

Nonstoichiometric Compounds VI

Santa Fe, New Mexico, USA
4-8 September 2016

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ISBN: 978-1-5108-3252-7

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



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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 principles1**
Steffen Grieshammer, Forschungszentrum Juelich, Germany

10:00 - 10:20 **Peroxide as a mechanism to accommodate excess oxygen2**
Robin Grimes, Imperial College London, United Kingdom

10:20 - 10:40 **Non-stoichiometries in the bulk and at boundaries13**
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-scale14**
William Chueh, Stanford University, USA

11:30 - 11:50 **Potential energy landscape for oxygen vacancy dynamics in ceria-based solid electrolytes15**
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 gas16**
Shu Yamaguchi, The University of Tokyo, Japan

14:20 - 14:40 **Surface oxygen nonstoichiometry depends non-monotonically on biaxial strain in ultrathin ceria films17**
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 cells18**
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 films19**
Manfred Martin, RWTH Aachen University, Germany

16:20 - 16:40 **Electrical properties of an amorphous zirconium oxide thin film and structure
formation during crystallization20**
Ralph Andreas Henning, Justus-Liebig University, Germany

16:40 - 17:00 **Understanding oxygen anionic-electronic defects under high electric fields:
Resistive switches devices21**
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 methods22**
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 CALPHAD23**
Alexander H. Bork, ETH Zurich, Switzerland

09:40 - 10:00 **Solar-driven thermochemical CO₂ reduction using nonstoichiometric perovskite24**
Yoshihiro Yamazaki, Kyushu University, Japan

10:00 - 10:20 **Incorporating finite temperature into materials by design for nonstoichiometric complex functional oxides25**
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 cycle26**
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 kinetics27**
Rotraut Merkle, MPI for Solid State Research, Germany
- 09:20 - 09:40 **Pressure-induced defects in zirconates28**
Hitoshi Takamura, Tohoku University, Japan
- 09:40 - 10:00 **First principles calculations of defect clustering in acceptor-doped BaZrO₃29**
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 solutions30**
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}Co₂O_{6-δ}31**
Einar Vøllestad, University of Oslo, Norway
- 11:10 - 11:30 **Chemistry of hydride ion and proton in anion-encaging crystals: Mayenite and apatite32**
Katsuro Hayashi, Kyushu University, Japan
- 11:30 - 11:50 **Anion diffusion in mixed-anionic perovskite systems33**
Hiroshi Kageyama, Kyoto University, Japan
- 11:50 - 12:10 **NASICON materials - a long neglected class of solid electrolytes34**
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 cells35**
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 applications36**
Alessandro Senocrate, Max-Planck-Institut FKF, Germany
- 14:40 - 15:00 **Local heterogeneity and radiative efficiency in hybrid perovskite thin films47**
Raj Giridharagopal, University of Washington, USA
- 15:00 - 15:20 **Leveraging off-stoichiometry to defeat n-type degeneracy in zinc tin nitride48**
Angela N. Fioretti, Colorado School of Mines/National Renewable Energy Lab, USA

Wednesday, September 7, 2016 (continued)

- 15:20 - 15:40 **Developing new functional TCs57**
Lauren Garten, NREL, USA
- 15:40 – 16:10 Coffee Break
- 16:10 - 16:30 **From defects to alloys: Computational design of non-stoichiometric materials58**
Stephan Lany, NREL, USA
- 16:30 - 16:50 **A structural perception about intrinsic point defects in nonstoichiometric
compound semiconductors59**
Susan Schorr, Helmholtz-Zentrum Berlin, Germany
- Nuclear Materials**
- 16:50 - 17:10 **Order, disorder and stability in Be intermetallics for fusion applications71**
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 materials83**
Eric Toberer, Colorado School of Mines, USA
- 09:20 - 09:40 **Structural influences in thermoelectric materials84**
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 materials85**
Vladan Stevanovic, Colorado School of Mines, USA
- 10:00 - 10:20 **The effect of extended strain fields on point defect scattering86**
Brenden R. Ortiz, Colorado School of Mines, USA
- 10:20 - 10:50 Coffee break
- 10:50 - 11:10 **Thermopower and conductivity of aerosol deposited $\text{BaFe}_{1-x}\text{Ta}_x\text{O}_{3-\delta}$ films114**
Murat Bektas, University of Bayreuth, Germany
- 11:10 - 11:30 **Control of defects for optimizing performance in thermoelectric alloys115**
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**116
Ralph Andreas Henning, Justus-Liebig University, Germany
2. **The effect of cluster reconfiguration and non-stoichiometry on uranium vacancy migration in UO_2** 117
Robin Grimes, Imperial College London, United Kingdom
3. **Stoichiometry relaxation in oxides with mobile oxygen vacancies, protons and holes: Temperature dependence and trapping effects**118
Rotraut Merkle, MPI for Solid State Research, Germany
4. **The non-stoichiometric perovskite BaPbO_{3-x} : Crystal structure and cation - anion distribution**119
Alexandra Franz, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
5. **Synthesis and sintering of ZrC_{1-x} powders with variable stoichiometry ($0 < x < 0.4$)**120
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**121
Enkhsetseg Dashjav, Research Center Juelich, Germany
7. **Environmental monitoring of CO_2 concentration flows with novel fast Li-Garnet based electrochemical sensor**122
Alexander Bork, Swiss Federal Institute of Technology (ETH Zurich), Switzerland
8. **Promising cerium-doped barium manganate perovskite for solar thermochemical hydrogen production**123
Débora R. Barcellos, Colorado School of Mines, USA