

9-4-2016

## Conference Program

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## *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**

(Justus-Liebig-University Giessen, Germany)

**Yoshihiro Yamazaki**

(Kyushu University, Japan)

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Dr. Joseph Berry, National Renewable Energy Laboratory, USA

# 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-Il 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.
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- 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<sub>2</sub> 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<sub>3</sub>**  
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<sub>1-x</sub>Gd<sub>0.8</sub>La<sub>0.2+x</sub>Co<sub>2</sub>O<sub>6-δ</sub>**  
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  $\text{BaFe}_{1-x}\text{Ta}_x\text{O}_{3-\delta}$  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  $\text{UO}_2$**   
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  $\text{BaPbO}_{3-x}$ : Crystal structure and cation - anion distribution**  
Alexandra Franz, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
5. **Synthesis and sintering of  $\text{ZrC}_{1-x}$  powders with variable stoichiometry ( $0 < x < 0.4$ )**  
Eugenio Zapata-Solvas, Imperial College London, United Kingdom
6. **Li distribution in the ionic conductor  $\text{Li}_{1+x}\text{Al}_x\text{Ti}_{2-x}(\text{PO}_4)_3$  with  $0 \leq x \leq 0.6$  studied by neutron diffraction**  
Enkhsetseg Dashjav, Research Center Juelich, Germany
7. **Environmental monitoring of  $\text{CO}_2$  concentration flows with novel fast Li-Garnet based electrochemical sensor**  
Alexander Bork, Swiss Federal Institute of Technology (ETH Zurich), Switzerland
8. **Promising cerium-doped barium manganate perovskite for solar thermochemical hydrogen production**  
Débora R. Barcellos, Colorado School of Mines, USA