Program

Nonstoichiometric Compounds VI

September 4 - 8, 2016

LaFonda on the Plaza
Santa Fe, New Mexico, USA

Conference Chairs

Ryan O'Hayre
(Colorado School of Mines, USA)

Juergen Janek
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Yoshihiro Yamazaki
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Nonstoichiometric Compounds Conferences History

An ECI Conference Series

Nonstoichiometric Ceramics and Intermetallics (1998)
Jules Routbort, Rudiger Dieckmann, and Thomas Mason
Kona, Hawaii

Nonstoichiometric Ceramics and Intermetallics II (2001)
Rudiger Dieckmann and C.T. Liu
Barga, Italy

Nonstoichiometric Compounds III (2005)
Manfred Martin, Thomas O. Mason, and Junichiro Mizusaki
Kauai, Hawaii

Nonstoichiometric Compounds IV (2009)
Han-Ill Yoo, Shu Yamaguchi, Juergen Janek, and Sossina M. Haile
Jeju Island, Korea

Nonstoichiometric Compounds V (2012)
Juergen Janek, Lorenzo Malavasi, Tatsuya Kawada, and Ryan O'Hayre
Sicily, Italy

Conference Sponsor

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Sunday, September 4, 2016

16:30 - 18:30	Conference check-in (Mezzanine)
18:30 - 19:15	Reception (La Terraza Terrace)
19:15 - 21:00	Dinner (La Terraza Room)

NOTES

- Technical Sessions will be held in Lumpkins Ballroom South.
- The Poster Session will be held in Lumpkins Ballroom North.
- Vouchers will be provided for breakfast each day in the restaurant.
- Lunches on Monday and Wednesday will be in La Terraza Room and Terrace. Dinners on Monday and Wednesday will be in La Terraza Room. Lunch on Thursday will be in Lumpkins Ballroom North.
- Audiotaping, videotaping and photography of presentations are prohibited.
- Speakers – Please leave at least 5 minutes for questions and discussion.
- Please do not smoke at any conference functions.
- Turn your cellular telephones to vibrate or off during technical sessions.
- After the conference, ECI will send an updated participant list to all participants. Please check your listing now and if it needs updating, you may correct it at any time by logging into your ECI account.
- Please do not smoke at any conference functions.
- Please write your name in the front of this program booklet so it can be returned if misplaced.

Monday, September 5, 2016

07:30 - 09:00	Breakfast
09:25 - 09:40	Opening Remarks
	Oxide Ion Conductors I: Bulk
09:40 - 10:00	**Defect interaction in non-stoichiometric doped ceria from first principles** Steffen Grieshammer, Forschungszentrum Juelich, Germany
10:00 – 10:20	**Peroxide as a mechanism to accommodate excess oxygen** Robin Grimes, Imperial College London, United Kingdom
10:20 – 10:40	**Non-stoichiometries in the bulk and at boundaries** Joachim Maier, Max Planck Institute for Solid State Research, Germany
10:40 - 11:10	Coffee break
	Oxide Ion Conductors II: Surfaces/Interfaces
11:10 - 11:30	**Ion insertion electrochemistry at the molecular and nano-scale** William Chueh, Stanford University, USA
11:30 - 11:50	**Potential energy landscape for oxygen vacancy dynamics in ceria-based solid electrolytes** Sangtae Kim, University of California, Davis, USA
11:50 - 12:20	**Discussion Panel: Oxide Ion Conductors (Bulk)**
12:20 - 14:00	Lunch break
	Oxide Ion Conductors II: Surfaces/Interfaces
14:00 - 14:20	**Surface reaction of nonstoichiometric oxide with oxygen gas** Shu Yamaguchi, The University of Tokyo, Japan
14:20 - 14:40	**Surface oxygen nonstoichiometry depends non-monotonically on biaxial strain in ultrathin ceria films** Chirranjeevi Balaji Gopal, Stanford University, USA
14:40 - 15:00	**Surface Sr segregation behaviors in a model thin film perovskite cathode for solid oxide fuel cells** Woo Chul Jung, KAIST, South Korea

Monday, September 5, 2016 (continued)

15:00 - 15:30	**Discussion Panel: Oxide Ion Conductors (Surfaces/Interfaces)**
15:30 - 16:00	Coffee break
	Resistive Switching/Memristors
16:00 - 16:20	**Resistive switching in highly disordered thin oxide films** Manfred Martin, RWTH Aachen University, Germany
16:20 - 16:40	**Electrical properties of an amorphous zirconium oxide thin film and structure formation during crystallization** Ralph Andreas Henning, Justus-Liebig University, Germany
16:40 - 17:00	**Understanding oxygen anionic-electronic defects under high electric fields: Resistive switches devices** Rafael Schmitt, ETH Zurich, Switzerland
17:00 - 17:30	**Discussion Panel: Memristors**
18:00 - 20:00	Dinner
20:00 - 21:30	Poster Session/Social hour

Tuesday, September 6, 2016

07:30 - 09:00	Breakfast
	Nonstoichiometric Oxides for Solar Thermochemistry
09:00 - 09:20	**Solar thermochemical water splitting: Advances in materials and methods** Anthony McDaniel, Sandia National Laboratories, USA
09:20 - 09:40	**Two-step thermochemical solar-to-fuel efficiency computation of strontium and chromium doped lanthanum manganite perovskite oxides using CALPHAD** Alexander H. Bork, ETH Zurich, Switzerland
09:40 - 10:00	**Solar-driven thermochemical CO_2 reduction using nonstoichiometric perovskite** Yoshihiro Yamazaki, Kyushu University, Japan
10:00 - 10:20	**Incorporating finite temperature into materials by design for nonstoichiometric complex functional oxides** Vladan Stevanovic, Colorado School of Mines, National Renewable Energy Laboratory, USA
10:20 - 10:40	**Driving the solar thermal reforming of methane via a nonstoichiometric ceria redox cycle** Jonathan R. Scheffe, University of Florida, USA
10:40 - 11:10	**Discussion Panel: Solar Thermochemistry**
11:30	**Pick up boxed lunch (Mezzanine) and depart for excursion**
	After excursion: Dinner on your own in Santa Fe

Wednesday, September 7, 2016

07:30 - 09:00	Breakfast
	Proton Conductors
09:00 - 09:20	**Cathode materials for protonic ceramic fuel cells: Bulk defect chemistry and surface reaction kinetics** Rotraut Merkle, MPI for Solid State Research, Germany
09:20 - 09:40	**Pressure-induced defects in zirconates** Hitoshi Takamura, Tohoku University, Japan
09:40 - 10:00	**First principles calculations of defect clustering in acceptor-doped $BaZrO_3$** Akihide Kuwabara, Japan Fine Ceramics Center, Japan
10:00 - 10:20	**Comparing the electrical and protonic conductivity of mesoporous and nanocrystalline thin films of ceria-zirconia solid solutions** Matthias Thomas Elm, University of Giessen, Germany
10:20 - 10:50	Coffee Break
10:50 - 11:10	**Tailoring the properties of a-site substituted $Ba_{1-x}Gd_{0.8}La_{0.2+x}Co_2O_{6-\delta}$** Einar Vøllestad, University of Oslo, Norway
11:10 - 11:30	**Chemistry of hydride ion and proton in anion-encaging crystals: Mayenite and apatite** Katsuro Hayashi, Kyushu University, Japan
11:30 - 11:50	**Anion diffusion in mixed-anionic perovskite systems** Hiroshi Kageyama, Kyoto University, Japan
11:50 - 12:10	**NASICON materials - a long neglected class of solid electrolytes** Enkhtsetseg Dashjav, Forschungszentrum Jülich GmbH, Germany
12:10 - 12:40	**Discussion Panel: Proton Conductors**
12:40 - 14:00	Lunch
	PV Absorbers/Perovskite PV/TCOs
14:00 - 14:20	**Importance of interfaces in hybrid perovskite solar cells** Philip Schulz, National Renewable Energy Laboratory, USA
14:20 - 14:40	**Detection and relevance of ion conduction in hybrid organic-inorganic halide perovskites for photovoltaic applications** Alessandro Senocrate, Max-Planck-Institut FKF, Germany
14:40 - 15:00	**Local heterogeneity and radiative efficiency in hybrid perovskite thin films** Raj Giridharagopal, University of Washington, USA
15:00 - 15:20	**Leveraging off-stoichiometry to defeat n-type degeneracy in zinc tin nitride** Angela N. Fioretti, Colorado School of Mines/National Renewable Energy Lab, USA

Wednesday, September 7, 2016 (continued)

15:20 - 15:40	**Developing new functional TCs** Lauren Garten, NREL, USA
15:40 – 16:10	Coffee Break
16:10 - 16:30	**From defects to alloys: Computational design of non-stoichiometric materials** Stephan Lany, NREL, USA
16:30 - 16:50	**A structural perception about intrinsic point defects in nonstoichiometric compound semiconductors** Susan Schorr, Helmholtz-Zentrum Berlin, Germany
	Nuclear Materials
16:50 - 17:10	**Order, disorder and stability in Be intermetallics for fusion applications** Robin Grimes, Imperial College London, United Kingdom
17:10 - 17:40	**Discussion Panel: PV**
19:00	Reception followed by Conference Banquet

Thursday, September 8, 2016

07:30 - 09:00	Breakfast
	Thermoelectrics
09:00 - 09:20	**Harnessing non-stoichiometry and disorder in thermoelectric materials** Eric Toberer, Colorado School of Mines, USA
09:20 - 09:40	**Structural influences in thermoelectric materials** Wolfgang Zeier, Justus-Liebig-University Giessen, Germany
09:40 - 10:00	**Integrating high-throughput computations and experimental knowledge to advance design and discovery of novel functional materials** Vladan Stevanovic, Colorado School of Mines, USA
10:00 - 10:20	**The effect of extended strain fields on point defect scattering** Brenden R. Ortiz, Colorado School of Mines, USA
10:20 - 10:50	Coffee break
10:50 - 11:10	**Thermopower and conductivity of aerosol deposited $BaFe_{1-x}Ta_xO_{3-\delta}$ films** Murat Bektas, University of Bayreuth, Germany
11:10 - 11:30	**Control of defects for optimizing performance in thermoelectric alloys** G. Jeffrey Snyder, Northwestern University, USA
11:30 - 12:00	**Discussion Panel: Thermoelectrics**
12:00	Closing Remarks
	Lunch and Departures

Poster Presentations

1. **Structure formation and electrical properties of thin films: The Ce-Ti-O system**
   Ralph Andreas Henning, Justus-Liebig University, Germany

2. **The effect of cluster reconfiguration and non-stoichiometry on uranium vacancy migration in UO_2**
   Robin Grimes, Imperial College London, United Kingdom

3. **Stoichiometry relaxation in oxides with mobile oxygen vacancies, protons and holes: Temperature dependence and trapping effects**
   Rotraut Merkle, MPI for Solid State Research, Germany

4. **The non-stoichiometric perovskite $BaPbO_{3-x}$: Crystal structure and cation - anion distribution**
   Alexandra Franz, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

5. **Synthesis and sintering of ZrC_{1-x} powders with variable stoichiometry ($0<x<0.4$)**
   Eugenio Zapata-Solvas, Imperial College London, United Kingdom

6. **Li distribution in the ionic conductor Li1+xAlxTi2-x(PO4)3 with $0 \leq x \leq 0.6$ studied by neutron diffraction**
   Enkhtsetseg Dashjav, Research Center Juelich, Germany

7. **Environmental monitoring of CO_2 concentration flows with novel fast Li-Garnet based electrochemical sensor**
   Alexander Bork, Swiss Federal Institute of Technology (ETH Zurich), Switzerland

8. **Promissing cerium-doped barium manganate perovskite for solar thermochemical hydrogen production**
   Débora R. Barcellos, Colorado School of Mines, USA