Program

Nonstoichiometric Compounds VII

March 10-14, 2019
Phoenix Seagaia Resort
Miyazaki (Kyushu Island), Japan

Conference Chairs
Hitoshi Takamura
Tohoku University, Japan

Roger De Souza
RWTH Aachen University, Germany

Ryan O’Hayre
Colorado School of Mines, Colorado

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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

Nonstoichiometric Compounds VI (2016)
Ryan O’Hayre, Juergen Janek, Yoshihiro Yamazaki
Santa Fe, New Mexico, USA
The conference organizers would like to acknowledge the Miyazaki Convention and Visitors Bureau for its financial support.
Sunday, March 10, 2019

17:30 – 18:45 Conference Check-in (Foyer of Fountain Room, 2nd Floor of Seagaia Convention Center)

19:00 – 20:30 Dinner (Pine Terrace - first floor of the Sheraton Grande Ocean Resort)

Locations and Notes

- Technical sessions will be in the Seagaia Convention Center in the Fountain Room on the 2nd Floor.
- The poster session will be in Seagaia Convention Center in the Orchard Room on the 2nd Floor.
- Breakfasts will be at the Pine Terrace at the Sheraton Grande Ocean Resort
- Lunches and Monday’s dinner will be in the Seagaia Convention Center in the Gibraltar Room on the 2nd Floor.
- The conference banquet on Wednesday will be in the Seagaia Convention Center in the Zuiyo Room on the 3rd Floor.
- The ECI office is in the Business Lounge – Room 4 on the 2nd Floor of the convention center.
- Audio, still photo and video recording by any device (e.g., cameras, cell phones, laptops, PDAs, watches) is strictly prohibited during the technical sessions, unless the author and ECI have granted prior permission.
- Speakers – Please have your presentation loaded onto the conference computer prior to the session start (preferably the day before).
- Speakers – Please leave at least 3-5 minutes for questions and discussion.
- Please do not smoke at any conference functions.
- Turn your mobile telephones to vibrate or off during technical sessions.
- Please write your name on your program so that it can be returned to you if lost or misplaced.
- 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.
- Emergency Contact Information: Because of privacy concerns, ECI does not collect or maintain emergency contact information for conference participants. If you would like to have this information available in case of emergency, please use the reverse side of your name badge.
Monday, March 11, 2019

07:30 – 09:00  Breakfast

Session 1: Interface and photo-induced phenomena in nonstoichiometric oxides
Chairs: Roger A. De Souza and Tatsuya Kawada

09:00 – 09:30  Stoichiometry effects in bulk and at interfaces: Solid state ionics and beyond
Joachim Maier, MPI for Solid State Research, Germany

09:30 – 09:50  Photoconductivity analyzed in the frequency domain - an introductory case study of strontium titanate
Dino Klotz, I2CNER/Kyushu University, Japan

09:50 – 10:20  The electrochemical interface and stochastic functions: A data-driven approach to modeling non-ideal behavior in concentrated systems
David Mebane, West Virginia University, USA

10:20 – 10:40  Effect of grain boundaries on ion migration in stabilized δ-Bi2O3 thin-film electrolyte
Seung Jin Jeong, KAIST, South Korea

10:40 – 11:00  Coffee Break

Session 2: Defects and transport properties of nanoscale oxides
Chairs: Manfred Martin and David Mebane

11:00 – 11:30  Engineering electrochemical nanoscale oxides
Harry L. Tuller, Massachusetts Institute of Technology, USA

11:30 – 11:50  Transport properties of mixed ionic and electronic conductors - from bulk to nanostructure
Kathrin Michel, Center for Materials Research, Justus Liebig University Giessen, Germany

11:50 – 12:10  Tailoring non-stoichiometry and mixed ionic-electronic conductivity in nanostructured Pr-substituted ceria
George Harrington, Kyushu University, MIT, Japan

12:10 – 13:00  Panel discussion

13:00 – 14:00  Lunch

Session 3: Defects and surface exchange kinetics of mixed conductors
Chairs: Koji Amezawa and Jong-Ho Lee

14:00 – 14:20  Departure from solid solution behavior in double perovskites
David N. Mueller, Forschungszentrum Jülich, Peter Gruenberg Institute, Germany

14:20 – 14:40  A high-temperature Mössbauer study into ionic and electronic disorder in BSCF5582
Klaus-Dieter Becker, Technische Universität Braunschweig, Germany
### Monday, March 11, 2019 (continued)

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker(s)</th>
<th>Institution(s)</th>
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<tbody>
<tr>
<td>14:40 – 15:00</td>
<td>Preparation of Ba_{1-x}Ln_xFeO_{3-δ} and BaFe_{1-x}Ln_xO_{3-δ} (Ln: trivalent ion) with cubic perovskite structure and random distribution of oxide ion vacancy</td>
<td>Takuya Hashimoto, Nihon University, Japan</td>
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<td>15:00 – 15:20</td>
<td>Enhanced oxygen exchange of perovskite oxide surfaces through strain-driven chemical stabilization</td>
<td>WooChul Jung, KAIST, South Korea</td>
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<td>15:20 – 15:40</td>
<td>Surface modification through oxide ALD to improve oxygen exchange rate on perovskite surface</td>
<td>Jongsu Seo, KAIST, South Korea</td>
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<td>15:40 – 16:00</td>
<td>Chemical strain in perovskite-like materials</td>
<td>Dmitry Tsvetkov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia</td>
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<td>16:00 – 16:20</td>
<td>Coffee Break</td>
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<td>16:20 – 16:40</td>
<td>Session 4: Electronic structure and bonding in oxides</td>
<td>Chairs: Harry L. Tuller and Matthias T. Elm</td>
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<td>16:40 – 17:00</td>
<td>The Fermi energy in oxides: assessing and understanding the limits using XPS</td>
<td>Andreas Klein, TU Darmstadt, Germany</td>
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<td>17:00 – 17:20</td>
<td>Non-innocent role of fluorine as an electron donor in oxides</td>
<td>Tomas Duchon, Forschungszentrum Jülich GmbH, Germany</td>
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<td>17:20 – 17:40</td>
<td>Evolutionally search with density functional calculations for a new class of one-dimensional electride</td>
<td>Tomofumi Tada, Tokyo Institute of Technology, Japan</td>
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<td>17:40 – 18:10</td>
<td>Different defects formation modes under sevier reducing condition in primitive cubic perovskites, BaZr_{1-x}Y_xO_{3-x/2} and BaSn_{1-x}Y_xO_{3-x/2}</td>
<td>Katsuro Hayashi, Kyushu University, Japan</td>
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<tr>
<td>18:10 – 18:30</td>
<td>Panel discussion</td>
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<td>18:30 – 20:00</td>
<td>Dinner (Gibraltar Room)</td>
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<td>20:00 – 21:30</td>
<td>Poster session</td>
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Tuesday, March 12, 2019

07:30 – 09:00  Breakfast

**Session 5: Oxide-ion conductors**
Chairs: Han-Ill Yoo and Tomofumi Tada

09:00 – 09:30  Oxide ion transport and phase stability in the excess oxygen scheelite phases
Stephen Skinner, Imperial College London, United Kingdom

09:30 – 09:50  Structure-conductivity relation in oxygen ion conductors: Doped ceria and La-mellilites
Steffen Grieshammer, Forschungszentrum Jülich, Germany

09:50 – 10:20  Local distortion by dopants and percolation conductivity in oxides
Shu Yamaguchi, The University of Tokyo, NIAD-EQ, Japan

10:20 – 10:40  Computational and experimental studies of diffusion in monoclinic HfO₂
Michael P. Müller, RWTH Aachen University, Germany

10:40 – 11:00  Coffee Break

**Session 6: Inorganic-organic hybrid materials and their applications**
Chairs: Shu Yamaguchi and Andreas Klein

11:00 – 11:20  Non-stoichiometry and ion transport in halide perovskites: Equilibrium situation and light effects
Alessandro Senocrate Max-Planck-Institut FKF, Germany

11:20 – 11:40  Iodide-ion transport in methylammonium lead iodide perovskite: Some surprising aspects
Roger A. De Souza, RWTH Aachen University, Institute of Physical Chemistry, Germany

11:40 – 12:00  Inorganic/Organic hybrid superlattice films toward next-generation flexible/wearable thermoelectric devices
Kunihito Koumoto, Nagoya Industrial Science Research Institute, Japan

12:00 – 12:20  Experimental thermochemical verification of trends in thermodynamic stability of hybrid perovskite-type organic-inorganic halides
Dmitry Tsvetkov, Ural Federal University, Russia

12:20 – 12:45  Panel discussion

12:45  Pick up Bento Box Lunch (Fountain Room Foyer)

13:00  Board buses for Excursion – Meet in front of the first floor entrance of the Seagaia Convention Center

(Aya Teruha Suspension Bridge, Unkai Brewery Tour, Aya Castle)

Dinner on your own

Buses will drop off in the downtown area of Miyazaki for attendees who want to have dinner there and explore the area. Buses will then continue back to the Sheraton Grande Ocean Resort, returning by 18:30.
Wednesday, March 13, 2019

07:30 – 09:00  Breakfast

**Session 7: Proton and mixed conducting oxides I**
Chairs: Ryan O’Hayre and Stephen Skinner

09:00 – 09:30  Mixed-conducting cathode materials for protonic ceramic fuel cells: Proton uptake and defect interactions
Rotraut Merkle, Max Planck Institute for Solid State Research, Germany

09:30 – 09:50  Defect thermodynamics and lattice site basicity of proton and mixed conducting oxides
Tor Svendsen Bjørheim, University of Oslo, Norway

09:50 – 10:10  Defect chemistry of mixed conducting double Perovskites
Ragnar Strandbakke, University of Oslo, Norway

10:10 – 10:30  Manganese oxide base electrocatalysts for proton-conducting ceramic cells
Yoshitaka Aoki, Hokkaido University, Japan

10:30 – 10:50  Coffee Break

**Session 8: Proton and mixed conducting oxides II**
Chairs: Rotraut Merkle and William C. Chueh

10:50 – 11:20  Hydration in fluorite-related rare-earth cerates
Truls Norby, University of Oslo, Norway

11:20 – 11:50  Percolation effects during ionic motion
Manfred Martin, RTWH Aachen University, Germany

11:50 – 12:10  Molecular dynamics and kinetic Monte Carlo hybrid approach for efficient dynamics and proton conduction in phosphoric acid
Albert Iskandarov, Materials Research Center for Element Strategy, Tokyo Institute of Technology, Japan

12:10 – 13:00  Panel discussion

13:00 – 14:00  Lunch

**Session 9: Reactions and materials for high-temperature electrochemical devices I**
Chairs: Truls Norby and Yoshitaka Aoki

14:00 – 14:30  Investigation of cathodic reaction in SOFCs and PCFCs by using patterned thin film model electrodes
Koji Amezawa, Tohoku University, Japan

14:30 – 14:50  Comprehensive understanding of cathodic and anodic polarization effects on stability of nanoscale oxygen electrode for reversible solid oxide cells
Jong-Ho Lee, Korea Institute of Science and Technology (KIST), South Korea

14:50 – 15:10  Oxygen diffusion of non-stoichiometric (La, Sr)MnO₃ /CERIA NANO-composite SOFC cathode
Seiichi Suda, Shizuoka University, Department of Engineering, Japan
15:10 – 15:30  
La$_{1-x}$Sr$_x$MnO$_{3+δ}$ as a nonstoichiometric model system for the catalysis of oxygen evolution reaction  
Raika Oppermann, Physikalisches Institut Giessen, Germany

15:30 – 15:50  
Coffee Break

15:50 – 16:20  
Session 10: Reactions and materials for high-temperature electrochemical devices II  
Chairs: Tor S. Bjørheim and WooChul Jung

15:50 – 16:20  
Equivalent circuit analysis of a three-carrier electrolyte/electrode system  
Tatsuya Kawada, Tohoku University, Japan

16:20 – 16:40  
A highly active and redox stable novel ceramic anode with in-situ exsolution of nanocatalysts  
Kyeong Joon Kim, DGIST, South Korea

16:40 – 17:00  
Defect structure and transport properties of ceria-zirconia-based oxides  
Hitoshi Takamura, Tohoku University, Japan

17:00 – 19:00  
Panel discussion

19:00 – 21:00  
Banquet
Thursday, March 14, 2019

07:30 – 09:00  Breakfast

Session 11: Highly Nonstoichiometric Compounds
Chairs: Jürgen Janek and Takuya Hashimoto

09:00 – 09:30  Demystification of Mizusaki’s α-factor for the positively-deviated defect behavior of hyperstoichiometric oxides
H.-I. Yoo, Daegu-Gyeongbuk Institute of Science and Technology, South Korea

09:30 – 09:50  Non-stoichiometry in monoclinic zirconia and amorphous zirconia
Simon C. Middleburgh, Bangor University, United Kingdom

09:50 – 10:10  Synthesis and crystal structure of novel nonstoichiometric suboxide solid solutions, Ti_{12-δ}Ga_{x}Bi_{3-x}O_{10}
Hisanori Yamane, Tohoku University, Japan

10:10 – 10:30  Coffee Break

Session 12: Materials for Li and Na Secondary Batteries
Chairs: Joachim Maier and Katsuro Hayashi

10:30 – 11:00  Nonstoichiometry and reactivity of lithium solid electrolytes for solid state batteries
Jürgen Janek, Justus Liebig University Gießen, Germany

11:00 – 11:20  Electrochemical properties of micro-batteries with single NCM-111 secondary particles as cathode
Matthias Thomas Elm, University of Giessen, Center for Materials Research, Germany

11:20 – 11:40  Mechanism of oxygen release from Li-rich cathode material for lithium ion batteries
Takashi Nakamura, Tohoku University, Japan

11:40 – 12:00  Nonstoichiometry and defect structure of γ-NaxCoO2
Wonyo Joo, Department of Materials Science and Engineering, Seoul National University, South Korea

12:00 – 12:20  Development of complex hydrides for fast ionic conduction
Motoaki Matsuo, School of Science and Technology, Kwansei Gakuin University, Japan

12:20 – 12:40  Panel discussion

12:40  Closing

12:50 – 14:00  Lunch
Posters

Nonstoichiometric Compounds VII

Engineering Conferences International
Poster Presentations

1. **The Fermi energy in acceptor doped SrTiO$_3$ and BaTiO$_3**
   Andreas Klein, TU Darmstadt, Germany

2. **Self-assembled graphene derivatives used as HTLs for highly efficient inverted perovskite solar cells**
   Hong Lin, Tsinghua University, China

3. **Thermoelectric properties of graphene incorporated thermoelectric materials**
   Won Seon Seo, Korea Institute of Ceramic Engineering and Technology, South Korea

4. **Proton uptake in the mixed ionic and electronic conductors Ba$_{1-x}$Sr$_x$FeO$_{3-d}$**
   Rotraut Merkle, MPI for Solid State Research, Germany

5. **Crystal structure, oxygen nonstoichiometry, hydration and conductivity BaZr$_{1-x}$MxO$_{3-d}$ (M=Pr, Nd, Y, Co)**
   Ivan Ivanov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia

6. **Local structural analysis on hydration behavior in doped AZrO$_3$ (A = Ba, Ca) protonic conductors**
   Itaru Oikawa, Tohoku University, Japan

7. **Defect structure of BZCYYb17 and theoretical behavior and performance of SOFC’s with BZCYYb17 electrolyte**
   In-Ho Kim, Chonnam national university, South Korea

8. **Reversible water uptake and release of pseudo-cubic type La$_{0.7}$Sr$_{0.3}$Mn$_{1-x}$Ni$_x$O$_3$ at intermediate temperatures**
   Ning Wang, Hokkaido University, Japan

9. **Measurement of the active width in Sr-doped lanthanum manganate Sfc Cathodes using Nano-ct, impedance spectroscopy and Bayesian calibration**
   David S. Mebane, West Virginia University, USA

10. **Evaluation of the high temperature solid Oxide cells using La$_{0.1}$Sr$_{0.9}$Co$_{0.8}$Fe$_{0.2}$O$_{3-δ}$**
    Jaewoon Hong, Chonnam National University, South Korea

11. **Oxygen nonstoichiometry and thermodynamic quantities of Perovskite-Type La$_{1-x}$Sr$_x$FeO$_{3.5}$ (x=0.2, 0.5, 0.8)**
    Hohan Bae, Chonnam National University, South Korea

12. **High resolution thermochemical study of phase stability and rapid oxygen incorporation in YBaCo$_{6.4}$Zn$_x$O$_{7+δ}$ 114-cobaltites**
    Dmitry Tsvetkov, Ural Federal University, Russia

13. **Structure and properties of the layered perovskites in Sm-Ba-Co-Fe-O System**
    Nadezhda E. Volkova, Ural Federal University, Russia

14. **3-point measurement in solid state devices: (Novel) artifacts and how to avoid them**
    Tobias Huber, TU Wien, Austria

15. **Discussion on electrode reaction in partial equilibrium state by EMF measurements**
    Tomoyuki Yamasaki, The University of Tokyo, Japan

16. **DFT+U studies including spin-orbit coupling - a case study for f-electrons in praseodymium-doped ceria**
    Kathrin Michel, Center for Materials Research, Justus Liebig University Giessen, Germany
17. **Origin of the surface-orientation dependence of the reduction kinetics of ultrathin ceria**  
   Tomas Duchon, Forschungszentrum Jülich GmbH, Germany

18. **A highly active and durable lanthanum strontium cobalt ferrite cathode for Intermediate-Temperature solid Oxide fuel cells**  
   Jin Wan Park, DGIST, South Korea

19. **Hydration thermodynamics of proton-conducting perovskite Ba$_4$Ca$_2$Nb$_2$O$_{11}$**  
   Vladimir Sereda, Ivan Ivanov, Dmitry Tsvetkov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia

20. **In situ and ex situ study of cubic La$_{0.5}$Ba$_{0.5}$CoO$_{3-\delta}$ to double perovskite LaBaCo$_2$O$_{6-\delta}$ transition**  
   Dmitry Malyshkin, Ivan Ivanov, Dmitry Tsvetkov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia

21. **Heat increments and oxidation enthalpies of (Y,Pr,Gd)BaCo$_2$O$_{6.5}$ double perovskites**  
   Anton Sednev, Ivan Ivanov, Dmitry Tsvetkov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia