

**International FOXSI Conference, May 23-25, 2016**  
**TUtheSky Lounge, TU Vienna**

**Monday, May 23<sup>th</sup>, 2016**

- 9:00 – 09:15      **Günther Rupprechter**      Welcome Address
- 09:15 – 10:15      **Miquel Salmeron** (University of California, Berkeley, USA) INV01  
Structure and Reactions on Catalysts Surfaces in Ambient Gas  
Pressure and Under Liquids
- 10:15 – 11:00      **COFFEE BREAK**
- 11:00 – 11:30      **Shamil Shaikhutdinov** (Fritz-Haber-Institut, Max-Planck-Gesellschaft, DE)  
Ultrathin Oxide Films on Metal Substrates: Case Studies
- 11:30 – 12:00      **Michael Schmid** (TU Wien)  
From Ultrathin to Thin Zirconia Films
- 12:00 – 13:30      **BREAK**
- 13:30 - 13:45      **Johannes Fröhlich** (Vice Rector of Research, TU Wien)  
Welcome Address
- 13:45 – 14:45      **Joachim Sauer** (Humboldt University, Berlin, DE) INV02  
Oxygen Defects and the Reactivity of Ceria
- 14:45 – 15:15      **Lutz Hammer** (Universität Erlangen-Nürnberg, DE)  
LEED Intensity Analyses of Oxide Films - Structural Surprises &  
Reliability
- 15:15 – 15:45      **Detre Teschner** (Fritz-Haber-Institut, Max-Planck-Gesellschaft, DE)  
Ir-Based Electrocatalysts for the Oxygen Evolution Reaction
- 15:45 – 16:30      **COFFEE BREAK (16:25 CONFERENCE PHOTOGRAPH)**
- 16:30 – 17:00      **Martin Sterrer** (Graz University, AT)  
Hydroxylation and Dissolution of Model Thin Film Oxides: MgO, CaO  
and SiO<sub>2</sub>
- 17:00 – 17:30      **Günther Rupprechter** (TU Wien)  
Interaction of Water with Ultrathin ZrO<sub>2</sub> Films
- 17:30 – 18:00      **Josef Redinger** (TU Wien)  
Theory of Oxide Surfaces and Metal/oxide Interfaces – Adsorption on  
ZrO<sub>2</sub> Films and Bulk Surfaces
- 19:30 – 22:00      **RECEPTION (Terrace 11<sup>th</sup> floor)**

**Tuesday, May 24<sup>th</sup>, 2016**

- 09:15 – 10:15 **Joachim Maier** (Max Planck Institute for Solid State Research, Stuttgart DE)  
INV03  
Mass Transport and Mass Storage in Functional Oxides
- 10:15 – 11:00 **COFFEE BREAK**
- 11:00 – 11:30 **Bilge Yildiz** (MIT, USA)  
Elastic Strain and Dislocations in Oxide Thin Films: Hand-in-Hand or Counter in Oxide Ion Conduction?
- 11:30 – 12:00 **Yakun Gao** (University of Oxford, UK)  
Nucleation and Growth of Anatase TiO<sub>2</sub>(001) on the SrTiO<sub>3</sub>(001) Surface
- 12:00 – 13:30 **BREAK**
- 13:30 – 14:30 **Harry L. Tuller** (Dpt. of Materials Science and Engineering, MIT, US) INV04  
Coupled Optical and Electrochemical Investigation of Oxygen Exchange and Diffusion at Oxide Thin Film Surfaces
- 14:30 – 15:00 **Jürgen Fleig** (TU Wien)  
Voltage and Light Affecting Defects in Oxides
- 15:00 – 15:30 **Federico Baiutti** (Max Planck Institute for Solid State Research, Stuttgart, DE)  
High-Temperature Superconductivity in La<sub>2</sub>CuO<sub>4</sub>-Based Heterostructures Induced by Interface Effects
- 15:30 – 16:15 **COFFEE BREAK**
- 16:15 – 16:45 **Ulrike Diebold** (TU Wien)  
Homoepitaxial Growth and Surface Reactivity of SrTiO<sub>3</sub>(110)
- 16:45 – 17:15 **Marco Moors** (Peter Grünberg Institut, FZ Jülich, DE)  
SrRuO<sub>3</sub> Thin Films as Active Layers for Resistive Switching
- 17:15 – 17:45 **Florian Mittendorfer** (TU Wien)  
Theory of Perovskite Surfaces
- 20:00 – 22:00 **POSTER DISCUSSION (11<sup>th</sup> floor)**

**Wednesday, May 25<sup>th</sup>, 2016**

- 09:15 – 10:15 **Mischa Bonn** (Max Planck Institute for Polymer Research, Mainz, DE)  
INV05  
Charge Transfer Across Quantum Dot-Oxide Interfaces for High Efficiency Photovoltaics
- 10:15 – 11:00 **COFFEE BREAK**
- 11:00 – 11:30 **Yuri Suchorski** (TU Wien)  
In Situ Mesoscopic and Microscopic Visualisation of Catalytic Reactions on Metal-Oxide Systems
- 11:30 – 12:00 **M. Verónica Ganduglia-Pirovano** (Instituto de Catálisis y Petroleoquímica-CSIC, Madrid, ES)  
The Non-Innocent Role of Cerium Oxide in Heterogeneous Catalysis: A Theoretical Perspective
- 12:00 – 13:30 **BREAK**
- 13:30 – 14:00 **Bernhard Klötzer** (University Innsbruck, AT)  
Promotional Zr-Metal Interactions in Fuel Reforming Processes
- 14:00 – 14:30 **Andreas Stierle** (University Hamburg and DESY, DE)  
Pt/ZrO<sub>2</sub> Interfaces: From Ultrathin Films to Ion Transport Conditions
- 14:30 – 15:00 **Dominik Eder** (TU Wien)  
Interfacial Dynamics in Nanocarbon-Inorganic Hybrid Photocatalysts
- 15:00 – 15:45 **COFFEE BREAK**
- 15:45 – 16:15 **Michael Stöger-Pollach** (TU Wien)  
Cerenkov Spectrometry and Electron Energy Loss Spectrometry for Quantitative Bandgap Determination in Oxides
- 16:15 – 16:45 **Martin Setvin** (TU Wien)  
Surface Chemistry of Oxygen and Water on Anatase TiO<sub>2</sub> (101)
- 16:45 – 17:15 **Xiao Hu** (University of Oxford, UK)  
Surface Structures of Ultrathin Ti<sub>2</sub>O<sub>3</sub> Films on Au (111)
- 17:15 **CLOSING**

## Poster Program

**Fabian Kollhoff** (Friedrich-Alexander-Universität Erlangen-Nürnberg, DE)  
Adsorption and Thermally Activated Metalation of Carboxy-Functionalized Porphyrins on MgO Nanoparticles

**Christian Berger** (Montanuniversität Leoben, Lehrstuhl für Physikalische Chemie, AT)  
Oxygen Exchange Kinetics of  $\text{La}_{0.9}\text{Ca}_{0.1}\text{FeO}_{3-\delta}$

**Denis Gryaznov** (Institute for Solid State Physics, University of Riga, Riga, LV)  
Mechanism of the Oxygen Reduction Reaction at SOFC Cathodes:  
Combined Experimental and Ab-Initio Investigations

**Wolfgang Wallisch** (TU Wien, University Service Centre for Transmission Electron Microscopy, AT)  
Determining Optical Properties of  $\text{LaSrMnO}_3$ - $\text{LaAlO}_3$  Interfaces by VEELS Investigations

**Eva-Maria Köck, Michaela Kogler** (Institut für Physikalische Chemie, Universität Innsbruck, AT)  
Water Chemistry on  $\text{Y}_2\text{O}_3$ , YSZ and  $\text{ZrO}_2$

**Kevin Ploner** (Institut für Physikalische Chemie, Universität Innsbruck, AT)  
Structure-Activity Relationships in Methanol Steam Reforming on Cu/t-ZrO<sub>2</sub>-Catalysts

I. Bepalov, M. Datler, S. Buhr, J. Zeininger, M. Stöger-Pollach, J. Bernardi, G. Rupprechter, **Y. Suchorski** (TU Wien)  
Catalytic CO Oxidation on Stepped Rh Surfaces

**Peter Lackner** (TU Wien)  
The Influence of the Substrate on Zirconia Thin Films

Nevzat Yigit, Liliana Lukashuk, **Karin Föttinger**, Günther Rupprechter (TU Wien)  
Operando Spectroscopy Studies of  $\text{Co}_3\text{O}_4$  and  $\text{LaCoO}_3$  Catalysts During Preferential CO Oxidation

**Daniel Halwidl**, Florian Mittendorfer, Wernfried Mayr-Schmölzer, Michael Schmid, Josef Redinger, Ulrike Diebold (TU Wien)  
Adsorption of Water and Oxygen on  $\text{Ca}_3\text{Ru}_2\text{O}_7(001)$

**Edvinas Navickas** (TU Wien)  
Water Induced Decoupling of Tracer and Electrochemical Oxygen Exchange Kinetics on Mixed Conducting Oxides

Wernfried Mayr-Schmölzer, Jakub Planer, Tobias Hruby, Oleg Feyta, Florian Mittendorfer, and **Josef Redinger** (TU Wien)  
DFT Calculations on Zirconia Films of Increasing Thickness

**Julia Kunze-Liebhäuser** (Institut für Physikalische Chemie, Leopold-Franzens-Universität Innsbruck, AT)  
Ethanol Electro-Oxidation on Valve Metal (oxy) Carbide Supported Pt (alloy) Catalysts

**Björn Arndt** (University Hamburg and DESY, DE)  
Water Adsorption on Magnetite (001)

**Gregor Feldbauer** (Institute of Advanced Ceramics, Hamburg University of Technology, DE)  
Dimerization of Benzoic Acid on TiO<sub>2</sub> Surfaces - an Ab-Initio Study

**Thomas Kropp** (Humboldt University, Berlin, DE)  
C–H Bond Activation at Ceria-Supported Vanadia Clusters

**Noelia Barrabés** (TU Wien)  
New Atomically Designed Catalytic Active Phases: Co<sub>x</sub>(SR)<sub>m</sub> and Co Doped Au<sub>n</sub>(SR)<sub>m</sub> Clusters

**Alexey Cherevan** (TU Wien)  
Crystalline Mesoporous Tantalum Oxide Photocatalysts: Tuning Pore Sizes and Injection Barriers

**Greta Haselmann** (TU Wien)  
Strong-Metal Support Interaction (SMSI) Effects Under Ambient Conditions in Liquid-Phase Photocatalysis

**C. Rameshan**, H. Li, K. Anic, V. Pramhaas, M. Roiaz, R. Blume, M. Hävecker, R. Rameshan, J. Knudsen, A. Knop-Gericke, G. Rupprechter (TU Wien)  
Methane Dry Reforming Studied on Inverse Pt/ZrO<sub>2</sub> Model Catalyst