



TECHNISCHE  
UNIVERSITÄT  
WIEN

## Program



## 33. Workshop

on

# Novel Materials and Superconductivity

## BSFZ Obertraun

**11. - 17. February 2018**

*Sponsored by TU Wien*

<b>Location:</b>	<b>Bundessportheim und Freizeitzentrum BSFZ Obertraun</b> <b>Winkl 49 (Oberösterreich, A – 4831 Obertraun</b> Tel: [+43] (6131) 239-0 international Fax: [+43] (6131) 239-423 international
<b>Date:</b>	<b>Arrival: Sunday, February 11th, 2018</b> (Dinner 18:00, Get Together 19:30) <b>Departure: Saturday, February 17<sup>th</sup>, 2018</b>

**Organizers:**

**Univ.Prof. Dr. Günther Rupprechter**

Ao.Univ.Prof.Dr. Peter Blaha

Mag.phil. Ulrike Prohaska

**Institute of Materials Chemistry**

**TU Wien, Getreidemarkt 9/E165, A-1060 Vienna**

Tel: [+43] (1) 58801-165101

Fax: [+43] (1) 58801-16599

E-Mail: [guenther.rupprechter@tuwien.ac.at](mailto:guenther.rupprechter@tuwien.ac.at)

**Programme Committee:**

B. Batlogg  
F. Kubel  
G. Rupprechter

U. Diebold  
W. Lang  
K. Schwarz

P. Knoll  
S. Paschen  
P. Weinberger

**World Wide Web:** <http://wien2k.at/theochem/obertraun/>

**Wednesday, Feb. 14th, 2018 *Novel Materials and Simulations***

*(Chair: Karlheinz Schwarz)*

**14:00 Jan Kotakoski** (University of Vienna, Austria)

*Structure and Manipulation of 2D Materials at the Atomic Level*

**15:00 Short Break**

**15:15 Florian Libisch** (TU Wien, Austria)

*Simulating Quantum Transport Through Disordered Graphene Nanodevices*

**16:15 Coffee Break**

**16:45 Georg Madsen** (TU Wien, Austria)

*Transport in Defected Materials*

**17:45 Break**

**18:15 Dinner**

*Evening Session (Chair: Peter Blaha)*

**19:30 POSTER SHORT PRESENTATIONS AND POSTER SESSION**

## POSTER CONTRIBUTIONS:

- **Noelia Barrabes – Rabanal** (TU Wien)  
*N. Barrabés, S. Pollitt, G. Rupprechter*  
*Insights on the Reactivity and Stability of Oxide Supported Au<sub>n</sub>(SR)<sub>m</sub> Clusters*
- **Lorenz Bergen** (TU Wien)  
*L. Bergen, E. Constable, L. Weymann, A.A. Mukhin, I.A. Gudim, L.N. Bezmaternykh, Anna Pimenov, A. Pimenov*  
*Phonon Spectroscopy of Magnetoelectric Langasite*
- **Thomas Fabian** (TU Wien)  
*T. Fabian, J. Burgdörfer, F. Libisch*  
*An Efficient Basis set for Large – Scale Quantum Transport Calculations: Applications to Electron – Phonon Coupling*
- **Georg Gravogel** (TU Wien)  
*Moisture-triggered Carbonization of Main Group II Metal Oxides under Elevated CO<sub>2</sub> Pressure*
- **Leila Kalantari** (TU Wien)  
*L. Kalantari, F. Tran, P. Blaha*  
*Testing Nonlocal van der Waals Functionals for Layered Materials*
- **Pawel Kulesza** (University of Warsaw)  
*P.J. Kulesza, I.A. Rutkowska, S. Zoladek, B. Dembinska, K. Miecznikowski*  
*Development of Graphene-Based Supports for Platinum Catalysts Active at Low Loadings During Oxygen Reduction*
- **Peter Kovacs** (TU Wien)  
*P. Kovacs*  
*Why Does SCAN Fail on Alkali Metals?*
- **Alexander Liebig** (University of Regensburg)  
*A.Liebig, A. Peronio, D. Meuer, A.J. Weymouth, F. J. Giessibl*  
*Coulomb's Law at the Nanoscale: Imaging CaF<sub>2</sub>(111) by Atomic Force Microscopy With Atomically Characterized Tips*
- **Franz Renz** (University of Hannover)  
*M. Kumar, D. Wengerowsky, D. Unruh, R. Sindelar, G. Klingelhöfer, F. Renz*  
*Applied Molecular Switches in Drug Release and Gas Separation*