

Special Research Program SFB F45 Functional Oxide Surfaces and Interfaces (FOXSI)

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

Monday, May 23th, 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
SiO₂
- 17:00 – 17:30 **Günther Rupprechter** (TU Wien)
Interaction of water with ultrathin ZrO₂ films
- 17:30 – 18:00 **Josef Redinger** (TU Wien)
Theory of oxide surfaces and metal/oxide interfaces – Adsorption on
ZrO₂ films and bulk surfaces
- 19:30 – 22:00 **RECEPTION (Terrace 11th floor)**

Tuesday, May 24th, 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 TiO₂ (001) on the SrTiO₃ (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 La₂CuO₄-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 SrTiO₃(110)
- 16:45 – 17:15 **Marco Moors** (Peter Grünberg Institut, FZ Jülich, DE)
SrRuO₃ 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 (10th and 11th floor)**

Wednesday, May 25th, 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/ZrO₂ 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 TiO₂ (101)
- 16:45 – 17:15 **Xiao Hu** (University of Oxford, UK)
Surface Structures of Ultrathin Ti₂O₃ 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 Y_2O_3 , YSZ and ZrO_2

Kevin Ploner (Institut für Physikalische Chemie, Universität Innsbruck, AT)
Structure-activity relationships in methanol steam reforming on Cu/t-ZrO₂-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 Co_3O_4 and 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 TiO₂ 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_x(SR)_m and Co doped Au_n(SR)_m 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/ZrO₂ model catalyst