peter K. Davies, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA.

DD11.10

THERMODYNAMICS OF SOLID SOLUTION FORMATION IN CoO-MgO. Lan Wang and Alexandra Navrotsky, University of California-Davis, Davis, CA.

DD11.11

LOCAL STRUCTURE AND PROPERTIES OF THE $(1-x)\text{Pb}(\text{Sc}_{2/3}\text{W}_{1/3})\text{O}_3 - (x)\text{Pb}(\text{Ti}/\text{Zr})\text{O}_3$ RELAXOR PEROVSKITES. Pavol Juhás, Wojciech Dmowski, Takeshi Egami, Peter K. Davies, Dept. of Materials Science, Univ. of Pennsylvania, Philadelphia, PA.

DD11.12

OPTICAL PROPERTIES OF RUTILE AND ANATASE PHASES OF TiO_2 THIN FILMS GROWN AT ROOM TEMPERATURE BY RF MAGNETRON SPUTTERING. V.M. Naik, Department of Natural Sciences, University of Michigan-Dearborn, Dearborn, MI; D.B. Haddad and R. Naik, Department of Physics and Astronomy, Wayne State University, Detroit, MI; J. Benci and G.W. Auner, Department of Electrical and Computer Engineering, Wayne State University, Detroit, MI.

DD11.13

A VARIABLE-EMITTANCE RADIATOR BASED ON A METAL-INSULATOR TRANSITION OF $(\text{La},\text{Sr})\text{MnO}_3$. Y. Shimakawa, T. Yoshitake, and Y. Kubo, Fund. Res. Labs., NEC Corporation, Tsukuba, JAPAN; T. Machida and K. Shinagawa, Dep. of Phys. Toho Univ., Funabashi, JAPAN; A. Okamoto and Y. Nakamura, NEC TOSHIBA Space Systems, Ltd., Yokohama, JAPAN; A. Ochi, Func. Mat. Res. Labs., NEC Corporation, Kawasaki, JAPAN; S. Tachikawa and A. Ohnishi, ISAS, Sagami-hara, JAPAN.

DD11.14

USING A NOVEL METHOD COMBINING SOL-GEL AND COMBUSTION SYNTHESIS TECHNIQUES FOR PREPARATION OF Y-Ba-Cu-O SUPERCONDUCTOR. Chyi-Ching Hwang, Ching-Kai Hong, Department of Applied Chemistry, Chung Cheng Institute of Technology, National Defense University, Ta-Hsi, Tao-Yuan, TAIWAN, ROC; Cheng-Hsiung Peng, San-Yuan Chen, Department of Materials Science and Engineering, National Chao Tung University, Hsin-Chu, TAIWAN, ROC.

DD11.15

STRUCTURAL, DIELECTRIC AND PIEZOELECTRIC PROPERTIES OF THE CdTiO_3 - PbTiO_3 - PbZrO_3 AND CdTiO_3 - PbTiO_3 - $(\text{Na}_{0.5}\text{Bi}_{0.5})\text{TiO}_{0.5}$ SYSTEMS. D.Y. Suárez-Sandoval, P.K. Davies, Dept. of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA.

DD11.16

CRYSTAL CHEMISTRY AND ENERGETICS OF PEROVSKITES

ALONG THE NaNbO_3 - SrTiO_3 JOIN. Hongwu Xu, Alexandra Navrotsky, Univ of California at Davis, Dept of Chemical Engineering and Material Sciences, Davis, CA; Yali Su, M. Lou Balmer, Pacific Northwest National Lab, Richland, WA.

DD11.17

ELECTROMAGNETIC AND THERMOELECTRIC CHARACTERISTICS OF Na_xCoO_2 OF PRECISELY CONTROLLED Na-NONSTOICHIOMETRY. Teruki Motohashi, Maarit Karppinen, and Hisao Yamauchi, Tokyo Inst. Tech., Materials & Structures Lab., Yokohama, JAPAN.

DD11.18

THEORETICAL STUDY OF THE ELECTRONIC STRUCTURE OF TIN COMPOUNDS. Pierre-Emmanuel Lippens, Laboratoire des Agregats Moleculaires et Materiaux Inorganiques, CNRS UMR 5072, Universite Montpellier II, Montpellier, FRANCE.

DD11.19

ELECTRICAL AND DIELECTRIC PROPERTIES OF $\text{Bi}_6\text{Ti}_3\text{Mn}_2\text{O}_{18}$. S.V. Suryanarayana, M.B. Suresh, K. Srinivas, E.V. Ramanamurthy, Materials Research Laboratory, Physics Department, Osmania University, Hyderabad, INDIA; G. Swaminathan, BHEL R&D, Hyderabad, INDIA.

DD11.20

OXIDATION-PROTECTION METHODOLOGY FOR LONG-TERM USE OF CARBON-CARBON FIBER-MATRIX COMPOSITES IN OXIDIZING AMBIENTS. Ilan Golecki, Honeywell International (formerly AlliedSignal) Inc., Morristown, NJ; Karen Fuentes, Honeywell International Inc., Torrance, CA; Terence Walker, Honeywell International Inc., South Bend, IN.

DD11.21

STRUCTURE AND DIELECTRIC PROPERTIES OF $\text{Ba}_9\text{ZnTa}_6\text{O}_{24}$. Meganathan Thirumal, Peter K. Davies, University of Pennsylvania, Dept of Materials Science and Engineering, Philadelphia, PA.

DD11.22

THERMOCHEMISTRY OF PEROVSKITE OXIDES LaMO_3 (M = Al, Ga, In AND Sc). Jihong Cheng, Alexandra Navrotsky, University of California at Davis, Thermochemistry Facility, Dept of Chemical Engineering and Materials Science, Davis, CA.

DD11.23

GENERATION OF A LARGE AMOUNT OF ACTIVE OXYGENIC RADICALS O^- AND O_2^- IN AN ANION-ENCAGING CRYSTAL $12\text{CaO}\cdot 7\text{Al}_2\text{O}_3$. Satoru Matsui^{a,b}, Katsuro Hayashi^b, Masahiro Hirano^b and Hideo Hosono^{a,b}; ^aMaterials and Structures Laboratory, Tokyo Institute of Technology, JAPAN; ^bHosono Transparent Electro-Active Materials Project, ERATO, JST, JAPAN.

DD11.24

MODIFIED MATERIAL PROPERTY IN THE Ta/Nb PEROVSKITES BY ALLOVALENT ANIONIC SUBSTITUTION. Young-il Kim, Patrick M. Woodward, Dept of Chemistry, The Ohio State Univ, Columbus, OH.

DD11.25

EVALUATION OF THE THERMODYNAMIC PROPERTIES AND PHASE EQUILIBRIA OF THE Ni-Al-Ta SYSTEM FOR Ni-BASED SUPERALLOYS. Sihuai Zhou, Longqing Chen, Zi-Kui Liu, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA.

DD11.26

HIGH-PRESSURE VOLUME EXPANSION IN THE DEFECT PYROCHLORES ANbWO_6 (A= NH_4^+ , H^+ , Rb^+ , K^+). Paris W. Barnes, Patrick M. Woodward, The Ohio State University, Dept. of Chemistry, Columbus, OH; Yongjae Lee, Thomas Vogt, Brookhaven National Laboratory, Physics Dept., Upton, NY.

DD11.27

MICROSTRUCTURAL STUDIES OF HIGH DIELECTRIC CONSTANT COPPER TITANATE BULK MATERIALS. D.X. Huang, C.Y. Park, L. Chen, and A.J. Jacobson, Materials Research Science and Engineering Center, University of Houston, Houston, TX.

DD11.28

EDGE-DEFINED FILM-FED GROWTH (EFG) AND CHARACTERIZATION OF SINGLE CRYSTAL PIEZOELECTRIC FIBERS. Jian Shen, Benjamin P. Nunes, Andrey N. Soukhovjak, Yet-Ming Chiang, Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, MA.

DD11.29

BAND GAPS OF D⁰ OXIDES: FROM Ti TO W. H.W. Eng, P.M. Woodward, The Ohio State Univ, Dept of Chemistry, Columbus, OH.

DD11.30

THERMOELECTRIC PROPERTIES OF MAGNETICALLY *c*-AXIS ALIGNED POLYCRYSTALS IN (Ca₂Co_mO_{m+2-δ})_{~0.62}CoO₂ (*m*=1 and 2). Shigeru Horii, M. Sano, M. Suzuki, K. Otszchi, J. Shimoyama, and K. Kishio, Univ. of Tokyo, Dept. of Superconductivity, JAPAN; I. Matsubara, M. Shikano, and R. Funahashi, National Institute of Advanced Industrial Science and Technology, Osaka, JAPAN.

DD11.31

SYNTHESIS AND CHARACTERIZATION OF RARE-EARTH SUBSTITUTED BISMUTH IRON TITANATE CERAMIC SYSTEM (R-BIT). Srinivas Adiraj, Dong-Wan Kim, Kug Sun Hong, Seoul National University, School of Materials Science & Engineering, Seoul, SOUTH KOREA.

DD11.32

STRUCTURAL AND MAGNETIC PROPERTIES OF NdBaCo₂O_{5+δ}. Jonathan Burley, John Mitchell, Materials Science Division, Argonne National Laboratory, IL.

SESSION DD12: SYNTHESIS, CRYSTAL GROWTH

Chairs: Arthur W. Sleight and Paul Alivisatos
Friday Morning, December 6, 2002
Back Bay C (Sheraton)

8:30 AM *DD12.1

CRYSTAL GROWTH OF QUATERNARY RUTHENIUM AND OSMIUM CONTAINING PEROVSKITES FROM REACTIVE HYDROXIDE FLUXES. H.-C. zur Loye, K.E. Stitzer, M.D. Smith, University of South Carolina, Department of Chemistry and Biochemistry, Columbia, SC.

9:00 AM DD12.2

BOND VALENCE SUMMATIONS FOR PARTIALLY-DISORDERED PYROCHLORE SOLID SOLUTIONS A₂(B'_yB_{1-y})₂O₇ AND (A'_zA_{1-z})₂B₂O₇. David J. Davis and Bernhardt J. Wuensch, Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, MA; and Kevin W. Eberman, 3M Center, St. Paul, MN.

9:15 AM DD12.3

NEW MATERIALS FROM POLYCHALCOARSENATE FLUXES. Ratnasabapathy G. Iyer and Mercouri G. Kanatzidis, Department of Chemistry, Michigan State University, East Lansing, MI.

9:30 AM DD12.4

SYNTHESIS OF A NEW CLASS OF HYBRID SOLIDS VIA SALT INCLUSION. Qun Huang, Mutlu Kartir, Xunhua Mo, Shiou-Jyh Hwu, Clemson University, Dept of Chemistry, Clemson, SC.

9:45 AM BREAK**10:15 AM DD12.5**

GAS ABSORPTION IN RIGID NANOPOROUS GLASSY NETWORKS PRODUCED BY ORGANIC-INORGANIC SYNTHESIS AND COMPUTER SIMULATION. C.A. Angell, X.-G. Sun, W. Xu, A. Chizmeshya, and A. Kahn, Depts. of Chemistry and Materials Science, Arizona State University, Tempe, AZ.

10:30 AM DD12.6

MODULATED STRUCTURES IN VANADIUM OXIDE INTERCALATES. Peter Y. Zavalij, M. Stanley Whittingham, Institute for Materials Research and Chemistry Department, State University of New York at Binghamton, Binghamton, NY.

10:45 AM DD12.7

UNDERSTANDING OF Li ORDER-DISORDER TRANSITIONS IN Li_xV₂(PO₄)₃ PHASES (x=3.0~0.0) by ⁷Li SOLID STATE NMR AND NEUTRON DIFFRACTION. Shih-Chieh Yin, Linda F. Nazar, Department of Chemistry, University of Waterloo, CANADA; Hiltrud Grondy, Department of Chemistry, University of Toronto, CANADA; Robert Hammond, Chalk River Laboratories, CANADA; Pierre Strobel, ILL, Grenoble, FRANCE.

11:00 AM DD12.8

REINVESTIGATION OF THE INCOMMENSURATE STRUCTURE OF LITHARGE. Gianguido Baldinozzi, Jean-Marc Raultot, Structures, propriétés et modélisation des solides, CNRS-Ecole Centrale Paris, Châtenay-Malabry, FRANCE; Vaclav Petricek, Dept of Physics, Czech Academy of Sciences, Praha, CZECH REPUBLIC;

Georgette Petot, Structures, propriétés et modélisation des solides, CNRS-Ecole Centrale Paris, Châtenay-Malabry, FRANCE.

11:15 AM DD12.9

READY REACTIVITY AND UNEXPECTED PHASE TRANSFORMATION AT THE NANOMETER SCALE. James L. Gole and John Stout, School of Physics, and Zurong Dai and Z.L. Wang, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA; Clemens Burda and Frank Ernst, Case Western Reserve University, Cleveland, OH.

11:30 AM DD12.10

SYNTHESIS AND LATTICE DISTORTION OF FERROELECTRIC/ANTIFERROELECTRIC BISMUTH(III)-CONTAINING PEROVSKITES. Yoshiyuki Inaguma, Atsushi Miyaguchi, and Tetsuhiro Katsumata, Dept. of Chemistry, Gakushuin Univ., Tokyo, JAPAN.

SESSION DD13: SYNTHESIS AND PROPERTIES

Chairs: Hans-Conrad zur Loye and
Bernhardt J. Wuensch
Friday Afternoon, December 6, 2002
Back Bay C (Sheraton)

1:30 PM *DD13.1

DIRECT FABRICATION OF PATTERNED FILMS OF FUNCTIONAL CERAMICS BY ADVANCED SOFT SOLUTION PROCESSING WITHOUT FIRING. Masahiro Yoshimura, Tomoaki Watanabe, Takeshi Fujiwara, and Ryo Teranishi, Materials and Structures Laboratory, Tokyo Institute of Technology, Yokohama, JAPAN.

2:00 PM DD13.2

SYNTHESIS AND PROPERTIES OF ANATASE AND RUTILE Ti_{1-x}Co_xNF. Robert Butterick, Chris Lanci, Samuel Lofland, and K.V. Ramanujachary, Rowan University, Dept of Chemistry and Physics, Glassboro, NJ.

2:15 PM DD13.3

SYNTHESES OF DENSE, NEAR NET-SHAPED, ULTRA-HIGH-MELTING CARBIDE/METAL AND BORIDE/METAL COMPOSITES AT <1300°C BY THE DISPLACIVE COMPENSATION OF POROSITY PROCESS. Matthew Dickerson, Zbigniew Grzesik, Robert Snyder, Ken Sandhage, Dept of Materials Science and Engineering, Ohio State Univ, Columbus, OH.

2:30 PM DD13.4

INTERFACING SOLID STATE AND SOFT MATERIALS. Ulrich Wiesner, Cornell Univ, Dept of Materials Science and Engineering, Ithaca, NY.

2:45 PM BREAK**3:15 PM DD13.5**

RATIONAL DESIGN AND SYNTHESIS OF NEW OXY-HALIDES AND OXIDES THROUGH LOW TEMPERATURE SYNTHETIC STRATEGIES. Thomas A. Kodenkandath, Liliana Viciu, Andrew Bankston and John B. Wiley, Department of Chemistry & Advanced Materials Research Institute, University of New Orleans, New Orleans, LA.

3:30 PM DD13.6

EXPLORATION OF CATION SUBSTITUTION IN THE LAYERED COMPOUND CHROMIUM TUNGSTEN DINITRIDE. K. Scott Weil, Pacific Northwest National Laboratory, Department of Materials Science, Richland, WA; Prashant Kumta, Carnegie Mellon University, Department of Materials Science, Pittsburgh, PA; Jekabs Grins, Stockholm University, Department of Inorganic Chemistry, Stockholm, SWEDEN.

3:45 PM DD13.7

SYNTHESIS AND CHARACTERIZATION OF HETERO-POLYNILOBATES. May Nyman, Francois Bonhomme, Brian R. Cherry, Todd M. Alam, Mark A. Rodriguez, Louise J. Criscenti, Randall T. Cygan, Sandia National Laboratories, Albuquerque, NM.

4:00 PM DD13.8

TEMPLATED GROWTH OF COMPLEX NITRIDE ISLAND DISPERSIONS BY CONTROLLED INTERNAL REACTIONS. Michael Brady, Peter Tortorelli, Joseph Horton, Sarah Wrobel, David Hoelzer, Andrew Payzant, Ian Anderson, Larry Walker, Oak Ridge National Laboratory, Oak Ridge, TN.

4:15 PM DD13.9

NOVEL URANYL MOLYBDATE TRIAZOLATES AND THEIR RELATIONSHIP TO MINERAL STRUCTURES.

Christopher L. Cahill, Nils Schnor, Jacquelynn Danek and Lauren Borkowski, George Washington University, Dept. of Chemistry, Washington, DC.

4:30 PM DD13.10

Abstract Withdrawn

4:45 PM DD13.11

PREPARATION OF IRON(III) OXIDE AND ITS HYDRATES FROM IRON(III) VERSUS THE REACTION PARAMETERS. Meriadeg Charlou, Georges Denes and Andre L. Yonkeu, Concordia University, Department of Chemistry and Biochemistry, Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, Laboratories for Inorganic Materials, Montreal, Quebec, CANADA.