



TECHNISCHE  
UNIVERSITÄT  
WIEN



## Program



### 34th Workshop

on

## Novel Materials and Superconductors

### JUFA Schladming February 10 – 15, 2019

*Sponsored by TU Wien*

<b>Location:</b>	<b>JUFA Hotel Schladming</b> <b>Coburgstrasse 253, A – 8970 Schladming</b> Tel: +43(0) 5/7083-330 international Fax: +43(0) 5/7083-331 international
<b>Date:</b>	<b>Arrival: Sunday, February 10th, 2019</b> (Dinner 18:00, Get Together 19:30) <b>Departure: Friday, February 15th, 2019</b>

**Organizers:**

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

Ao.Univ.Prof.Dr. Peter Blaha

Mag.phil. Ulrike Prohaska

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**Program Committee:**

B. Batlogg

U. Diebold

P. Knoll

F. Kubel

W. Lang

S. Paschen

G. Rupprechter

K. Schwarz

P. Weinberger

**World Wide Web:** <https://www.imc.tuwien.ac.at/konferenzen/>

## Scientific Program

**Monday, Feb. 11th, 2019** *Surface Phenomena*

(Chair: Günther Rupprechter)

**14:00** **Günther Rupprechter** (TU Wien, Austria)

*Opening 34th Workshop*

**14:10** **Ulrike Diebold** (TU Wien, Austria)

U. Diebold et al.

*Surface Science Investigation of Oxides*

**14:50** **Coffee Break**

**15:10** **Franz Gießibl** (Univ. Regensburg, Germany)

F. Huber, S. Polesya, S. Mangkovsky, H. Ebert, F.J. Gießibl

*Transition from Physisorption to Chemisorption Observed by AFM*

**15:50** **Coffee Break**

**16:10** **Thomas Greber** (Univ. Zürich, Switzerland)

*Single Layer Boron Nitride: An Ultimate Membrane*

**16:50** **Break**

**18:00** **Dinner**

*Evening Session (Chair: Ulrike Diebold)*

**19:30** **Peter Weinberger** (TU Wien, Austria)

*Thermochemical Energy Storage – From Concept to Application*

**20:00** **Clara Garcia** (TU Wien, Austria)

C. Garcia , N. Barrabes, G. Rupprechter

*Thiolate Protected Gold Cluster as Catalyst*

**20:30** **End**

**Tuesday, Feb. 12th, 2019** *Interface Science*

(Chair: Peter Knoll)

**14:00** **Jörg Libuda** (Univ. Erlangen-Nürnberg, Germany)

*Model System in Catalysis and Energy Science: From Surface Science to Electrochemistry and Photoelectrochemistry*

**14:40** **Coffee Break**

**15:00** **Markus Valtiner** (TU Wien, Austria)

C. Merola, D. Dworschak, H.W. Cheng, M. Valtiner

*Adsorption and Reactivity at Electrified Solid/Liquid Interfaces: High Resolution Imaging and Single Molecule Studies*

**15:40** **Coffee Break**

**16:00** **Christoph Rameshan** (TU Wien, Austria)

L. Lindenthal, J. Popovic, R. Rameshan, J. Raschofer, T. Ruh, A.K. Opitz, C. Rameshan

*Metal Nanoparticle Exsolution on Perovskite Type Catalyst Materials - Enhancing Catalytic Activity*

**16:40** **Break**

**18:00** **Dinner**

*Evening Session (Chair: Peter Blaha)*

**19:30** **Julia Kunze - Liebhäuser** (Univ. Innsbruck, Austria)

E.-M. Wernig, C. Griesser, T. Götsch, N. Shakibi-Nia, J. Kunze-Liebhäuser

*Activation of Small Molecules at Transition Metal Carbide / Electrolyte Interfaces*

**20:00** **Pawel Kulesza** (Univ. Warsaw, Poland)

P.J. Kulesza, I.A. Rutkowska, A. Wadas, E. Szaniawska, E. Seta

*Functional Electrocatalytic Materials: Conversion of CO<sub>2</sub> and other Inert Reactants*

**20:30** **End**

**Wednesday, Feb. 13th, 2019** *Surface Reactions*

(Chair: Karlheinz Schwarz)

**14:00** **Johannes Lercher** (TU München, Germany)

*A Bridge to Enzymes? – Role of Steric Constraints and Chemical Environment for Catalysis*

**14:40** **Coffee Break**

**15:00** **Christophe Copéret** (ETH Zürich, Switzerland)

*Catalyst Design Through the Controlled Functionalization of Surfaces*

**15:40** **Coffee Break**

**16:00** **Günther Rupprechter** (TU Wien, Austria)

*Applied and Model Catalysts Monitored under Operation*

**16:40** **Break**

**18:00** **Dinner**

*Evening Session (Chair: Christoph Rameshan)*

**19:30** **Meeting of the Program Committee**

**20:00** **POSTER SHORT PRESENTATIONS AND POSTER SESSION**

**Thursday, Feb. 14th, 2019** *Superconductors and Multiferroics*

(Chair: Bertram Batlogg)

**14:00 Georg Madsen** (TU Wien, Austria)

G. Madsen, P. Kovacs, F. Tran, P. Blaha

*Kinetic Energy Dependent Functionals in Density Functional Theory*

**14:40 Coffee Break**

**15:00 Florian Libisch** (TU Wien, Austria)

V. Smejkal, L. Linhart, J. Burgdörfer, F. Libisch

*High Harmonic Generation in Low-Dimensional Materials*

**15:40 Coffee Break**

**16:00 Andrei Pimenov** (TU Wien, Austria)

*Voltage Control of Magnetoelectric Excitations*

**16:40 Break**

**18:00 Dinner**

*Evening Session* (Chair: Andrei Pimenov)

**19:30 Jesús Carrete Montana** (TU Wien, Austria)

J. Carrete, A. van Roekeghem, N. Mingo, G. Madsen

*Atomistic Modeling of Phonon Transmission at Interfaces*

**20:00 Bertram Batlogg** (ETH Zürich, Switzerland)

*Physics in the Smartphone*

**21:00 End**

**Friday, Feb. 15th, 2019** *Short Presentations*

(Chair: Peter Weinberger)

**14:00 Helge Rosner** (Max-Planck-Institut für Chemische Physik fester Stoffe, Germany)

*Physical Properties and Electronic Structure of Delafossites*

**14:20 Christian Knoll** (TU Wien, Austria)

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

*Enlarged Spin Switchable Hoffman-Type Networks for Sensing Applications*

**14:40 Leonie Deilmann** (TU Wien, Austria)

L. Deilmann, D. Eder

*Mesostructuring of Semiconduction Photocatalysts*

**15:00 Coffee Break**

**15:20 Alexey Cherevan** (TU Wien, Austria)

*Towards Surface-Immobilized Non-Noble-Metal Oxide Co-Catalysts for Photocatalytic Water Splitting*

**15:40 Marco Arrigoni** (TU Wien, Austria)

M. Arrigoni, J. Carrete, N. Mingo, G. Madsen

*Role of Force-Constant Disorder in the Lattice Thermal Conductivity of Semiconductor Alloys: a First-Principles Study*

**16:00 Iwona Rutkowska** (Univ. of Warsaw, Poland)

*Graphene Nanostructures in Electrocatalysis*

**16:20 End**

## POSTER CONTRIBUTIONS:

- **Andrea Auer** (Univ. Innsbruck)  
A. Auer, N.S. Nia, C. Griesser, J. Kunze-Liebhäuser  
*Electrochemical Scanning Tunneling Microscopy Study of Cu Single Crystals in CO Saturated Alkaline Solutions*
- **Andreas Baum** (Walther-Meißner-Institut München)  
A. Baum, H.N. Ruiz, N. Lazarevic, Yao Wang, T. Böhm, R. Hosseinian Ahangharnejhad, P. Adelman, T. Wolf, Z.V. Popovic, B. Moritz, T.P. Deveraux, R. Hackl  
*Frustrated Spin Order and Stripe Fluctuations in FeSe*
- **Sohaib Ehsan** (TU Wien)  
S. Ehsan, M. Arrigoni, G. Madsen, P. Blaha  
*First Principles Phonon Calculations for High Temperature Phase of Perovskites*
- **Rezek Estaiteh** (Palestine Technical University)  
M. Rezek, S. Katircioglu  
*Structural Stability and Electronic Properties of Different Cross Sectional Unstrained and Rectangular Cross Section Strained GaP Nanowires*
- **Clara Freytag** (TU Wien)  
Y. Suchorski, M. Datler, I. Bepalov, C. Freytag, J. Zeininger, G. Rupprechter  
*Hydrogen Oxidation on ZrO<sub>2</sub> Supported Rh: Metal-Oxide Interaction Transmitted by Solitary Chemical Waves*
- **Georg Gravogl** (TU Wien)  
*Hydration Behaviour and Cycle Stability of Magnesium Oxide as Thermochemical Energy Storage Material*
- **Shaimaa Habib** (Univ. Graz)  
Shaimaa A. Habib, C. Strablegg, J. Reynvaan, C. Prietl, P. Knoll  
*Ferrite-Graphene Nano-Composites Promising in Energy Management Application*
- **Leila Kalantari** (TU Wien)  
L. Kalantari, P. Blaha  
*Water Adsorption on the CuOx and NiOx Attached to the Anatase TiO<sub>2</sub> (101) Surface by DFT Calculation*
- **Frieda Maria Kapsamer** (TU Wien)  
F.M. Kapsamer, M. Seifried, C. Knoll, D.Müller, G.Giester, M.Reissner, P.Weinberger  
*Imidazole-Based Scorpionate Ligands in Iron (II) Complexes and Their Spin-Crossover Behaviour*
- **Lorenz Lindenthal** (TU Wien, Austria)  
L. Lindenthal, R. Rameshan, C. Rameshan  
*Structural and Chemical Characterisation of Doped Perovskites by XPS and XRD - Tailored Exsolution of Metal Nanoparticles*
- **Franz Renz** (Leibniz Univ. Hannover)  
*Concerted Spin State Switching*
- **Paolo Rudatis** (TU Wien)  
P. Rudatis, D. Eder  
*Composites in Photoelectrochemical Water Splitting*

- **Thomas Ruh** (TU Wien)  
T. Ruh, L. Lindenthal, R. Rameshan, C. Rameshan, P. Blaha  
*Structural Relaxation of Doped Rare Earth Perovskites*
  - **Marco Seifried** (TU Wien)  
M. Seifried, C. Knoll, G. Giester, M. Reissner, D. Müller P. Weinberger  
*Towards Functionalized N1-Substituted 1H-Tetrazoles – A Cross-Coupling Approach*
  - **Vera Truttmann** (TU Wien)  
V. Truttmann, N. Barrabes, G. Rupprechter  
*Reaction of Supported Au11 Nanoclusters with Thiolates*
  - **Dagmar Wengerowsky** (Leibniz Univ. Hannover)  
D. Wengerowsky, R. Lehmann, H-J. Schmidt, G. Klingelhöfer, R. Sindelar, B.F.O. Costa, F. Renz  
*News From "Trompetenden Putto"*
  - **Willi Zeni** (TU Wien)  
W. Zeni, C. Knoll, J.M. Welch, M. Reissner, G. Giester, D. Müller, P. Weinberger  
*Bifunctional Fe(II) SCO-Complexes Based on  $\omega$ -(1H-Tetrazol-1-yl) Carboxylic Acids*
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**General Information:**

*Breakfast: 07.00 – 10.30*

*Lunch: 12.30 – 13:30*

*Dinner: 18.00 – 20.00*

*Afternoon Talks: 30min talk, 10min discussion suggested*

*Evening Talks: 20min talk, 10min discussion suggested*

*Students Talks on Friday: 15min talk, 5min discussion suggested*