

Solid-State Chemistry of Inorganic Materials VIII

**MATERIALS RESEARCH SOCIETY
SYMPOSIUM PROCEEDINGS VOLUME 1309**

**Solid-State Chemistry
of Inorganic Materials VIII**

Symposium held November 29–December 3, Boston, Massachusetts, U.S.A.

EDITORS

P. Shiv Halasyamani

University of Houston
Houston, Texas, U.S.A.

Simon J. Clarke

University of Oxford
Oxford, United Kingdom

David G. Mandrus

The University of Tennessee
Knoxville, Tennessee, U.S.A.

Kyoung-Shin Choi

Purdue University
West Lafayette, Indiana, U.S.A.



Materials Research Society
Warrendale, Pennsylvania



CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town,
Singapore, São Paulo, Delhi, Tokyo, Mexico City

Cambridge University Press
32 Avenue of the Americas, New York, NY 10013-2473, USA

www.cambridge.org
Information on this title: www.cambridge.org/9781605112862

Materials Research Society
506 Keystone Drive, Warrendale, PA 15086, USA
<http://www.mrs.org>

© Materials Research Society 2011

This publication is in copyright. Subject to statutory exception
and to the provisions of relevant collective licensing agreements,
no reproduction of any part may take place without the written
permission of Cambridge University Press.

This book has been registered with Copyright Clearance Center, Inc.
For further information please contact the Copyright Clearance Center,
Salem, Massachusetts.

First published 2011

Printed in the United States of America

This work was supported in part by the National Science Foundation, Division
of Materials Research - Solid-State Chemistry under grant number DMR-1041307.
The views, opinions, and/or findings contained in this report are those of
the author(s) and should not be construed as an official position, policy, or
decision by the supporter, unless so designated by other documentation.

Single article reprints from this publication are available through
University Microfilms Inc., 300 North Zeeb Road, Ann Arbor, MI 48106

CODEN: MRSPDH

ISBN: 978-1-605-11286-2 Hardback

Cambridge University Press has no responsibility for the persistence or
accuracy of URLs for external or third-party Internet Web sites referred to
in this publication and does not guarantee that any content on such Web sites
is, or will remain, accurate or appropriate.

CONTENTS

Preface ix

Materials Research Society Symposium Proceedings xi

NOVEL SYNTHETIC METHODS

Superconducting Parent Compound Pr_2CuO_4 Achieved
by Special Post-reduction 3

Hideki Yamamoto, Osamu Matsumoto,
Keitaro Yamagami, Michio Naito,
and Yoshiharu Krockenberger

Controlled Hydrothermal Synthesis of Complex Mixed Oxides
Using Solution Redox Chemistry 9

Richard I. Walton, Kripasindhu Sardar,
Helen Y. Playford, Deena R. Modeshia,
Richard J. Darton, Janet Fisher,
and David Thompsett

Building 3D Materials from Adjustable 2D-units; Towards
the Design of New Bi-based Compounds 15

M. Colmont, D. Endara, M. Huvé,
S.V. Krivovichev, and O. Mentré

POSTER SESSION: SOLID STATE CHEMISTRY OF INORGANIC MATERIALS VIII

Growth of Ruthenium and Ruthenium Oxide Nanoplates 23
Lamartine Meda and Geoffrey D. Stevens

Synthesis of Layered Titanate Micro/Nano-materials for Efficient
Pollutant Treatment in Aqueous Media 27

Y.X. Tang, Y.K. Lai, D.G. Gong,
Zhili Dong, and Z. Chen

Thermodynamic Aspects of Transition Metals Doped ZnO 33
David Sedmidubský, Zdeněk Sofer,
Štěpán Huber, and Jindřich Leitner

What is the True Nature of Conducting Proton in Perovskite Ceramic Membrane: Hydroxyl Ion or Interstitial Proton?	39
Aneta Slodczyk, Philippe Colomban, Oumaya Zafrani, Olivier Lacroix, Johan Loricourt, Frederic Grasset, and Beatrice Sala	
Thermodynamics of Oxygen Chemistry on PbTiO₃ and LaMnO₃ (001) Surfaces.....	45
Ghanshyam Pilania and R. Ramprasad	
The Effect of Boron on Processing and Phosphorescence Behavior of SrAl₄O₇ (SA₂) Co-doped with Eu²⁺ and Dy³⁺	51
Murat G. Eskin, Hasan Kurt, Mehmet Ali Gulgur, and Cleva W. Ow-Yang	
pO₂ stability of Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-δ}	57
Stefan F. Wagner, Simon Taufall, Christian Niedrig, Holger Götz, Wolfgang Meneskou, Stefan Baumann, and Ellen Ivers-Tiffée	

THERMOELECTRICS AND RELATED MATERIALS

* Thermoelectric Properties of New Thallium Tellurides	67
Cheriyedath Raj Sankar, Savitree Bangarigadu-Sanasy, and Holger Kleinke	

POSTER SESSION: SOLID STATE INORGANIC MATERIALS CHEMISTRY - VIII

DLC-coated Substrate for Infrared Absorption Spectroscopy in Supercritical Water	79
Takuji Ube and Takashi Ishiguro	
Two-step Sintering Process for Lutetium Oxide Transparent Ceramics	85
Xiaomei Guo, Kewen K. Li, Yanyun Wang, Yingyin K. Zou, and Hua Jiang	
Low Temperature Phase Diagram of NH₃BH₃	91
Bertil Sundqvist, Ove Andersson, Issam Quwar, and Alexandr Talyzin	

*Invited Paper

Growth and Characterization of Shape-controlled Single Crystals by a Micro-pulling-down Method.....	97
Yuu Yokota, Hidehiko Tanaka, Masato Sato, Valery Chami, Kazushige Tota, Ko Onodera, Takayuki Yanagida, and Akira Yoshikawa	
Correlation between Deep-Level Defects and Current Collapses in AlGaN/GaN Heterostructures Probed by Steady-State Photo-Capacitance Spectroscopy.....	101
Yoshitaka Nakano, Yoshihiro Irokawa, Yasunobu Sumida, Shuichi Yagi, and Hiroji Kawai	
Deep-Level Characterization of Free-Standing HVPE-grown GaN Substrates Using Transparent Conductive Polyaniline Schottky Contacts	107
Yoshitaka Nakano, Nobuyuki Matsuki, Mickael Lozac'h, Kazuaki Sakoda, and Masatomo Sumiya	
Hydrogen Atom Adsorption on Aluminum Clusters: An Electronic Structures Density Functional Study.....	113
Phung Thi Viet Bac and Hiroshi Ogawa	
Synthesis and Characterization of Indium Oxide-doped Hematite $x\text{In}_2\text{O}_3 \cdot (1-x)\alpha\text{-Fe}_2\text{O}_3$ Solid Solution.....	119
Monica Sorescu, Tianhong Xu, and Lucian Diamandescu	
Periodically Ordered Mesoporous Co_3O_4/Heteropoly Acid Composite Frameworks for Catalytic Applications	125
Gerasimos S. Armatas, Ioannis Tamiolakis, and Dimitris E. Petrakis	
Preparation of Protonated Titanate Nanotube Films with an Extremely Large Wetting Contrast	133
Y.K. Lai, Y.X. Tang, D.G. Gong, J.J. Gong, Y.C. Chen, C.J. Lin, and Z. Chen	
 <i>WIDE-BAND-GAP SEMICONDUCTORS AND CATALYTIC MATERIALS</i>	
A DFT and HRTEM Study on MoS_2/Co: Locating Promoters in Catalytic Nanostructures	141
Manuel Ramos, Gilles Berhault, Jose Rurik Farias, Jose Trinidad Elizalde, Domingo Ferrer, Brenda Torres, and R.R. Chianelli	

POROUS MATERIALS AND METAL-ORGANIC FRAMEWORKS

Covalently Interconnected and Separated Vanadosilicate Shells	151
Xiqu Wang, Lumei Liu, and Allan J. Jacobson	
Author Index	157
Subject Index	159

PREFACE

Symposium EE, "Solid-State Chemistry of Inorganic Materials VIII," was held Nov. 29–Dec. 3 at the 2010 MRS Fall Meeting in Boston, Massachusetts. Solid-state chemistry is a truly interdisciplinary field, attracting investigators from chemistry, condensed-matter physics, materials science engineering, ceramics, metallurgy, chemical engineering, and mineralogy/geology, to name but a few. Solid-state chemistry encompasses synthesis of new materials, preparation of materials in new forms (nanocrystalline, thin-film heterostructures, porous, etc.), investigations of the relationships between composition, structure and properties, as well as the application of cutting-edge characterization methods. The scope and importance of solid-state chemistry has grown not only with the discovery of new materials but also through the advancement of techniques for preparing and studying them, and in advanced computational predictions for structures and properties. Our knowledge of the diverse properties of solids continues to expand. The intent of the symposium was to provide researchers from academics, government, and industrial laboratories an interdisciplinary forum for interaction, discussion, and exchange of ideas on recent fundamental advances in Solid-State Chemistry and their impact on the development and application of inorganic materials.

Important topics that were covered in this symposium included:

- Synthetic methods for new and novel materials.
- Structure-property-theory relationships
- Crystal chemistry, including incommensurate structures
- New computational and theoretical methods in solid-state materials
- Battery, fuel cell, and materials for energy
- Dielectric and multiferroic materials
- Microporous and nanostructural materials
- Novel magnetic, optical and electronic properties

The organizers thank the National Science Foundation – Division of Materials Research (DMR-1041307), The University of Houston, and Materials Research Society for financial support.

P. Shiv Halasyamani
Simon J. Clarke
David G. Mandrus
Kyoung-Shin Choi

February 2011

MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS

- Volume 1275— Structural and Chemical Characterization of Metals, Alloys and Compounds, R. Pérez Campos, A. Contreras Cuevas, R.A. Esparza Muñoz, 2011, ISBN 978-1-60511-252-7
- Volume 1276— Advanced Structural Materials—2010, H.A. Calderon, A. Salinas Rodriguez, H. Balmori-Ramirez, 2010, ISBN 978-1-60511-253-4
- Volume 1277E— Biomaterials—2010, S.E. Rodil, A. Almaguer-Flores, K. Anselme, 2010, ISBN 978-1-60511-254-1
- Volume 1278E— Composite, Hybrid Materials and Ecomaterials, R. Bernal, C. Cruz Vazquez, L.E. Rendon Diaz Miron, V.M. Castaño, 2010, ISBN 978-1-60511-255-8
- Volume 1279— New Catalytic Materials, J.A. Wang, J. Manuel Domínguez, 2010, ISBN 978-1-60511-256-5
- Volume 1280E— Nanomaterials for Biomedical Applications, L. Zhang, T.J. Webster, A. Salinas Rodriguez, 2010, ISBN 978-1-60511-257-2
- Volume 1282— Diamond Electronics and Bioelectronics—Fundamentals to Applications IV, P. Bergonzo, J.E. Butler, C.E. Nebel, M. Nesladek, A.T.S. Wee, 2011, ISBN 978-1-60511-259-6
- Volume 1283E— Carbon-Based Electronic Devices—Processing, Performance and Reliability, M. Chhowalla, R.R. Keller , M. Meyyappan, W.J. Ready, 2011, ISBN 978-1-60511-260-2
- Volume 1284— Fundamentals of Low-Dimensional Carbon Nanomaterials, J.J. Boeckl, L. Dai, W. Lu, M.H. Rummeli, J. Warner, 2011, ISBN 978-1-60511-261-9
- Volume 1285E— Challenges in Roll-to-Roll (R2R) Fabrication for Electronics and Other Functionalities, T. Blauddeck, G. Cho, J.H. Daniel, M.R. Dokmeci, 2011, ISBN 978-1-60511-262-6
- Volume 1286E— Molecular and Hybrid Materials for Electronics and Photonics, J. Liu, 2011, ISBN 978-1-60511-263-3
- Volume 1287E— Low-Temperature-Processed Thin-Film Transistors, E. Fortunato, 2011, ISBN 978-1-60511-264-0
- Volume 1288E— Novel Fabrication Methods for Electronic Devices, P. Andrew, 2011, ISBN 978-1-60511-265-7
- Volume 1289E— Controlling Material Properties and Charge-Carrier Interactions with Quantum-Dot Coupling, 2011, ISBN 978-1-60511-266-4
- Volume 1290E— Magnetism and Correlated Electronic Structure of Nitrides—Rare-Earth and Transition Metals as Constituents and Dopants, W.R.L. Lambrecht, A. Ney, K. Smith, H.J. Trodahl, 2011, ISBN 978-1-60511-267-1
- Volume 1291E— Integrated Nonreciprocal Photonics—Materials, Phenomena and Devices, V. Fratello, M. Levy, B. Stadler, M. Vanwolleghem, 2011, ISBN 978-1-60511-268-8
- Volume 1292— Oxide Nanoelectronics, H. Hwang, J. Levy, P. Makysymovych, G. Medeiros-Ribeiro, R. Waser, 2011, ISBN 978-1-60511-269-5
- Volume 1293E— Liquid-Crystal Materials—Beyond Displays, N.L. Abbott, D.J. Broer, T. Kato, T.J. White, 2011, ISBN 978-1-60511-270-1
- Volume 1294E— Resonant Optical Antennas—Sensing and Shaping Materials, K.B. Crozier, N. Engheta, G. Ju, R. Quidant, R. Zia, 2011, ISBN 978-1-60511-271-8
- Volume 1295— Intermetallic-Based Alloys for Structural and Functional Applications, M. Palm, B. Bewlay, S. Kumar, K. Yoshimi, 2011, ISBN 978-1-60511-272-5
- Volume 1296E— New Methods in Steel Design—Steel Ab Initio, Y. Adachi, R. Dronskowski, D. Raabe, P.E.A. Turchi, 2011, ISBN 978-1-60511-273-2
- Volume 1297— Deformation Mechanisms, Microstructure Evolution and Mechanical Properties of Nanoscale Materials, J.R. Greer, D.S. Gianola, B.G. Clark, T. Zhu, A.H.W. Ngan, 2011, ISBN 978-1-60511-274-9
- Volume 1298— Advanced Materials for Applications in Extreme Environments, T.S. Byun, R. Smith, M. Li, 2011, ISBN 978-1-60511-275-6
- Volume 1299— Microelectromechanical Systems—Materials and Devices IV, M.P. de Boer, F.W. DelRio, C. Eberl, E.P. Gusev, 2011, ISBN 978-1-60511-276-3
- Volume 1300E— Bulk Metallic Glasses and their Applications, K.F. Yao, 2011, ISBN 978-1-60511-277-0

MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS

- Volume 1301— Soft Matter, Biological Materials and Biomedical Materials—Synthesis, Characterization and Applications, A.J. Nolte, K. Shiba, R. Narayan, D. Nolte, 2011, ISBN 978-1-60511-278-7
- Volume 1302E—Nanowires—Growth and Device Assembly for Novel Applications, 2011, ISBN 978-1-60511-279-4
- Volume 1303— Nanomaterials Integration for Electronics, Energy and Sensing, D. E. Perea, Y. Jung, J. B. Hannon, M. A. Reed, S. T. Picraux, 2011, ISBN 978-1-60511-280-0
- Volume 1304E—Hierarchical Materials and Composites—Combining Length Scales from Nano to Macro, J.H. Moon, G.M. Odegard, M.S.P. Shaffer, B.L. Wardle, 2011, ISBN 978-1-60511-281-7
- Volume 1305E—Group IV Semiconductor Nanostructures and Applications, L. Dal Negro, 2011, ISBN 978-1-60511-282-4
- Volume 1306E—Aerogels and Aerogel-Inspired Materials, S. Brock, G. Gould, A. Roig, D. Rolison, 2011, ISBN 978-1-60511-283-1
- Volume 1307E—Boron and Boron Compounds—From Fundamentals to Applications, M. Dudley, J.H. Edgar, M. Kuball, 2011, ISBN 978-1-60511-284-8
- Volume 1308E—Artificially Induced Crystalline Alignment in Thin Films and Nanostructures, A.T. Findikoglu, R. Huehne, T. Shimada, J.Z. Wu, 2011, ISBN 978-1-60511-285-5
- Volume 1309— Solid-State Chemistry of Inorganic Materials VIII, K-S. Choi, S.J. Clarke, P.S. Halasyamani, D.G. Mandrus, 2011, ISBN 978-1-60511-286-2
- Volume 1310E—Magneto Calorics and Magnetic Cooling, A. Fujita, K. Gschneidner Jr., O. Gutfleisch, K.G. Sandeman, A. Yan, 2011, ISBN 978-1-60511-287-9
- Volume 1311— Next-Generation Fuel Cells—New Materials and Concepts, T. He, K. Swider-Lyons, B. Park, P.A. Kohl, 2011, ISBN 978-1-60511-288-6
- Volume 1312— Polymer-Based Materials and Composites—Synthesis, Assembly, Properties and Applications, V. Bharti, M. Chipara, D. Venkataraman, 2011, ISBN 978-1-60511-289-3
- Volume 1313— Materials for Advanced Lithium Batteries, G.-A. Nazri, J-M Tarascon, D. Guyomard, A. Yamada, 2011, ISBN 978-1-60511-290-9
- Volume 1314E—Thermoelectric Materials for Solid-State Power Generation and Refrigeration, Y. Grin, G.S. Nolas, J. Sharp, T.M. Tritt, 2011, ISBN 978-1-60511-291-6
- Volume 1315— Transparent Conducting Oxides and Applications, J.J. Berry, E. Fortunato, J. Medvedeva, Y. Shigesato, 2011, ISBN 978-1-60511-292-3
- Volume 1316E—Nanofunctional Materials, Nanostructures and Nanodevices for Biomedical Applications II, R. Rao, 2011, ISBN 978-1-60511-293-0
- Volume 1317E—Interdisciplinary Approaches to Safe Nanotechnologies, C. Chaneac, S. Harper, G.V. Lowry, R.I. MacCuspie, 2011, ISBN 978-1-60511-294-7
- Volume 1318— Advances in Spectroscopy and Imaging of Surfaces and Nanostructures, J. Cumings, J. Guo, F.M. Granozio, O.V. Kolosov, 2011, ISBN 978-1-60511-295-4
- Volume 1319— Materials Issues in Art and Archaeology IX, P.B. Vandiver, C.L. Reedy, J.L. Ruvalcaba Sil, W. Li, 2011, ISBN 978-1-60511-296-1
- Volume 1320— Materials Education Development and Outreach—From K-Grad, D. Bahr, K. Jones, M. Glass, E. Allen, 2011, ISBN 978-1-60511-297-8

Prior Materials Research Society Symposium Proceedings available by contacting Materials Research Society