



TECHNISCHE
UNIVERSITÄT
WIEN



Program



34th Workshop

on

Novel Materials and Superconductors

JUFA Schladming February 10 – 15, 2019

Sponsored by TU Wien

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

Organizers:

Univ.Prof. Dr. Günther Rupprechter

Ao.Univ.Prof.Dr. Peter Blaha

Mag.phil. Ulrike Prohaska

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Program Committee:

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U. Diebold

P. Knoll

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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 CO₂ 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. Adelmann, 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 ZrO₂ 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 TiO₂ (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 ω -(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