

# **Nonstoichiometric Compounds VII**

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10 - 14 March 2019

## **Editors:**

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**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...1**

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...2**

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...3**

David Mebane, West Virginia University, USA

10:20 – 10:40 **Effect of grain boundaries on ion migration in stabilized  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> thin-film electrolyte...4**

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...5**

Harry L. Tuller, Massachusetts Institute of Technology, USA

11:30 – 11:50 **Transport properties of mixed ionic and electronic conductors - from bulk to nanostructure...6**

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...7**

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...8**

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...9**

Klaus-Dieter Becker, Technische Universität Braunschweig, Germany

**Monday, March 11, 2019 (continued)**

- 14:40 – 15:00      **Preparation of  $Ba_{1-x}Ln_xFeO_{3-\delta}$  and  $BaFe_{1-x}Ln_xO_{3-\delta}$  ( $Ln$ : trivalent ion) with cubic perovskite structure and random distribution of oxide ion vacancy...10**  
Takuya Hashimoto, Nihon University, Japan
- 15:00 – 15:20      **Enhanced oxygen exchange of perovskite oxide surfaces through strain-driven chemical stabilization...11**  
WooChul Jung, KAIST, South Korea
- 15:20 – 15:40      **Surface modification through oxide ALD to improve oxygen exchange rate on perovskite surface...12**  
Jongsu Seo, KAIST, South Korea
- 15:40 – 16:00      **Chemical strain in perovskite-like materials...13**  
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...14**  
Andreas Klein, TU Darmstadt, Germany
- 16:40 – 17:00      **Non-innocent role of fluorine as an electron donor in oxides...15**  
Tomas Duchon, Forschungszentrum Jülich GmbH, Germany
- 17:00 – 17:20      **Evolutionally search with density functional calculations for a new class of one-dimensional electrider...16**  
Tomofumi Tada, Tokyo Institute of Technology, Japan
- 17:20 – 17:40      **Different defects formation modes under sevier reducing condition in primitive cubic perovskites,  $BaZr_{1-x}Y_xO_{3-x/2}$  and  $BaSn_{1-x}Y_xO_{3-x/2}$ ...17**  
Katsuro Hayashi, Kyushu University, Japan
- 17:40 – 18:10      **Modulating metal-oxygen bonding in lithiated metal oxides with point defects...18**  
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...19**  
Stephen Skinner, Imperial College London, United Kingdom

09:30 – 09:50 **Structure-conductivity relation in oxygen ion conductors: Doped ceria and La-melilites...20**  
Steffen Grieshammer, Forschungszentrum Jülich, Germany

09:50 – 10:20 **Local distortion by dopants and percolation conductivity in oxides...21**  
Shu Yamaguchi, The University of Tokyo, NIAD-EQ, Japan

10:20 – 10:40 **Computational and experimental studies of diffusion in monoclinic HfO<sub>2</sub>...22**  
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...23**  
Alessandro Senocrate Max-Planck-Institut FKF, Germany

11:20 – 11:40 **Iodide-ion transport in methylammonium lead iodide perovskite: Some surprising aspects...24**  
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...25**  
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...26**  
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...27**  
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...28**  
Tor Svendsen Bjørheim, University of Oslo, Norway

09:50 – 10:10 **Defect chemistry of mixed conducting double Perovskites...29**  
Ragnar Strandbakke, University of Oslo, Norway

10:10 – 10:30 **Manganese oxide base electrocatalysts for proton-conducting ceramic cells...30**  
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...31**  
Truls Norby, University of Oslo, Norway

11:20 – 11:50 **Percolation effects during ionic motion...32**  
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...33**  
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...34**  
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...35**  
Jong-Ho Lee, Korea Institute of Science and Technology (KIST), South Korea

14:50 – 15:10 **Oxygen diffusion of non-stoichiometric (La, Sr)MnO<sub>3</sub> /CERIA NANO-composite SOFC cathode...36**  
Seiichi Suda, Shizuoka University, Department of Engineering, Japan

**Wednesday, March 13, 2019 (continued)**

15:10 – 15:30      **La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3±δ</sub> as a nonstoichiometric model system for the catalysis of oxygen evolution reaction...37**  
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...38**  
Tatsuya Kawada, Tohoku University, Japan

16:20 – 16:40      **A highly active and redox stable novel ceramic anode with in-situ exsolution of nanocatalysts...39**  
Kyeong Joon Kim, DGIST, South Korea

16:40 – 17:00      **Defect structure and transport properties of ceria-zirconia-based oxides...40**  
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  $\alpha$ -factor for the positively-deviated defect behavior of hyperstoichiometric oxides...41**  
H.-I. Yoo, Daegu-Gyeongbuk Institute of Science and Technology, South Korea

09:30 – 09:50 **Non-stoichiometry in monoclinic zirconia and amorphous zirconia...42**  
Simon C. Middleburgh, Bangor University, United Kingdom

09:50 – 10:10 **Synthesis and crystal structure of novel nonstoichiometric suboxide solid solutions,  $Ti_{12-6}Ga_xBi_{3-x}O_{10}$ ...43**  
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...44**  
Jürgen Janek, Justus Liebig University Gießen, Germany

11:00 – 11:20 **Electrochemical properties of micro-batteries with single NCM-111 secondary particles as cathode...45**  
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...46**  
Takashi Nakamura, Tohoku University, Japan

11:40 – 12:00 **Nonstoichiometry and defect structure of  $\gamma$ - $Na_xCoO_2$ ...47**  
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...48**  
Motoaki Matsuo, School of Science and Technology, Kwansai Gakuin University, Japan

12:20 – 12:40 Panel discussion

12:40 Closing

12:50 – 14:00 Lunch