

# 32. Workshop: Novel Materials and Superconductivity

**Monday, 13.Feb. Chair: Günther Rupprechter**

**14:00** K. Schwarz (TU Wien): *Opening, 32<sup>nd</sup> WS*

**14:10** Klaus Wandelt (Uni Bonn):  
*Steering Molecular Order at Interfaces*

**15:10** Short Break

**15:30** Franz Giessibl (Uni Regensburg):  
*Maxing out Atomic Force Microscopy:  
Subatomically Resolved Single Atoms, Spins  
and Superconductors*

**16:30** Coffee Break

**17:00** Erik Vesseli (Uni Triest):  
*Low-Dimensional Model Catalysts at Near-Ambient Pressure*

**Evening session Chair: Ulrike Diebold**

**19:30** Julia Kunze-Liebhäuser (Uni Innsbruck):  
*Electrochemical Surface Science Study of  
TiO<sub>2</sub> Nanotube Lithiation and Delithiation*

**20:10** Pawel Kulesza (Uni Warsaw):  
*Mixed-Metal-Oxide-Based Materials for  
Efficient Electrocatalysis and  
Photoelectrocatalysis*

**Thursday, 16.Feb. Chair: Bertram Batlogg**

**14:00** Gregor Tkachov (Uni Würzburg):  
*Topological Insulators and the  
2016 Nobel Prize in Physics in Retrospect*

**15:00** Short Break

**15:15** Andrei Pimenov (TU Wien):  
*Magneto-optics of Topological Insulators*

**16:15** Coffee Break

**16:45** Martin Claassen (Stanford U.):  
*Topology in Condensed Matter Physics*

**Evening session Chair: Andrei Pimenov**

**19:30** Alexey Shuvaev (TU Wien):  
*Magneto-optical Band Structure Mapping of  
Dirac Fermions*

**20:10** Nicholas Plumb (P.Scherrer I., Villingen):  
*Electronic Structure of BaBiO<sub>3</sub>: A Different  
Paradigm for Insulating Parent Compounds of  
HTSCs*

**Tuesday, 14.Feb. Chair: Peter Knoll**

**14:00** Rudi Hackl (W.Meissner Inst., Garching):  
*Magnetism in FeSe*

**15:00** Short Break

**15:15** Marisa Medarde (P.Scherrer Inst, Villingen):  
*Towards Ferroelectricity From Spiral  
Magnetic Order Beyond RT in Layered  
Perovskites*

**16:15** Coffee Break

**16:45** Jan Ingo Flege (Uni Bremen):  
*In Situ Microscopy of Ultrathin Rare-Earth  
Oxide Films and Nanostructures*

**Evening session Chair: Peter Blaha**

**19:30** Andreas Tröster (TU Wien):  
*Landau Theory Meets DFT*

**20:10** Sohaib Ehsan (TU Wien):  
*Calculation of Cubic and Tetragonal Phases  
of RbCaF<sub>3</sub>: A DFT Study*

**Friday, 17.Feb. Chair: Peter Weinberger**

**14:00** Thomas Greber (Uni Zürich):  
*4f Single Molecule Magnets*

**15:00** Short Break

**15:15** Ulrike Diebold (TU Wien):  
*Surface Science Investigations of Metal  
Oxides*

**16:15** Coffee Break

**16:45** Christoph Rameshan (TU Wien):  
*Cobalt Oxides Model Catalysts -  
Surface Reactivity Towards CO and H<sub>2</sub>O*

**Evening session Chair: Günther Rupprechter**

**19:30** Peter Weinberger (TU Wien)  
*Miraculous Chemistry: a few Astonishing  
Demonstration Experiments*

**Posters (continued):**

**T. Ruh** (TU Wien)  
*DFT Study of Water Adsorption on Alkaline-Earth-Oxide Surfaces*  
**S. Schwab** (TU Wien)  
*Reduction of Ion Conductivity in Polymers by Sodium Getter Substances*  
**J. Wang** (TU Wien)  
*Solution Processed Hybrid Lead-free Perovskite and its Solar Application*

**Wednesday, 15.Feb. Chair: Karlheinz Schwarz**

**14:00** Dominik Eder (TU Wien):  
*Hybridisation and Mesostructuring as Tools  
Toward new Functional Materials*

**15:00** Short Break

**15:15** Peter Weinberger (TU Wien):  
*The Spin Crossover Phenomenon and its  
Possible Application – Challenges and Chances*

**16:15** Coffee Break

**16:45** Helge Rosner (MPI Dresden):  
*Electronic Structure of Fe-pnictid  
Superconductors and Related Compounds*

**Evening session Chair: Peter Blaha**

**19:30** Poster session:

**M. Bagheri** (TU Wien)  
*Energy Dependence XPS Valence Band Spectroscopy, DFT Calculation in  
Compression with Hard X-Ray Photo Emission Experiment*  
**K. Belbase** (TU Wien)  
*Calculation of Stress Tensor Within the ab-initio Full Potential Linearized  
Augmented Plane Wave Method*  
**M. Bichler** (TU Wien)  
*DFT Study of the (012) Surface of Hematite*  
**H. Boller** (JKU Uni Linz)  
*The Ternary System Cr-As-N- The Crystal Structure of Cr<sub>6</sub>AsN*  
**L. Deilmann** (TU Wien)  
*Highly Ordered Mesoporous Niobium Oxide and Nitrides*  
**K. Dobrezberger** (TU Wien)  
*Kinetic, Microscopic and Spectroscopic Studies of Carbon Supported  
Palladium and Platinum Catalysts*  
**U. Dziom** (TU Wien)  
*Dynamic Quantum Hall Effect in 2D Electron gas*  
**M. Gollwitzer** (TU Wien)  
*Synthetic Approaches to Novel Crystalline Sponges*  
**G. Gravogl** (TU Wien)  
*Pressure Dependence of Thermochemical Energy Storage Materials*  
**L. Kalantari** (TU Wien)  
*Computational Study of Y NMR Shielding in Intermetallic Yttrium  
Compounds*  
**C. Knoll** (TU Wien)  
*Transition Metal Oxide Redox Couples for High Temperature  
Thermochemical Energy Storage*  
**P. Knoll** (Uni Graz)  
*Multilayer Graphene Deposited by Inverted Fireballs*  
**G. Madsen** (TU Wien)  
*Predictive Calculation of the Lattice Thermal Conductive*  
**D. Meuer** (Uni Regensburg)  
*Building Metal Tips Atom by Atom Characterized With an Extended COFI  
Method*  
**Anna Pimenov** (TU Wien)  
*Magnetolectric Phase Diagrams of Multiferroic GdMn<sub>2</sub>O<sub>5</sub>*  
**F. Renz** (Leibniz Uni Hannover)  
*Molecular Switches for Stimuli-Responsive Drug Release*