

P. WEINBERGER

## Program



# 32. Workshop

on

## Novel Materials and Superconductivity

### BSFZ Obertraun

**Feb. 12. – 18. 2017**

*Sponsored by TU Wien*

<b>Location:</b>	<b>Bundessportheim und Freizeitzentrum BSFZ Obertraun Winkl 49 (Oberösterreich, A – 4813 Obertraun Tel: [+43] (6131) 239-0 international Fax: [+43] (6131) 239-423 international</b>
<b>Date:</b>	<b>Arrival: Sunday, February 12th, 2017 (Dinner 18:00, Get Together 19:30) Departure: Saturday, February 18th, 2017</b>

#### Organizers:

**Univ.Prof. Dr. Günther Rupprechter**  
Univ.Prof.i.R. Dr. Karlheinz Schwarz  
Mag.phil. Ulrike Prohaska  
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#### Programme Committee:

U. Diebold  
W. Lang  
K. Schwarz  
P. Knoll  
S. Paschen  
P. Weinberger

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

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

(Chair: Karlheinz 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: Peter Blaha)*

**19:30** POSTER SESSION

**Friday, Feb. 17th, 2017 Nanostructured Surfaces**

*(Chair: Peter 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 CO and H<sub>2</sub>O*

**17:25** End

**18:15** Dinner

*Evening Session (Chair: Günther Rupprechter)*

**19:30** Social Evening

Peter Weinberger (TU Wien, Austria)

**„Miraculous Chemistry: a few Astonishing Demonstration Experiments“**

## POSTER CONTRIBUTIONS:

- **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 Cr<sub>6</sub>AsN*
- **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*
- **Anna Pimenov** (TU Wien)  
*Anna Pimenov, S.H. Bukhari, Th. Kain, M. Schiebl, A. Shuvaev, A. Pimenov*  
*Magnetoelectric Phase Diagrams of Multiferroic GdMn<sub>2</sub>O<sub>5</sub>*