

Program



32. Workshop

on

Novel Materials and Superconductivity

BSFZ Obertraun

Feb. 12. – 18. 2017

Sponsored by TU Wien

Location:	Bundessportheim und Freizeitzentrum BSFZ Obertraun Winkl 49 (Oberösterreich, A – 4813 Obertraun Tel: [+43] (6131) 239-0 international Fax: [+43] (6131) 239-423 international
Date:	Arrival: Sunday, February 12th, 2017 Departure: Saturday, February 18th, 2017

Organizers:

Univ.Prof. Dr. Günther Rupprechter
Univ.Prof.i.R. Dr. Karlheinz Schwarz
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Programme Committee:

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World Wide Web: <http://www.wien2k.at/theochem/obertraun/index.html>

Scientific Program

Monday, Feb. 13th, 2017 **Surface Science and Electrochemistry**
(Chair: G. Rupprechter)

- 14:00** Karlheinz **Schwarz** and Günther **Rupprechter** (TU Wien, Austria)
Opening 32nd Workshop
- 14:10** Klaus **Wandelt** (University of Bonn, Germany)
Steering Molecular Order at Interfaces
- 15:10** **Short Break**
- 15:30** Franz **Giessibl** (University of Regensburg, Germany)
Maxing out Atomic Force Microscopy: Subatomically Resolved Single Atoms, Spins and Superconductors
- 16:30** **Coffee Break**
- 17:00** Erik **Vesselli** (University of Trieste, Italy)
Low-Dimensional Model Catalysts at Near-Ambient Pressure
- 17:40** **Break**

18:15 **Dinner**

Evening Session (Chair: U. Diebold)

- 19:30** Julia **Kunze – Liebhäuser** (University of Innsbruck, Austria)
Electrochemical Surface Science at Energy Conversion and -Storage Relevant Materials
- 20:10** Pawel **Kulesza** (University of Warsaw, Poland)
Mixed-Metal-Oxide-Based Materials for Efficient Electrocatalysis and Photoelectrocatalysis
- 20:50** **End**

Tuesday, Feb. 14th, 2017 **Novel Materials I**

(Chair: P. Knoll)

- 14:00** Rudi **Hackl** (Walther Meißner Institute, Germany)
A. Baum, N. Lazarevic, T. Böhm, H.R. Ruiz, Y. Wang, T. P. Devereaux, T. Wolf, R. Hackl
Magnetism in FeSe
- 15:00** **Short Break**
- 15:15** Marisa **Medarde** (Paul Scherrer Institute, Switzerland)
Towards Ferroelectricity From Spiral Magnetic Order Beyond RT in Layered Perovskites
- 16:15** **Coffee Break**
- 16:45** Jan Ingo **Flege** (University of Bremen, Germany)
In Situ Microscopy of Ultrathin Rare-Earth Oxide Films and Nanostructures
- 17:25** **Break**

18:15 **Dinner**

Evening Session (Chair: P. Blaha) **ATTENTION: Small Conference Room!**

- 19:30** Andreas **Tröster** (TU Wien, Austria)
Landau Theory meets DFT
- 20:10** Sohaib **Ehsan** (TU Wien, Austria)
S. Ehsan, A. Tröster, P. Blaha
Calculation of Cubic and Tetragonal Phases of RbCaF₃. A DFT Study
- 20:50** **End**

Wednesday, Feb. 15th, 2017 **Novel Materials II**

(Chair: K. Schwarz)

14:00 Dominik **Eder** (TU Wien, Austria)

Hybridisation and Mesostructuring as Tools Toward new Functional Materials

15:00 **Short Break**

15:15 Peter **Weinberger** (TU Wien, Austria)

D. Müller, C. Knoll, M. Seifried, M. Reissner, G. Giester, P. Weinberger

The Spin Crossover Phenomenon and its Possible Application - Challenges and Chances

16:15 **Coffee Break**

16:45 Helge **Rosner** (Max Planck Institut für chemische Physik fester Stoffe, Germany)

H. Rosner, S.L. Drechsler, I. Kraft, K. Goetze, V. Petzold, C. Geibel

Electronic Structure of Fe-pnictide Superconductors and Related Compounds

17:45 **Break**

18:15 **Dinner**

Evening Session (Chair: P. Blaha)

19:30 **POSTER SESSION**

*Thursday, Feb. 16th, 2017 **Topological Insulators***

(Chair: B. Batlogg)

- 14:00** Dr Gregor **Tkachov** (Würzburg University, Germany)
Topological Insulators and the 2016 Nobel Prize in Physics in Retrospect
- 15:00** **Short Break**
- 15:15** Andrei **Pimenov** (TU Wien, Austria)
Magneto-optics of Topological Insulators
- 16:15** **Coffee Break**
- 16:45** Martin **Claassen** (Stanford University, USA)
Topology in Condensed Matter Physics
- 17:45** **Break**

18:15 **Dinner**

Evening Session (Chair: A. Pimenov)

- 19:30** Alexey **Shuvaev** (TU Wien, Austria)
A. Shuvaev, V. Dziom, N. Mikhailov
Magneto-optical Band Structure Mapping of Dirac Fermions
- 20:10** Nicholas **Plumb** (Paul Scherrer Institut, Switzerland)
Electronic Structure of BaBiO₃: A different Paradigm for Insulating Parent Compounds of HTSCs
- 20:50** **End**

*Friday, Feb. 17th, 2017 **Nanostructured Surfaces***
(Chair: P. Weinberger)

14:00 Thomas **Greber** (University of Zürich, Switzerland)
4f Single Molecule Magnets

15:00 **Short Break**

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

16:15 **Coffee Break**

16:45 Christoph **Rameshan** (TU Wien, Austria)
C.Rameshan, K. Anic, G. Rupprechter
Cobalt Oxides Model Catalysts – Surface Reactivity Towards VO and H₂O

17:25 **End**

18:15 **Dinner**

19:30 **Social Evening**
Peter **Weinberger** (TU Wien, Austria)
„Miraculous Chemistry: a few Astonishing Demonstration Experiments“

POSTER:

- **M. Bagheri** (TU Wien)
M. Bagheri, P. Blaha
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)
Magdalena Bichler, Florian Kraushofer, Zdenek Jakub, Gareth Parkinson, Peter Blaha
DFT Study of the (012) Surface of Hematite
- **H. Boller** (JKU Universität Linz)
H. Boller, H.S Effenberger
The Ternary System Cr-As-N- The Crystal Structure of Cr₆AsN
- **L. Deilmann** (TU Wien)
L. Deilmann, A. Cherevan, D. Eder
Highly Ordered Mesoporous Niobium Oxide and Nitrides
- **K. Dobrezberger** (TU Wien)
Klaus Dobrezberger, Karin Föttinger, Günther Rupprechter
Kinetic, Microscopic and Spectroscopic Studies of Carbon Supported Palladium and Platinum Catalysts
- **U. Dziom** (TU Wien)
U. Dziom, A. Shuvaev, A. Pimenov
Dynamic Quantum Hall Effect in 2D Electron gas
- **M. Gollowitzer** (TU Wien)
Martin Gollowitzer, Danny Müller, Peter Weinberger
Synthetic Approaches to Novel Crystalline Sponges
- **G. Gravogl** (TU Wien)
Georg Gravogl, Danny Müller, Christian Knoll, Peter Weinberger, Ronald Miletich, Andreas Werner
Pressure Dependence of Thermochemical Energy Storage Materials
- **L. Kalantari** (TU Wien)
L. Kalantari, P. Blaha
Computational Study of Y NMR Shielding in Intermetallic Yttrium compounds
- **C. Knoll** (TU Wien)
Christian Knoll, Danny Müller, Michael Harasek, Peter Weinberger
Transition Metal Oxide Redox Couples for High Temperature Thermochemical Energy Storage
- **P. Knoll** (Universität Graz)
J. Reynvaan, M. Mayer, I. Letofsky-Papst, C. Prietl, P. Knoll, A. Hohenau, K. Krenn
Multilayer Graphene Deposited by Inverted Fireballs
- **G. Madsen** (TU Wien)
Predictive Calculation of the Lattice Thermal Conductive
- **D. Meuer** (Universität Regensburg)
Building Metal Tips Atom by Atom Characterized With an Extended COFI Method
- **A. Pimenov** (TU Wien)
A. Pimenov, S.H. Bukhari, Th. Kain, M. Schiebl, A. Shuvaev
Magnetoelectric Phase Diagrams of Multiferroic GdMn₂O₅

- **F. Renz** (Leibniz Universität Hannover)
F. Renz, M. Kumar, R. Lehmann, D. Wengerowsky, R. Saadat, R. Sindelar, and G. Klingelhöfer
Molecular Switches for Stimuli-Responsive Drug Release
- **T. Ruh** (TU Wien)
Thomas Ruh, Christian Knoll, Danny Müller, Peter Weinberger, Peter Blaha
DFT Study of Water Adsorption on Alkaline-Earth-Oxide Surfaces
- **S. Schwab** (TU Wien)
S. Schwab, J. Appenroth, J. Jung, E. Pittenauer, S. Gruber, M. Bauer, S. Miethaner, M. Nelhiebel, H. Hutter
Reduction of ion Conductivity in Polymers by Using Sodium Getter Substances
- **J. Wang** (TU Wien)
J. Wang, G. Haselmann, L. Wan, A. Cherevan, D. Eder
Solution Processed Hybrid Lead-free Perovskite and its Solar Application