

Program

Nonstoichiometric Compounds V

Taormina, Sicily, Italy

September 23-28, 2012

Conference Co-Chairs

Professor Juergen Janek

Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany

Professor Lorenzo Malavasi

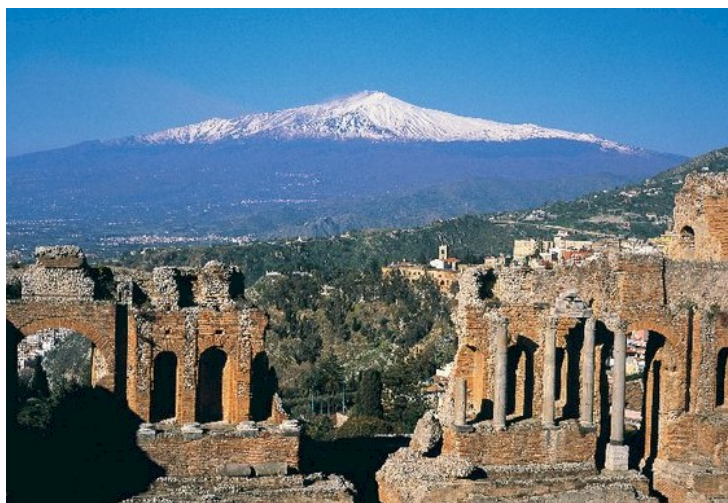
Department of Chemistry, University of Pavia, Italy

Professor Tatsuya Kawada

Graduate School of Environmental Studies, Tohoku University, Japan

Professor Ryan O'Hayre

Colorado Center for Advanced Ceramics Metallurgical and Materials
Engineering, Colorado School of Mines, USA



Engineering Conferences International

32 Broadway, Suite 314

New York, NY 10004, USA

Phone: 1-212-514-6760, Fax: 1-212-514-6030

www.engconfintl.org – info@engconfintl.org

Hotel Capo dei Greci
Riviera di Taormina
SS 114 - km 38
98030 Sant'Alessio Siculo (ME)
Tel: +39-045-627-9692
Fax: +39045-742-0513

Engineering Conferences International (ECI) is a not-for-profit global engineering conferences program, originally established in 1962, that provides opportunities for the exploration of problems and issues of concern to engineers and scientists from many disciplines.

ECI BOARD MEMBERS

Barry C. Buckland, President
Peter Gray
Michael King
Raymond McCabe
David Robinson
William Sachs
Eugene Schaefer
P. Somasundaran
Deborah Wiley

Chair of ECI Conferences Committee: William Sachs

ECI Technical Liaison for this conference: Manfred Martin

ECI Executive Director: Barbara K. Hickernell

ECI Associate Director: Kevin M. Korpics

Conference Sponsors

Samsung Electro-Mechanics Co.

BASF

SURFACE systems + technology GmbH & Co. KG

SCHMID Technology Center

Bruker

Sunday, September 23, 2012

17:00 – 18:30 Conference Check-in (Conference center)
19:00 – Welcome Reception / Dinner

NOTES

- Audiotaping, videotaping and photography of presentations are strictly prohibited.
- Please do not smoke at any conference functions.
- Turn your cellular telephones to vibrate or off during technical sessions.
- All technical and poster sessions will be in the conference center. Meals will be in the restaurant (except for the gala dinner – the location will be announced on site).
- Be sure to check your contact information on the Participant List in this program and make any corrections to your name/contact information online. A corrected copy will be sent to all participants after the conference.
- Speakers – Please leave at least 5 minutes for questions and discussion. Be available for discussion during meals and social periods

Monday, September 24, 2012

- 07:00 – 08:30 Breakfast
- 08:30 – 08:40 *Welcome and opening remarks*
J. Janek (Chair) and Manfred Martin (ECI Liaison)
- Session I: Fundamental studies of defects**
Session Chair: Ryan O'Hayre
- 08:40 – 09:15 *On the nature of positively-deviated defect structure of complex oxides*
Han-Il Yoo, Seoul National University, Korea
- 09:15 – 09:50 *Highly disordered oxides*
Manfred Martin, RWTH Aachen University, Germany
- 09:50 – 10:25 *First principles calculations of point defect formation in solid state ionic materials*
Akihide Kuwabara, Japan Fine Ceramics Center, Japan
- 10:25 – 10:55 Coffee break
- 10:55 – 11:30 *From lithium batteries to fuel cells: Atomic-scale insights into defects, transport and surfaces*
Saiful Islam, University of Bath, United Kingdom
- 11:30 – 11:50 *Bulk and surface defect properties in oxides from a tight-binding variable-charge model.*
Robert Tetot, ICMMO(LEMHE) CNRS/Univ. Paris-Sud, France
- 11:50 – 12:25 *Growth of nanoparticles through control of defect chemistry*
John T.S. Irvine, University of St Andrews, UK
- 12:30 – 14:00 Lunch
- 14:00 – 14:20 *Influence of mechanical stress on oxygen potential in nonstoichiometric oxides*
T. Masumitsu, Tohoku University, Japan
- 14:20 – 14:40 *Defect structure and defect-induced expansion of oxide materials*
A.Yu. Zuev, Ural Federal University, Russia
- Session II: SOFC materials: Cathodes and permeation layers**
Symposium in honor of the 65th birthday of J. Mizusaki
- Session Chair: Han-Il Yoo
- 14:40 – 14:50 *Opening of the SOFC-Session:
Some remarks on the work of J. Mizusaki.*
Han-Il Yoo, Seoul National University, Korea
- 14:50 – 15:35 *Oxygen nonstoichiometry and the related properties vs. electronic structure of Perovskite-related metallic oxides with two 3d-transition elements on B-site for SOFC cathodes and interconnectors*
Junichiro Mizusaki, Tohoku University, Japan

Monday, September 24, 2012 (continued)

- 15:35 – 16:00 Coffee break
- 16:00 – 16:20 *Enhanced oxygen diffusion kinetics in epitaxial Perovskite thin films for solid oxide fuel cells*
Jong-Ho Lee, Korea Institute of Science and Technology, Korea
- 16:20 – 16:55 *Site percolation and electron/ligand hole interaction in transition metal (Fe and Pr-doped BaZrO₃)*
S. Yamaguchi, The University of Tokyo, Japan
- 16:55 – 17:30 *Crystal structure and oxygen permeability of donor-doped Ba-Sr-Co-Fe-based oxides*
Hitoshi Takamura, Tohoku University, Japan
- 17:30 – 17:50 *In situ study of activation and deactivation of La_{1-x}Sr_xMnO₃ SOFC cathodes – electrochemistry and surface analysis of thin-film electrodes*
Anne-Katrin Huber, Justus-Liebig-Universität Gießen, Germany
- 18:00 – 19:30 Poster Session and Social Hour
- 19:30 – 21:00 Dinner

Tuesday, September 25, 2012

- 07:00 – 08:30 Breakfast
- Session Chair: Lorenzo Malavasi
- 08:30 – 08:50 *Oxygen nonstoichiometry of $\text{LaNi}_{1-x}\text{Fe}_x\text{O}_{3-f\text{Å}}$*
Eiki Niwa, Nihon University, Japan
- 08:50 – 09:10 *Oxygen nonstoichiometry and defect structure of $\text{LnBaCO}_{2-x}\text{Me}_x\text{O}_{6-D}$*
(LN = Nd, Sm, Ho and Y; Me = Fe, Ni, Cu)
V. A. Cherepanov, Ural Federal University, Russia
- 09:10 – 09:30 *Defect structure and related properties of double perovskites*
 $\text{REBaCo}_{2-x}\text{Fe}_x\text{O}_{6-d}$ (RE=Gd, Pr; x=0, 0.2)
Dmitry Tsvetkov, Ural Federal University, Russia
- 09:30 – 09:50 *Material characterization of nonstoichiometric layered perovskite-type oxides, $\text{Pr}_{2-x}\text{Sr}_x\text{NiO}_{4+d}$*
Keiji Yashiro, Tohoku University, Japan
- 09:50 – 10:20 Coffee break
- 10:20 – 10:40 *Preparation and defect equilibrium of donor-doped neodymium nickelates*
Kazuto Ohkoshi, Tohoku University, Japan
- 10:40 – 11:00 *Ab initio calculations of strongly nonstoichiometric perovskite solid solutions: Applications for oxygen permeation membranes and SOFC cathodes*
Eugene Kotomin, Max Planck Institute for Solid State Research, Germany
- 11:00 – 11:20 *Defect-chemistry based simulation of high-temperature membrane separation processes*
Michael Schroeder, RWTH Aachen University, Germany
- 11:20 – 11:55 *A high-temperature Mössbauer study of iron-doped Ruddlesden-Popper phases $\text{La}_{N+1}\text{Ni}_N\text{O}_{3N+1}$*
K. D. Becker, Technical University of Braunschweig, Germany
- Session III: SOFC materials: Electrolytes and interconnects**
Session Chair: Tatsuya Kawada
- 11:55 – 12:30 *Evaluation of stress conditions in operated anode supported type SOFCs based on raman scattering spectroscopy*
Hiroo Yugami, Tohoku University, Japan
- 12:30 – 14:00 Lunch
- 14:00 – 14:20 *Mechanism of low-temperature protonic conductivity in bulk nanometric transition metal oxides*
Filippo Maglia, University of Pavia, Italy
- 14:20 – 14:55 *Ionic conduction in oxides with fluorite-related structures, inherent oxygen deficiency, and peculiar defect chemistries*
Truls Norby, University of Oslo, Norway

Tuesday, September 25, 2012 (continued)

- 14:55 – 15:15 *The influence of electric current on the growth of the oxide scale on ZMG232L alloy at 1073 K*
Kenichi Kawamura, Tokyo Institute of Technology, Japan
- 15:15 – 15:50 *Analysis and control of electronic properties of ceria based oxides*
Hans Dieter Wiemhoefer, University of Muenster, Germany
- 15:50 – 16:20 Coffee break

Session Chair: Manfred Martin
- 16:20 – 16:40 *Effect of co-doping with Co or Zn on the electronic conductivity and polarization of acceptor doped CeO₂ at low temperatures*
Kerstin Schmale, University of Munster, Germany
- 16:40 – 17:00 *Analysis of crystal structure and chemical state of RE (RE = Rare Earth Ion) of BaCe_{1-x}Re_xO_{3-D}*
Tomomi Hosaka, Nihon University, Japan
- 17:00 – 17:20 *Mechanical properties of calcium-substituted lanthanum chromite at high temperature under controlled atmosphere*
Yoshikazu Shirai, Tohoku University, Japan
- 17:20 – 17:40 *Structural phase transition of Ba₂Fe₂O₅ involving oxidation and heat absorption*
Takuya Hashimoto, Nihon University, Japan
- 18:15 – Evening on your own (Explore Taormina or relax at the hotel)

Wednesday, September 26, 2012

07:00 – 08:30 Breakfast

08:30 – 13:00 Optional excursion to Mt. Etna / Free time

12:30 – 14:00 Lunch

Session IV: Energy Materials

Session Chair: Claude Delmas

14:00 – 14:35 *Lessons learned from transparent conducting oxides*
Thomas O. Mason, Northwestern University, USA

14:35 – 15:10 *Role of defective oxides in photovoltaics*
David Ginley, NREL, USA

15:10 – 15:30 *A density-functional approach to predicting non-stoichiometry:
applications to transparent-conducting oxides*
Giancarlo Trimarchi, Northwestern University, USA

15:30 – 15:50 *Properties of tin oxides (Sn_2O , SnO) synthesized by Ion-Beam-
Sputtering*
Bruno K. Meyer, Justus-Liebig-Universität Giessen, Germany

15:50 – 16:20 Coffee break

16:20 – 16:40 *Raman studies of binary copper oxide of different stoichiometry*
Peter J. Klar, Justus-Liebig-Universität Giessen, Germany

16:40 – 17:00 *Thermoelectric materials and modules for waste heat recovery*
Wilfried Hermes, BASF SE, Germany

17:00 – 17:20 *In situ crystallization of laser deposited nonstoichiometric titania*
Thomas Leichtweiss, Justus Liebig University Giessen, Germany

19:00 – 20:30 Dinner

Thursday, September 27, 2012

07:00 – 08:30 Breakfast

Session V: Emerging subjects and new applications

Session Chair: Joachim Maier

08:30 – 09:05 *Industrial hydrogen sensor for molten metals based on the protonic defect in alpha alumina.*
Norihiko Fukatsu, Nagoya Institute of Technology, Japan

09:05 – 09:25 *Phase stability, point defects and magnetic properties of non-stoichiometric $Sr_2FeMoO_{6-DELTA}$ double perovskites*
Jörg Töpfer, University of Applied Sciences Jena, Germany

09:25 – 09:45 *Defect chemistry in pure and anion-doped mayenite*
Jens-Peter Eufinger, Justus-Liebig Universität Giessen, Germany

09:45 – 10:05 *Raman studies of cerium dioxide employed in heterogeneous catalysis of the HCl oxidation by oxygen*
Limei Chen, Justus-Liebig-Universität Giessen, Germany

10:05 – 10:30 Coffee break

Session VI: Interfaces, surfaces and nanosize effects

Session Chair: Thomas O. Mason

10:30 – 11:05 *Field-assisted sintering of bulk nanometric functional oxides*
Umberto Anselmi-Tamburini, University of Pavia, Italy

11:05 – 11:25 *Size dependent p-type conductivity of $BaTiO_3$ ceramics with average grain sizes ranging from 35 nm to 5.6 μm*
Xin Guo, Huazhong University of Science and Technology, China

11:25 – 12:00 *The I-V characteristics of grain boundaries: A simple linear diffusion model*
Sangtae Kim, University of California, Davis, USA

12:30 – 14:00 Lunch

14:00 – 14:35 *Oxygen surface exchange kinetics on $SrTi_{1-x}Fe_xO_3$ mixed conducting oxides*
H.J.M. Bouwmeester, University of Twente, Netherlands

14:35 – 14:55 *The role of configurational entropy on the surface reactivity of mixed ionic and electronic conductor electrodes*
Zhuoluo Albert Feng, Stanford University, United States

14:55 – 15:25 Coffee break

Special presentation from sponsor Samsung-Electro-Mechanics Co. (time and location to be announced)

TBA *Multilayer Ceramic Capacitors (MLCC): Business and Vision*
Jaekyung Yoo, Senior Vice President /Chief of LCR division,
Samsung Electro-Mechanics Co, Korea

19:00 – 19:30 Reception

19:30 – 21:30 Conference Banquet

Friday, September 28, 2012

07:00 – 08:30 Breakfast

Session VII: Materials for Lithium-ion batteries

Session Chair: Juergen Janek

08:30 – 09:05 *Defect chemistry for lithium-based batteries*
Joachim Maier, Max Planck Institute for Solid State Research, Germany

09:05 – 09:40 *Layered NaMO₂ as positive electrode of sodium batteries*
Claude Delmas, Université de Bordeaux, France

09:40 – 10:00 *Doping effects on the behavior of β -eucryptite*
Ivar Reimanis, Colorado School of Mines, USA

10:00 – 10:30 Coffee break

10:30 – 11:05 *Electrochemical Li-extraction from intermetallic phases in Li-ion batteries*
Helmut Ehrenberg, Karlsruhe Institute of Technology (KIT), Germany

11:05 – 11:15 Concluding remarks

12:30 – 14:00 Lunch

14:00 – Departures

List of Posters

1. **OXYGEN NONSTOICHIOMETRY AND CRYSTAL STRUCTURE OF DOUBLE PEROVSKITES $\text{REBaCo}_{2-x}\text{Fe}_x\text{O}_{6-D}$ (RE=GD, PR; $x=0-0.6$)**
Dmitry Tsvetkov, Ural Federal University, Russia
2. **EFFECT OF CARBON-BASED FOR SULFONATED SOLID ACID CATALYSTS SYNTHESIS USING IN A BIODIESEL PRODUCTION**
Kanokwan Ngaosuwan, Rajamangala University of Technology Krungthep, Thailand
3. **TOTAL SCATTERING INVESTIGATION OF MATERIALS FOR CLEAN ENERGY APPLICATIONS: IMPORTANCE OF THE LOCAL STRUCTURE**
Lorenzo Malavasi, University of Pavia and INSTM, Italy
4. **IN SITU TIME-RESOLVED NEUTRON DIFFRACTION INVESTIGATION DURING OXYGEN EXCHANGE IN LAYERED COBALTITE CATHODE MATERIALS**
Lorenzo Malavasi, University of Pavia and INSTM, Italy
5. **EVALUATION OF ELECTROCHEMICALLY-ACTIVE THICKNESS OF A POROUS MIXED CONDUCTING ELECTRODE**
Tatsuya Kawada, Tohoku University, Japan
6. **CONTROLLING SURFACE PROPERTIES OF SOLIDS: IN-SITU PEEM AND CONTACT ANGLE MEASUREMENTS WITH SILVER SULFIDE**
Juergen Janek, Institute of Physical Chemistry, Justus Liebig University Giessen, Germany
7. **INVESTIGATION OF THE ELECTRONIC PARTIAL CONDUCTIVITY IN THE INTERFACES OF NANOSCALED OXIDE MULTILAYERS**
Juergen Janek, Institute of Physical Chemistry, Justus Liebig University Giessen, Germany
8. **TRANSPORT PROPERTIES OF SINGLE CRYSTALLINE $\text{CeO}_2\text{-ZrO}_2\text{-Y}_2\text{O}_3$ SOLID SOLUTIONS**
Jens-Peter Eufinger, Institute of Physical Chemistry, Justus Liebig University Giessen, Germany