

*Program*

# ***Nonstoichiometric Compounds***

**March 8-13, 2009  
Jeju Island, Korea**

## **Conference Chairs**

**Professor Han-Il Yoo**  
Seoul National University, Korea

**Professor Shu Yamaguchi**  
The University of Tokyo, Japan

**Professor Juergen Janek**  
Justus-Liebig-University, Germany

**Professor Sossina M. Haile**  
California Institute of Technology, U.S.A.



**Engineering Conferences International**  
32 Broadway, Suite 314  
New York, NY 10004, USA  
Phone: 1 - 212 - 514 - 6760, Fax: 1 - 212 - 514 - 6030  
[www.engconfintl.org](http://www.engconfintl.org) – [info@engconfintl.org](mailto:info@engconfintl.org)

Engineering Conferences International (ECI) is a not-for-profit global engineering conferences program, originally established in 1962, that provides opportunities for the exploration of problems and issues of concern to engineers and scientists from many disciplines.

#### ECI BOARD MEMBERS

Barry C. Buckland, President

Peter Gray

Allen I. Laskin

Raymond McCabe

David Robinson

Jules Routbort

William Sachs

Eugene Schaefer

P. Somasundaran

Chair of ECI Conferences Committee: William Sachs

ECI Technical Liaison for this conference: Manfred Martin

ECI Director: Barbara K. Hickernell

ECI Associate Director: Kevin M. Korpics

**Our thanks to**



**for their generous support  
of this conference.**

**Thank you also to**



**for their technical endorsement.**

## Sunday, March 8, 2009

- 16:00 - 18:00 Registration
- 18:00 - 20:00 Welcome Party/Dinner

## Monday, March 9, 2009

- 07:30 - 08:20 Breakfast
- 08:20 - 08:30 **Opening Remarks**
- Session I: Basics/Defects/ Defect driven phenomena**  
Session Chairs: S. Yamaguchi & X. Guo
- 08:30 - 09:00 DEFECT INTERACTIONS IN SrTiO<sub>3</sub> IN THE TEMPERATURE RANGE OF 25 TO 250 °C  
Xin Guo, Institute of Solid State Research, Germany
- 09:00 - 09:20 THE OXYGEN RELEASE BEHAVIOR OF CAF<sub>2</sub>-TYPE (PR<sub>0.75</sub>ZR<sub>0.25</sub>)O<sub>2-γ</sub> PHASE WITH WIDE OXYGEN NONSTOICHIOMETRY  
Shinya Otsuka-Yao-Matsuo, Osaka University, Japan
- 09:20 - 09:40 MICROSTRUCTURAL EVOLUTION IN PEROVSKITES BY OXYGEN PARTIAL PRESSURE CHANGE AND DONOR DOPING  
Suk-Joong L. Kang, KAIST, Korea
- 09:40 - 10:00 DISORDER, LATTICE DYNAMICS AND IONIC CONDUCTION IN SUPERIONIC COPPER CHALCOGENIDES  
S.A. Danilkin, ANSTO, Australia
- 10:00 - 10:30 Coffee break
- 10:30 - 11:00 ON THE ORIGIN OF ANOMALOUS V<sub>TH</sub> SHIFT IN HIGH-K MOSFETS  
Akira Toriumi, The University of Tokyo, Japan
- 11:00 - 11:20 DIRECT OBSERVATION OF REVERSIBLE OXIDATION AND REDUCTION AT BURIED OXIDE/METAL INTERFACES  
Andreas Klein, Technische Universität Darmstadt, Germany
- 11:20 - 11:40 STRUCTURAL FEATURES OF BATIO3 NANO-POWDERS AND NANO-GRAINED CERAMICS  
N.-H. Cho, Inha University, Korea
- 11:40 - 12:00 DEFECT COMPLEX AND DIELECTRIC PROPERTIES OF ACCEPTOR AND MNO-DOPED BATIO3  
Young Ho Han, Sungkyunkwan University, Korea

12:00 - 14:00	Lunch
	<b>Session II: Ferroelectrics</b>
	Session Chairs: H-I. Yoo & P. McIntyre
14:00 - 14:30	Effect of Acceptor (Mg) Concentration on the Resistance Degradation Behavior in BaTiO <sub>3</sub> Model Dielectrics: Impedance Spectroscopy and TSDC (Thermally Stimulated Depolarization Current) Analysis Seok-Hyun Yoon, Samsung Electro-Mechanics Co., Korea
14:30 - 14:50	DIFFUSION PROCESSES IN MULTI-LAYER CERAMIC CAPACITORS Markus Kessel, Institute of Physical Chemistry, RWTH Aachen University, Germany
14:50 - 15:10	ROLE OF ELECTRON EMISSION FROM THE RARE-EARTH METAL OXIDES IN DISPLAY DEVICE Ki-Woong Whang, Seoul National University, Korea
15:10 - 15:40	Coffee break
15:40 - 16:10	BULK AND INTERFACIAL OXYGEN DEFECTS IN HAFNIA DIELECTRIC STACKS: A CRITICAL ASSESSMENT Paul C. McIntyre, Stanford University, USA
16:10 - 16:30	ATOMIC-RESOLUTION STRUCTURAL ANALYSIS OF LA <sub>2/3-x</sub> LI <sub>3x</sub> TiO <sub>3</sub> BY HIGH RESOLUTION ELECTRON MICROSCOPY Takao Tsurui, Tohoku University, Japan
16:30 - 16:50	TRANSMISSION ELECTRON MICROSCOPY STUDY OF AN ELECTRON-BEAM-INDUCED ORDER TO DISORDER TRANSFORMATION OF NONSTOICHIOMETRIC NIOBIUM NITRIDE Jonghan Won, Los Alamos National Laboratory, USA
16:50 - 17:40	<b>Short Presentation for Poster Session I (Odd number)</b>
18:00 - 19:30	Dinner
19:30 - 20:30	<b>Poster Session I</b> and Social Hour

**Tuesday, March 10, 2009**

- 07:30 – 08:30            Breakfast
- Session III: Thermoelectric, Energy conv/storage**  
Session Chairs: K. Koumoto & M. Schroeder
- 08:30 - 09:00            NANOSTRUCTURED STRONTIUM TITANATE-BASED OXIDES FOR THERMOELECTRICS  
Kunihito Koumoto, Nagoya University, Japan
- 09:00 - 09:20            THERMOELECTRIC PROPERTIES OF NONSTOICHIOMETRIC CHALCOGENIDE COMPOUNDS: THEORETICAL AND EXPERIMENTAL STUDIES  
Min Wook Oh, Korea Electrotechnology Research Institute, Korea
- 09:20 - 09:40            COPPER INDIUM DISELENIDE AND DISULFIDE SEMICONDUCTOR NANOCRYSTALS; SYNTHESSES AND THEIR DEFECT RELATED OPTICAL PROPERTIES  
Takahisa Omata, Osaka University, Japan
- 09:40- 10:00            AVERAGE AND LOCAL STRUCTURE INVESTIGATION OF ION CONDUCTORS BY MEANS OF TOTAL NEUTRON SCATTERING  
Lorenzo Malavasi, University of Pavia, Italy
- 10:00 - 10:20            WORK FUNCTIONS OF TRANSPARENT CONDUCTING OXIDES  
Andreas Klein, Technical University of Darmstadt, Germany
- 10:20 - 10:50            Coffee break
- 10:50 - 11:20            KEY PROPERTIES OF INORGANIC MEMBRANES FOR PARTIAL OXIDATION AND ENERGY CONVERSION PROCESSES  
Michael Schroeder, RWTH Aachen University, Germany
- 11:20 - 11:40            DISORDER AND DIFFUSION IN VARIOUSLY DOPED MAYENITES  
Hans Boysen, LMU, Germany
- 11:40 - 12:00            DEFECT MODEL OF LIQUID APPLIED TO IONIC CONDUCTIVITY OF GLASS  
Junichi Kawamura, IMRAM, Tohoku University, Japan
- 12:00 - 12:20            DEFECT STRUCTURE AND TRANSPORT PROPERTIES OF MG-Y-BASED HYDRIDES PREPARED UNDER HIGH PRESSURE  
Hitoshi Takamura, Tohoku University, Japan
- 12:20 - 14:00            Lunch

**Session IV: Wuensch Symposium**

Session Chairs: Sossina Haile & Tom Mason

- 14:00 - 14:30 A CHEMICALLY DRIVEN INSULATOR-METAL TRANSITION IN AMORPHOUS AND NON-STOICHIOMETRIC GALLIUM OXIDE  
Manfred Martin, RWTH Aachen University, Germany
- 14:30 - 15:00 DISCOVERY AND PROGRESS OF IRON-BASED SUPERCONDUCTORS  
Hideo Hosono, Tokyo Institute of Technology, Japan
- 15:00 - 15:30 LOW-TEMPERATURE PROTONIC CONDUCTION IN NANOCRYSTALLINE FLUORITE-STRUCTURED OXIDES: CONDUCTION MECHANISM  
Sangtae Kim, University of California, Davis, USA
- 15:30 - 16:00 Coffee break
- 16:00 - 16:30 THE NANO-GRAIN COMPOSITE MODEL (N-GCM): AN ALTERNATIVE TO THE BRICK LAYER MODEL FOR ANALYZING NANOCERAMICS  
Thomas O. Mason, Northwestern University, USA
- 16:30 - 17:10 CRYSTAL CHEMISTRY AND STRUCTURE FOR ANION-DEFICIENT FLUORITE PHASES  
Bernhardt J. Wuensch, Massachusetts Institute of Technology, USA
- 17:10 - 18:00 **Short Presentation for Poster Session II (Even numbers)**
- 18:00 - 19:30 Dinner
- 19:30 - 20:30 **Poster Session II** and Social Hour

**Wednesday, March 11, 2009**

07:30 - 08:30 Breakfast

**Session V: Magnetic Materials**

Session Chairs: Manfred Martin & Klaus Becker

08:30 - 09:00 THE DEVELOPMENT OF A-SITE ORDERED MANGANITES UTILIZING OXYGEN NONSTOICHIOMETRY  
Yutaka Ueda, University of Tokyo, Japan

09:00 - 09:20 NONSTOICHIOMETRY AND PHYSICAL PROPERTIES OF  $\beta$ -PHASE  $\text{Ag}_x\text{V}_2\text{O}_5$  ( $0.65 < X < 0.90$ )  
Masahiko Isobe, University of Tokyo, Japan

09:20 - 09:40 STRUCTURE ANALYSIS OF COBALT OXIDE SUPERCONDUCTORS BASED ON COMPOSITE CRYSTAL MODELS  
Kazunori Takada, National Institute for Materials Science, Japan

09:40 - 10:00 DEFECT-CHEMICAL PROPERTIES AND ELECTRONIC STRUCTURE OF DOPED  $\text{BaPrO}_3$   
Shogo Miyoshi, The University of Tokyo, Japan

10:00 - 10:30 Coffee break

10:30 - 11:00 A HIGH-TEMPERATURE MÖSSBAUER STUDY INTO THE STRUCTURE, DISORDER, AND FORMATION KINETICS OF IRON NITRIDES  
K.-D. Becker, Technical University of Braunschweig, Germany

11:00 - 11:20 SURFACE MODIFICATION OF  $(\text{La,Sr})\text{CoO}_3$  FOR HIGH PERFORMANCE SOFC CATHODE  
Koji Amezawa, Tohoku University, Japan

11:20 - 11:40 CHEMICAL ROUTE FROM A SOLID ELECTROLYTE TO AN ELECTRIDE - DEFECT CHEMISTRY OF MAYENITE ( $\text{C}_{12}\text{A}_7$ )  
Juergen Janek, Justus-Liebig-University Giessen, Germany

12:00 - 13:00 Lunch

13:00 Optional excursions

Dinner on your own

**Thursday, March 12, 2009**

07:30 – 08:30 Breakfast

**Session VI: Mixed Conductors**

Session Chairs: H. Tuller & J. Mizusaki

08:30 - 09:00 INVESTIGATION OF CATHODE BEHAVIOR OF MODEL THIN FILM  $\text{SrTi}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$   
MIXED IONIC-ELECTRONIC CONDUCTING ELECTRODES AND CORRELATION  
WITH DEFECT PROPERTIES  
Harry Tuller, Massachusetts Institute of Technology, USA

09:00 - 09:20 OXIDATION STATES OF THE TRANSITION METAL CATIONS IN THE HIGHLY  
NONSTOICHIOMETRIC PEROVSKITE -TYPE OXIDE  $\text{Ba}_{0.1}\text{Sr}_{0.9}\text{CO}_{0.8}\text{Fe}_{0.2}\text{O}_{3-\delta}$   
David N. Mueller, RWTH Aachen, Germany

09:20 - 09:40 OXYGEN NONSTOICHIOMETRY IN MIXED CONDUCTORS FROM  
ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY IN A THIN FILM GEOMETRY  
Sossina M. Haile, California Institute of Technology, USA

09:40 - 10:00 ANALYSIS OF STRUCTURAL PHASE TRANSITION OF  $\text{BaCe}_{1-x}\text{Y}_x\text{O}_{3-f}$  BY  
THERMAL ANALYSES AND X-RAY DIFFRACTION AT HIGH TEMPERATURES  
Takuya Hashimoto, Nihon University, Japan

10:00 - 10:30 Coffee break

10:30 - 11:00 B-SITE CATION MIXING EFFECTS ON CHEMICAL STABILITY AND DEFECT  
EQUILIBRIUM OF  $\text{LaCrO}_3$  BASED PEROVSKITE -TYPE OXIDE ELECTRONIC  
CONDUCTORS  
Junichiro Mizusaki, Tohoku University, Japan

11:00 - 11:20 PHASE STABILITY AND PROTON CONDUCTIVITY OF BARIUM CERATES DOPED  
BY TRIVALENT CATIONS HAVING DIFFERENT IONIC RADII  
Byung-Kook Kim, Korea Institute of Science and Technology, Korea

11:20 - 11:40 OXYGEN TRANSPORT KINETICS IN PBCF DOUBLE PEROVSKITE MEMBRANE  
Ji Haeng Yu, Korea Institute of Energy Research, Korea

11:40 - 12:00 MONITORING OF CHEMICAL POTENTIAL OF OXYGEN ON THE SURFACE OF  
GROWING OXIDE SCALES IN HIGH TEMPERATURE OXIDATION OF METALS AND  
ALLOYS  
Toshio MARUYAMA, Tokyo Institute of Technology, Japan

12:00 - 14:00 Lunch

**Session VII: Interface/composite/nanosize effects**

Session Chairs: S-T. Kim & R. A. De Souza

- 14:00 - 14:30      STRUCTURE –PROPERTY RELATIONSHIPS FOR TILT GRAIN BOUNDARIES IN STRONTIUM TITANATE  
Roger A. De Souza, RWTH Aachen University, Germany
- 14:30 - 14:50      ELASTIC STRAIN IN INTERFACES AND ITS INFLUENCE ON THE INTERFACIAL IONIC TRANSPORT – EXPERIMENTAL STUDIES AND FORMAL CONSIDERATIONS  
N. Schichtel, Justus-Liebig-University Giessen, Germany
- 14:50 - 15:10      NANOSCALE CONTROL OF ELECTRODE MATERIALS FOR LI-ION BATTERY AND FUEL CELL  
Byungwoo Park, Seoul National University, Korea
- 15:10 - 15:30      OXYGEN PERMEATION PROPERTIES OF  $\text{GdBaC}_{0.2}\text{O}_{5+d}\text{-Ce}_{0.8}\text{Gd}_{0.2}\text{O}_2$  COMPOSITE MEMBRANE  
Sun-Ju Song, Chonnam National University, Korea
- 15:30 – 16:00      Coffee break
- 16:00 – 16:30      STOICHIOMETRY AND PROPERTIES OF COMPLEX OXIDE THIN FILMS  
Jun Woo Son, University of California, Santa Barbara, USA
- 16:30 – 16:50      RELATIONSHIP BETWEEN STRUCTURAL AND ELECTRICAL PROPERTIES ON PROTON CONDUCTING  $\text{BaZrO}_3$  THIN FILM  
Hiroo Yugami, Tohoku University, Japan
- 16:50 - 17:10      A COMPREHENSIVE ELECTRICAL CHARACTERIZATION OF ACCEPTOR DOPED  $\text{BaTiO}_3$  IN QUENCHED STATE  
Jong-Sook Lee, Chonnam National University, Korea
- 17:10 – 17:50      **Poster Discussion**
- 18:30 – 20:30      Conference Banquet with entertainment

**Friday, March 13, 2009**

- 07:30 – 08:30            Breakfast
- Session VIII: Solid State Devices**  
                              Session Chairs: T. Hasegawa & J. Janek
- 08:30 - 09:00            THREE-TERMINAL ATOMIC SWITCH USING Ta<sub>2</sub>O<sub>5</sub>  
                              Tsuyoshi Hasegawa, National Institute for Materials Science, Japan
- 09:00 - 09:20            NONSTOICHIOMETRIC OXIDES AND THEIR APPLICATION TO RESISTIVE  
                              SWITCHING MEMORY DEVICES  
                              Jinha Hwang, Hongik University, Korea
- 09:20 - 09:40            CONTROL OF LOCAL ION TRANSPORT TO DEVELOP UNIQUE FUNCTIONAL  
                              NANOIONICS DEVICES  
                              Kazuya Terabe, National Institute for Materials Science, Japan
- 09:40- 10:00            MIXED CONDUCTING SILVER(I) POLYCHALCOGENIDE HALIDES, COMPOUNDS  
                              WITH UNEXPECTED SWITCHING PROPERTIES  
                              Tom Nilges, University of Muenster, Germany
- 10:00 - 10:20            AB INITIO STUDY ON THE ELECTRONIC CONDUCTION PATHS IN SOLID  
                              ELECTROLYTE ATOMIC SWITCHES  
                              Satoshi Watanabe, The University of Tokyo, Japan
- 10:20 - 10:50            Coffee break
- 10:50 - 11:20            DEFECT CHEMISTRY AND TRANSPORT PROPERTIES OF NITROGEN-DOPED  
                              YSZ  
                              Juergen Janek, Justus-Liebig-University Giessen, Germany
- 11:20 – 11:40            FABRICATION AND CHARACTERIZATION OF THE NANO-STRUCTURED THIN  
                              FILM ELECTROLYTE  
                              Jong-Ho Lee, Korea Institute of Science and Technology, Korea
- 11:40 - 12:00            THERMAL ATOMIC OXYGEN EMISSION FROM ZIRCONIA  
                              Katsuro Hayashi, Tokyo Institute of Technology, Japan
- 12:00 – 12:10            **Closing Remarks**
- 12:10                      Lunch and Departures

## List of Posters

### Poster Session 1 (Monday)

- <01> REDOX REACTION AND ELECTROCHEMICAL CHARACTERISTIC OF PT-(CE,GD)O<sub>2</sub> MIXED SYSTEM  
Kenji Yoshimura, Department of Materials Engineering, University of Tokyo, Japan
- <03> IONIC/ELECTRONIC TRANSPORT PROPERTIES AND DEFECT/ELECTRONIC STRUCTURE OF  
Ba(Zr<sub>x</sub>Pr)<sub>1-x</sub>O<sub>3</sub>  
Mao Tamaru, Department of Materials Engineering, University of Tokyo, Japan
- <05> CONCENTRATION-DEPENDENT DIFFUSION OF DONORS IN ZINC OXIDE  
Tsubasa Nakagawa, National Institute for Materials Science, Japan
- <07> ELECTROCHEMICAL PROPERTIES OF ELECTRODE-SUPPORTED LA<sub>0.75</sub>SR<sub>0.25</sub>GA<sub>0.8</sub>MG<sub>0.16</sub>FE<sub>0.04</sub>O<sub>3-δ</sub>  
SOLID OXIDE FUEL CELLS  
Ji Haeng Yu, Korea Institute of Energy Research, Korea
- <09> QUANTITATIVE ESTIMATION OF VOLUME FRACTION OF VOID AT METAL/SCALE INTERFACE AND  
AT THE INTERFACE OF DUPLEX SCALE FORMED DURING HIGH TEMPERATURE OXIDATION  
OF METALS AND ALLOY  
Mitsutoshi Ueda, Tokyo Institute of Technology, Japan
- <11> TRANSPORT PROPERTIES OF La<sub>0.1</sub>Sr<sub>0.9</sub>Co<sub>0.8</sub>Fe<sub>0.2</sub>O<sub>3-δ</sub> MEMBRANE  
Moon-Bong Choi, Alternative Energy Materials Research Laboratory, School of Materials Science and  
Engineering, Chonnam National University, Korea
- <13> ELECTRICAL PROPERTY OF BaCe<sub>0.85-x</sub>Zr<sub>x</sub>Y<sub>0.15</sub>O<sub>3-δ</sub> (0 ≤ x ≤ 0.85) PROTON-CONDUCTORS  
Cheol-Jae Park, Alternative Energy Materials Research Laboratory, School of Materials Science and  
Engineering, Chonnam National University, Korea
- <15> FIRST PRINCIPLES SIMULATION OF STOICHIOMETRY AND INTERFACE/SURFACE EFFECTS ON  
IONIC CONDUCTIVITY OF YTTRIA-STABILIZED ZIRCONIA  
Shusuke Kasamatsu, Department of Materials Engineering, University of Tokyo, Japan
- <17> PREPARATION AND CHARACTERIZATION OF COMPLEX OXIDES FOR WATER PHOTOLYSIS  
Eui-Chol Shin, Chonnam National University, Korea
- <19> SYNTHESIS AND STRUCTURE OF NONSTOICHIOMETRIC COMPOUND V<sub>4</sub>O<sub>9</sub> AS A MISSING LINK  
OF WADSWORTH PHASES  
Satoshi Yamazaki, Institute for Solid State Physics, University of Tokyo, Japan

## Poster Session 2 (Tuesday)

- <02> EFFECT OF OXYGEN NON-STOICHIOMETRY ON THE MAGNETIC PROPERTIES OF TiO<sub>2</sub> THIN FILMS  
Lorenzo Malavasi, University of Pavia, Italy
- <04> THE MAGNETORESISTANCE OF METAL-RICH Ag<sub>2+x</sub>Se - A PROTOTYPE NANOSCALE METAL/SEMICONDUCTOR DISPERSION  
Juergen Janek, Justus-Liebig-University Giessen, Institute of Physical Chemistry, Germany
- <06> MOCVD GROWTH OF DOPED CERIA THIN FILMS  
Tae-Sik Oh, California Institute of Technology, USA
- <08> SYNTHESIS AND PHYSICAL CHARACTERIZATION OF NANO-GRAINED BaTiO<sub>3</sub> CERAMICS  
S.-M. Moon, Inha University, Korea
- <10> STRUCTURE OF Ti<sub>4</sub>O<sub>7</sub> PREPARED BY MECHANOCHEMICAL SYNTHESIS  
Kosuke O. Hara, Graduate School of Energy Science, Kyoto University, Japan
- <12> EFFECT OF SM AND W CO-DOPING ON PROPERTIES OF FAST OXYGEN ION  
Moon-Bong Choi, Alternative Energy Materials Research Laboratory, School of Materials Science and Engineering, Chonnam National University, Korea
- <14> FIRST PRINCIPLES STUDY ON THE ELECTRONIC STRUCTURE AND REACTIVITY OF Ni/H/ZrO<sub>2</sub> TRIPLE PHASE BOUNDARY IN SOLID OXIDE FUEL CELL  
Tomofumi Tada, Department of Materials Engineering, University of Tokyo, Japan
- <16> ROLES OF OXYGEN VACANCY AND INTERSTITIAL CU IN ATOMIC SWITCH OF Ta<sub>2</sub>O<sub>5</sub>: AN AB INITIO STUDY  
Tingkun Gu, Department of Materials Engineering, University of Tokyo, Japan
- <18> ACCEPTOR CENTERS IN Ga<sub>2</sub>O<sub>3</sub>  
Detlev M. Hofmann, Physics Institute, University of Giessen, Germany