

## *Program*

# **Nonstoichiometric Compounds**

**Sheraton Kauai Resort Hotel**  
2440 Hoonani Road, Koloa, Kauai, HI 96756  
Tel: 808-742-1661 Fax: 808-742-9777

**April 3-8, 2005**

### *Conference Chairs*

**Manfred Martin**  
RWTH Aachen University

**Thomas O. Mason**  
Northwestern University

**Junichiro Mizusaki**  
Tohoku University

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### **Sunday, April 3, 2005**

16:00 – 18:00	Registration
17:00 – 18:00	Meeting of Organizing Committee, Session Chairs and Keynote Speakers
18:00 – 19:00	Opening Reception
19:00 – 21:00	Dinner ( <i>BeachLawn</i> )

### **Notes**

- ? **Please observe “No Smoking” at ECI technical sessions, meals and social hours.**
- ? **Speakers should allow time at the end of their presentation for questions and discussion.**
- ? **Please silence your cell phone during sessions.**
- ? **Posters will remain on display throughout the conference**
- ? **All General Sessions will be held at the *Poipu Ballroom***
- ? **All Socials and Poster Sessions will be held at *Lawai***

**Monday, April 04, 2005**

- 07:30 – 08:15 Breakfast Buffet (*Shells*)
- 08:15 - 08:25 Welcome and Opening Remarks  
Manfred Martin, Conference Chair  
Jules Routbort, Conference Liaison
- Session I: Transport**  
Session Chair: Thomas O. Mason
- 08:25 – 09:05 **OXYGEN TRANSPORT IN NON-STOICHIOMETRIC OXIDES** (*keynote*)  
J.A. Kilner, Imperial College, London
- 09:05 – 09:30 **QUANTITATIVE PREDICTION OF VOID FORMATION IN A GROWING SCALE IN HIGH TEMPERATURE OXIDATION OF METALS** (*invited*)  
Toshio Maruyama, Tokyo Institute of Technology
- 09:30 – 09:55 **IONIC TRANSPORT AND NEARLY CONSTANT LOSS IN  $\text{Na}_{1.70}\text{Li}_{0.32}\text{Al}_{0.66}\text{O}_{17}$**  (*invited*)  
Klaus Funke, University of Münster
- 09:55 – 10:20 **SYNTHESIS AND CHARACTERISATION OF POTENTIAL SULPHIDE ION CONDUCTORS**  
K. Hellgardt, Loughborough University
- 10:20 – 10:45 **NONSTOICHIOMETRICAL EFFECTS ON THE DIFFUSION OF GROUP I ELEMENTS IN II-VI SEMICONDUCTORS**  
Thomas Wichert, Universität des Saarlandes
- 10:45 – 11:05 Coffee Break
- Session II: Transport**  
Session Chair: Junichiro Mizusaki
- 11:05 – 11:45 **BULK CATION DIFFUSION IN IONIC MATERIALS** (*keynote*)  
Rüdiger Dieckmann, Cornell University
- 11:45 – 12:10 **CREEP AND DIFFUSION IN NANO-YTTRIA TETRAGONAL ZIRCONIA POLYCRYSTALS (NANO-YTZP)** (*invited*)  
Diego Gómez-García, Universidad de Sevilla
- 12:10 – 12:35 **CATION DIFFUSION IN LITHIUM NIOBATE**  
H. Haneda, National Institute for Materials Science, Tsukuba
- 12:35 – 13:00 **DIFFUSION IN THE HIGH-TEMPERATURE MATERIAL MOLYBDENUM DISILICIDE**  
Helmut Mehrer, University of Münster
- 13:00 – 14:30 Lunch (*Shells*)
- 14:30 – 16:30 Ad hoc sessions / free time
- 16:30 – 17:00 Afternoon Coffee

**Monday, April 04, 2005**

**Session III: Transport**

Session Chair: Helmut Mehrer

- 17:00 – 17:40      **CHEMICAL DIFFUSION IN COMPLEX OXIDES** (*keynote*)  
H.-I. Yoo, Seoul National University
- 17:40 – 18:05      **OXYGEN NON-STOICHIOMETRY AND ASSOCIATED DIELECTRIC  
EVOLUTION OF BaTiO<sub>3</sub> BASE-METAL ELECTRODE MULTILAYER  
CERAMIC CAPACITORS**  
G.Y. Yang, The Pennsylvania State University
- 18:05 – 18:30      **HOST CATION TRANSPORT AND SURFACE RECONSTRUCTION OF  
UNDOPED AND DONOR DOPED STRONTIUM TITANATE AT HIGH  
TEMPERATURES**  
Karsten Gömann, Technical University of Clausthal
- 18:30 – 18:55      **ANION DIFFUSION IN Y- AND N-DOPED ZIRCONIA**  
Hans Boysen, LMU München
- 18:55 – 19:20      **DEFECT CHEMISTRY AND TRANSPORT PROPERTIES OF  
NONSTOICHIOMETRIC LANTHANUM NICKEL OXIDES**  
Michael Schroeder, RWTH Aachen University
- 19:30 – 21:00      Dinner (*BeachLawn*)
- 21:00 – 22:30      Poster Session and Social Hour (*Lawa*)

**Tuesday, April 05, 2005**

07:30 – 08:30 Breakfast Buffet (*Shells*)

**Session IV: Bulk Properties**

Session Chair: Neil Allan

08:30 – 09:10 **THERMOCHEMICAL STUDIES OF FLUORITE-BASED OXIDES: ENERGETICS OF DEFECTS IN YTTRIA-STABILIZED ZIRCONIA, HAFNIA, AND CERIA AND OF SOME RELATED NANOMATERIALS** (*keynote*)  
Alexandra Navrotsky, University of California at Davis

09:10 – 09:50 **SPECTROSCOPIC STUDIES OF HIGH-TEMPERATURE SOLID STATE PROCESSES** (*keynote*)  
K.D. Becker, Technical University of Braunschweig

09:50 – 10:15 **ELECTRICAL PROPERTIES OF SUBSTITUTED  $\text{Ca}_2\text{Fe}_2\text{O}_5$**  (*invited*)  
Tim Armstrong, Oak Ridge National Laboratory

10:15 – 10:40 **NONSTOICHIOMETRY, CONDUCTIVITY AND DEFECT CHEMISTRY OF  $(\text{La}, \text{Ca})(\text{Cr}, \text{Al})\text{O}_3$**   
Junichiro Mizusaki, Tohoku University

10:40 – 11:10 Coffee Break

**Session V: Bulk Properties**

Session Chair: Toshio Maruyama

11:10 – 11:50 **HYDROGEN IN OXIDES** (*keynote*)  
Truls Norby, University of Oslo

11:50 – 12:30 **LOCAL ELECTRONIC STRUCTURE OF NONSTOICHIOMETRIC OXIDES BY ELECTRON SPECTROSCOPY** (*keynote*)  
Shu Yamaguchi, The University of Tokyo

12:30 – 12:55 **SOLUTION HARDENING AND SOFTENING IN NON-STOICHIOMETRIC CERAMICS AND INTERMETALLICS** (*invited*)  
Terence E. Mitchell, Los Alamos National Laboratory

13:00 – 14:30 Lunch Buffet (*Shells*)

14:30 – 18:00 Ad hoc sessions / free time

18:30 – 20:00 Dinner (*Beachlawn*)

**Tuesday, April 05, 2005**

**Session VI: Transparent Conducting Oxides**

Session Chair: Tim Armstrong

- 20:00 – 20:40      **TRANSPARENT OXIDE SEMICONDUCTORS** (*keynote*)  
Hideo Hosono, Tokyo Institute of Technology
- 20:40 – 21:05      **TRANSPORT AND DEFECT MECHANISM IN P-TYPE TCO MATERIALS**  
Brian J. Ingram, Northwestern University
- 21:05 – 21:20      Break
- 21:20 – 21:45      ***IN SITU* AND *EX SITU* HIGH-TEMPERATURE STUDIES ON INDIUM-TIN OXIDE**  
G.B. González, European Synchrotron Radiation Facility
- 21:45 – 22:10      **USE OF JONKER PLOTS TO CHARACTERIZE THE TRANSPORT PROPERTIES OF TRANSPARENT OXIDE SEMICONDUCTORS**  
Thomas O. Mason, Northwestern University
- 22:10 – 23:00      Poster Session and Social Hour (*Lawa!*)

**Wednesday, April 06, 2005**

07:30 – 08:30 Breakfast Buffet (*Shells*)

**Session VII: Surfaces, Interfaces**

Session Chair: Bernhardt J. Wuensch

08:30 – 09:10 **SIZE EFFECTS IN CERAMIC NANO-MATERIALS: TRANSPORT, REACTIVITY AND STORAGE** (*keynote*)

Joachim Maier, Max Planck Institute for Solid State Research

09:10 – 09:50 **NON-STOICHIOMETRY AND ELECTRONIC PROPERTIES OF INTERFACES** (*keynote*)

Andreas Klein, Darmstadt University of Technology

09:50 – 10:15 **TWO STEP MECHANISM OF GRAIN BOUNDARY POTENTIAL BARRIER FORMATION IN DONOR-DOPED PEROVSKITES**

Rene Meyer, Research Centre Jülich

10:15 – 10:40 **STRUCTURE-PROPERTY RELATIONSHIPS FOR GRAIN BOUNDRIES IN ACCEPTOR-DOPED SrTiO<sub>3</sub>**

Roger A. De Souza, RWTH Aachen University

10:40 – 11:10

Coffee Break

**Session VIII: Surfaces, Interfaces**

Session Chair: Klaus Funke

11:10 – 11:50 **NITROGEN-DOPED ZIRCONIA – PREPARATION, SURFACE REACTIONS AND TRANSPORT PROPERTIES** (*keynote*)

Jürgen Janek, Justus-Liebig-University Giessen

11:50 – 12:30 **CHARACTERIZATION OF HIGH TEMPERATURE ELECTRODES UNDER OPERATION** (*keynote*)

Tatsuya Kawada, Tohoku University

12:30 – 12:55 **OXYGEN INCORPORATION INTO “ELECTRON-RICH” AND “ELECTRON-POOR” OXIDES: MECHANISTIC STUDIES ON Sr(Fe<sub>x</sub>Ti<sub>1-x</sub>)O<sub>3-?</sub>**

Rotraut Merkle, Max Planck Institute for Solid State Research

13:00 – 14:30

Lunch Buffet (*Shells*)

14:30 – 19:30

Ad hoc discussions / free time

19:30 – 21:00

Dinner (*Beachlawn*)

After dinner speech

**AN HISTORICAL PERSPECTIVE OF INSIGHT INTO STRUCTURE-PROPERTY CONNECTIONS FOR FAST-ION CONDUCTORS**

Bernhardt J. Wuensch, Massachusetts Institute of Technology

Poster Session and Social Hour (*Lawai*)

**Thursday, April 07, 2005**

07:30 – 08:30 Breakfast Buffet (*Shells*)

**Session IX: Theory**

Session Chair: Manfred Martin

08:30 – 09:10 **ATOMIC SCALE MODELS FOR DEFECT STRUCTURE AND TRANSPORT PREDICTIONS** (*keynote*)  
Robin W. Grimes, Imperial College London

09:10 – 09:35 **SIMULATION OF OXIDE SOLID SOLUTIONS** (*invited*)  
Neil L. Allan, University of Bristol

09:35 – 10:00 **ELECTRONIC STRUCTURE, PHASE STABILITY AND CHEMICAL BONDING OF TRANSITION-METAL OXYNITRIDES FROM FIRST-PRINCIPLES THEORY**  
Richard Dronskowski, RWTH Aachen University

10:00 – 10:25 **NANOSCALE ORDERING IN SCANDIUM DOPED ZIRCONIA**  
A.N. Cormack, Alfred University

10:25 – 10:50 Coffee Break

10:50 – 11:15 **LAYERED ATOM PATTERNS IN FLUORITE-STRUCTURED OXIDES**  
Kurt E. Sickafus, Los Alamos National Laboratory

11:15 – 11:40 **AB INITIO BASED MODELLING OF SUBSTOICHIOMETRIC TITANIUM OXY-CARBONITRIDES**  
D.A. Andersson, P.A. Korzhavyi, B. Johansson, Royal Institute of Technology

**Session X: Fuel Cells**

Session Chair: Jules Routbort

11:40 – 12:05 **INVESTIGATION OF THE INTERFACIAL STABILITY BETWEEN ELECTRODE AND ELECTROLYTE LAYER OF LSGM-BASED SOFCs** (*invited*)  
Jong-Ho Lee, Korea Institute of Science and Technology

12:05 – 12:30 **HIGH ELECTRIC CONVERSION EFFICIENCY AND IMPURITY-POISONING OF SOLID OXIDE FUEL CELLS** (*invited*)  
Yoshio Matsuzaki, Tokyo Gas Co., Ltd

12:30 – 12:55 **SUBSTOICHIOMETRIC PEROVSKITES AS CATHODES OR CATALYST IN SOLID OXIDE FUEL CELLS** (*invited*)  
Michael Krumpelt, Argonne National Laboratory

13:00 – 14:30 Lunch Buffet (*Shells*)

14:30 – 18:30 Ad hoc discussions / free time

18:30 Conference Banquet

**Friday, April 08, 2005**

07:30 – 08:30 Breakfast Buffet (*Shells*)

**Session XI: Intermetallics**

Session Chair: Klaus Hilpert

08:30 – 08:55 **A HIGH-RESOLUTION AND IN SITU ELECTRON MICROSCOPE STUDY OF DISLOCATION CLIMB AND STRUCTURAL CHANGES IN TWO-PHASE TITANIUM ALUMINIDE ALLOYS**  
Fritz Appel, GKSS Research Centre

08:55 – 09:20 **NONSTOICHIOMETRY IN LINE COMPOUNDS**  
Gary S. Collins, Washington State University

09:20 – 09:45 **SYNTHESIS OF AIBASED INTERMETALLIC COMPOUNDS WITH NONSTOICHIOMETRIC COMPOSITION BY MEAN OF ION IMPLANTATION OF Ni AND Ti**  
Heishichiro Takahashi, Hokkaido University

9:45 – 10:10 Coffee Break

**Session XII: Transition Metal Compounds**

Session Chair: R. Dieckmann

09:45 – 10:10 **DEFECT FORMATION AND MECHANICAL STABILITY OF PEROVSKITES ON THE BASIS OF  $\text{LaCrO}_3$**   
K. Hilpert, Research Center Jülich

10:10 – 10:35 **ROLE OF CATION VACANCY DISTRIBUTION ON THE PROPERTIES OF CMR MANGANITES**  
Lorenzo Malavasi, Università di Pavia

11:00 – 11:25 **OXYGEN PARTIAL PRESSURE CONTROL DURING SINTERING OF Mn-Zn-FERRITES**  
Jörg Töpfer, Fachhochschule Jena

11:25 – 11:50 **MODELING OF THE DEFECT STRUCTURE OF COPPER-DOPED LANTHANUM COBALTITES**  
A. Yu. Zuev, Ural State University

11:50 – 12:15 Concluding Remarks

12:30 – 14:00 Lunch (*Shells*)  
Departure

# POSTER PRESENTATIONS

- 1. DIFFUSION OF Al AND Fe IN IRON-ALUMINIDES**  
Helmut Mehrer, University of Münster
- 2. DIFFUSION OF Ni AND Mn IN NICKEL-MANGANESE ALLOYS**  
Helmut Mehrer, University of Münster
- 3. TUNEABLE CONDUCTIVITY AND CONDUCTION MECHANISM IN A UV LIGHT ACTIVATED ELECTRONIC CONDUCTOR**  
Mariana I. Bertoni, Julia E. Medvedeva, Thomas O. Mason, Arthur J. Freemann, Kenneth R. Poeppelmeier, Northwestern University
- 4. OXYGEN CONTENT VARIATION IN THE DOUBLE-LAYERED MANGANITES: EFFECT ON THE STRUCTURAL, TRANSPORT AND MAGNETIC PROPERTIES**  
Lorenzo Malavasi, Elena di Tullio, Christina Tealdi, Giorgio Flor, Maria Cristina Mozzati, Carlo B. Azzoni, Università di Pavia
- 5. JOINING ADVANCED MATERIALS BY PLASTIC FLOW**  
Jules Routbort, K. Goretta, D. Singh, Argonne National Laboratory, F. Gutierrez-Mora, A. Dominguez-Rodriguez, Universidad de Sevilla
- 6. THE STRUCTURE RELATED PROPERTIES OF MIXED-CONDUCTING La-Sr CUPRATES**  
G.N. Mazo, S.N. Savvin, Moscow State University
- 7. NONSTOICHIOMETRY AND SOLID SOLUTION FORMATION IN UN, ZrN AND TiN**  
Nicholas J. Ashley, Robin W. Grimes, Jonathan Ball, Imperial College London, Ken McClellan, Los Alamos National Laboratory
- 8. DEFECT STRUCTURE AND CHARGE TRANSFER IN DOPED LANTHANUM COBALTITES AND MANGANITES**  
A.N. Petrov, A.Yu. Zuev, A.I. Vylkov, A.N. Demina, T.V. Aksenova, Ural State University
- 9. ELEMENTARY MECHANISMS IN SOLID STATE REACTIONS**  
Francoise Valdivieso, Michéle Pijolat, Michel Soustelle, Ecole Nationale Supérieure des Mines de Saint-Etienne
- 10. DEFECT INTERACTIONS VIA PAIRWISE DECONVOLUTION**  
Jonathan A. Ball, Robin W. Grimes, Imperial College
- 11. NEUTRON RIETVELD REFINEMENT OF THE STRUCTURE OF OXYGEN-CONDUCTING PHASES IN THE Nd<sub>2</sub>O<sub>3</sub>-Yb<sub>2</sub>O<sub>3</sub> SYSTEM: A SEARCH FOR POSSIBLE PYROCHLORE-LIKE CATION ORDERING IN NdYb<sub>3</sub>O<sub>6</sub>**  
Emily B. Walton, Bernhardt J. Wuensch, Massachusetts Institute of Technology
- 12. INTERACTION BETWEEN OXYGEN, WATER VAPOUR AND LSM IN SOFC SCREEN-PRINTED CATHODES**  
Michele Pijolat, Ecole Nationale Supérieure des Mines de Saint-Etienne
- 13. THERMOCHROMIC PROPERTIES OF DOPED AND UNDOPED VO<sub>2</sub> FILMS**  
Bruno K. Meyer, Ganhua Fu, Angelika Polity, Justus-Liebig-Universität Giessen

14. **ELECTRICAL PROPERTIES OF  $\text{ZnO}_{1-x}\text{S}_x:(\text{H,Al})$**   
Angelika Polity, Thorsten Krämer, Changzhong Wang, Bruno K. Meyer, Justus-Liebig-Universität Giessen
15. **DEFECT ENERGIES REVISITED IN NON-STOICHIOMETRIC  $\text{BaTiO}_3$**   
Soonil Lee, Myong-Ho Kim, Zi-Kui Liu, The Pennsylvania State University
16. **THE EFFECT OF SOLUTIONIZATION OF OXIDE PRECURSORS ON NITRIDE SYNTHESIS**  
C.R. Stanek, K.J. McClellan, J.T. Dunwoody, R.W. Margevicius, Los Alamos National Laboratory, T. Hartmann, University of Nevada Las Vegas
17. **PHASE STABILITY PREDICTION OF PYROCHLORE AND PYROCHLORE RELATED COMPOUNDS**  
C.R. Stanek, K.E. Sickafus, K.J. McClellan, Los Alamos National Laboratory, M.J.D. Rushton, A.R. Cleave, R.W. Grimes, Imperial College London
18. **DEVELOPMENT OF A HIGH TEMPERATURE IONIC CONDUCTING SOLID ELECTROLYTE USING AC IMPEDANCE SPECTROSCOPY**  
V.S. Johnson, K. Hellgardt, S.E. Dann, R. White, Loughborough University
19. **OXYGEN PERMEATION STUDY OF PEROVSKITE HOLLOW FIBRE MEMBRANES FOR THE PARTIAL OXIDATION OF METHANE TO SYNGAS**  
Michael Schroeder, RWTH Aachen University, Cristina Tablet, Gerd Gruber, Haihui Wang, Jürgen Caro, University of Hannover, Thomas Schiestel, Fraunhofer Institut (IGB), Hartmut Hederer, Uhde GmbH
20. **DEGRADATION OF YTRIA-STABILIZED ZIRCONIA IN AN ELECTRIC FIELD**  
Dominik Samuelis, Roger De Souza, Manfred Martin, RWTH Aachen University
21. **INVESTIGATION OF THE PHASE STABILITY AND THE NONSTOICHIOMETRIC DEFECT STRUCTURE OF  $\text{Li-Mn-O}$  SPINEL**  
Chunhui Luo, Manfred Martin, RWTH Aachen University
22. **DEFECT CHEMISTRY AND REDOX PROPERTIES OF  $\text{NdCoO}_3$  PEROVSKITE-TYPE OXIDE**  
Cristina Tealdi, Lorenzo Malavasi, Giorgio Flor, Università degli Studi di Pavia
23. **EFFECT OF NITROGEN DOPING ON IONIC CONDUCTIVITY OF ZIRCONIA**  
Joachim Maier, Jong-Sook Lee, Max Planck Institute for Solid State Research, Martin Lerch, Technische Universität Berlin
24. **OXIDATION KINETICS OF ZIRCONIUM AT HIGH TEMPERATURES STUDIED BY *IN SITU* X-RAY DIFFRACTION**  
N. Lakshmi, M. Martin, RWTH Aachen University, H.-I. Yoo, Seoul National University
25. **INVESTIGATIONS OF THE OXYGEN REDUCTION KINETICS IN SOLID OXIDE FUEL CELLS BY MEANS OF THIN FILM MICROELECTRODES**  
J. Maier, F. Baumann, H.-R. Kim, J. Fleig, Max Planck Institute for Solid State Research
26. **THERMODYNAMIC ACTIVITY MEASUREMENTS IN THE B2 PHASES  $\text{Ni}_{1-x}\text{Al}_x$  and  $(\text{Ni,Fe})_{1-x}\text{Al}_x$**   
L. Bencze, D.D. Raj, T. Markus, W.A. Oates, D. Kath, L. Singheiser, and K. Hilpert  
Research Centre Jülich