

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



Engineering Conferences International

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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-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

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

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|---------------|--|
| 17:30 – 18:45 | Conference Check-in (Foyer of Fountain Room, 2 nd 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)

- 14:40 – 15:00 **Preparation of $\text{Ba}_{1-x}\text{Ln}_x\text{FeO}_{3-\delta}$ and $\text{BaFe}_{1-x}\text{Ln}_x\text{O}_{3-\delta}$ (Ln : trivalent ion) with cubic perovskite structure and random distribution of oxide ion vacancy**
Takuya Hashimoto, Nihon University, Japan
- 15:00 – 15:20 **Enhanced oxygen exchange of perovskite oxide surfaces through strain-driven chemical stabilization**
WooChul Jung, KAIST, South Korea
- 15:20 – 15:40 **Surface modification through oxide ALD to improve oxygen exchange rate on perovskite surface**
Jongsu Seo, KAIST, South Korea
- 15:40 – 16:00 **Chemical strain in perovskite-like materials**
Dmitry Tsvetkov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia
- 16:00 – 16:20 Coffee Break
- Session 4: Electronic structure and bonding in oxides**
Chairs: Harry L. Tuller and Matthias T. Elm
- 16:20 – 16:40 **The Fermi energy in oxides: assessing and understanding the limits using XPS**
Andreas Klein, TU Darmstadt, Germany
- 16:40 – 17:00 **Non-innocent role of fluorine as an electron donor in oxides**
Tomas Duchon, Forschungszentrum Jülich GmbH, Germany
- 17:00 – 17:20 **Evolutionally search with density functional calculations for a new class of one-dimensional electride**
Tomofumi Tada, Tokyo Institute of Technology, Japan
- 17:20 – 17:40 **Different defects formation modes under sever reducing condition in primitive cubic perovskites, $\text{BaZr}_{1-x}\text{Y}_x\text{O}_{3-x/2}$ and $\text{BaSn}_{1-x}\text{Y}_x\text{O}_{3-x/2}$**
Katsuro Hayashi, Kyushu University, Japan
- 17:40 – 18:10 **Modulating metal-oxygen bonding in lithiated metal oxides with point defects**
William C. Chueh, Stanford University, USA
- 18:10 – 18:30 Panel discussion
- 18:30 – 20:00 Dinner (Gibraltar Room)
- 20:00 – 21:30 Poster session

Tuesday, March 12, 2019

- 07:30 – 09:00 Breakfast
- Session 5: Oxide-ion conductors**
Chairs: Han-Il 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-melilites**
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, RWTH 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

Wednesday, March 13, 2019 (continued)

15:10 – 15:30 **La_{1-x}Sr_xMnO_{3±δ} as a nonstoichiometric model system for the catalysis of oxygen evolution reaction**
Raika Oppermann, Physikalisch Chemisches Institut Giessen, Germany

15:30 – 15:50 Coffee Break

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, $Ti_{12-\delta}Ga_xBi_{3-x}O_{10}$**
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 - Na_xCoO_2**
Wonhyo 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 SrTiO₃ and BaTiO₃**
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_xFeO_{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 AZrO₃ (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_xO₃ at intermediate temperatures**
Ning Wang, Hokkaido University, Japan
9. **Measurement of the active width in Sr-doped lanthanum manganate Sofc 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_xFeO_{3-δ} (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_{4-x}Zn_xO_{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 $\text{Ba}_4\text{Ca}_2\text{Nb}_2\text{O}_{11}$**
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 $\text{La}_{0.5}\text{Ba}_{0.5}\text{CoO}_{3-\delta}$ to double perovskite $\text{LaBaCo}_2\text{O}_{6-\delta}$ transition**
Dmitry Malyshkin, Ivan Ivanov, Dmitry Tsvetkov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia
21. **Heat increments and oxidation enthalpies of $(\text{Y,Pr,Gd})\text{BaCo}_2\text{O}_{6-\delta}$ double perovskites**
Anton Sednev, Ivan Ivanov, Dmitry Tsvetkov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia