



TECHNISCHE
UNIVERSITÄT
WIEN



36th Workshop

on

Novel Materials and Superconductors



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 5 th , 2023 (Dinner 18:00, Get Together 19:30) Departure: Friday, February 10 th , 2023
Organizers:	Univ.Prof. Dr. Günther Rupprechter Ao.Univ.Prof.Dr. Peter Blaha Institute of Materials Chemistry TU Wien, Getreidemarkt 9/E165, A-1060 Vienna Tel: [+43] (1) 58801-165101 Fax: [+43] (1) 58801-1659 E-Mail: guenther.rupprechter@tuwien.ac.at

Program Committee

B. Batlogg
F. Gießibl
S. Paschen
K. Schwarz

P. Blaha
P. Knoll
A. Pimenov
P. Weinberger

U. Diebold
J. Kunze-Liebhäuser
G. Rupprechter

<http://www.wien2k.at/theochem/schladming/>

Scientific Program

Monday, Feb. 6th, 2022

Surface science and catalysis

(Chair: **Ulrike Diebold**, TUW)

- 14:00** **Günther Rupprechter** (TUW)
Opening 36th Workshop
- 14:05** Introduction by **Ulrike Diebold** (TUW)
- 14:20** **Jörg Libuda** (FAU Erlangen)
Triggering the energy release in molecular solar thermal systems
- 15:00** *Coffee Break*
- 15:30** **Christophe Copéret** (ETH Zurich)
Bridging the gap between single sites and heterogeneous catalysts
- 16:15** **Johannes Zeininger** (TUW)
Field emission microscopy of catalytic reactions on nanotips
- 16:45** **End**

18:00 **Dinner**

Evening Session (Chair: **Günther Rupprechter**, TUW)

- 19:30** Introduction by **Günther Rupprechter** (TUW)
- 19:45** **Friedrich Esch** (TU Munich)
Monitoring the dynamics of cluster/oxide support systems
- 20:30** **Alexander Genest** (TUW)
Selectivity of 1-butene isomerization on Pd nanoparticles - a combined view from experiment and modeling
- 21:00** **End**

For all talks: 5-10 min discussion suggested !!

Tuesday, Feb. 7th, 2023

Advanced methods in theoretical chemistry

(Chair: **Georg Madsen**, TUW)

- 14:00** Introduction by **Georg Madsen** (TUW)
- 14:15** **Florian Libisch** (TUW)
Machine learning sparse tight-binding parameters for defects
- 15:00** *Coffee Break*
- 15:30** **Kristian Berland** (NMBU)
Computational discovery and modeling of novel ferroelectric organic molecular crystals
- 16:15** **Felix Hummel** (TUW)
Coupled cluster method for excited states and thermal mixtures
- 17:00** **End**

18:00 **Dinner**

Evening Session (Chair: **Peter Blaha**, TUW)

- 19:30** Introduction by **Peter Blaha** (TUW)
- 19:45** **Aleix Comas-Vives** (TUW)
Nature, Activity, and Evolution of Catalytic Sites for CO₂ Conversion based on Multiscale Modelling
- 20:15** **Maren Podewitz** (TUW)
Building Better Models to Improve the Accuracy of Computational Catalysis beyond Electronic Structure Theory
- 20:45** **End**

For all talks: 5-10 min discussion suggested !!

Wednesday, Feb. 8th, 2023

Highlights in advanced coordination and metal-organic chemistry

(Chair: **Peter Weinberger**, TUW)

- 14:00** Introduction by **Peter Weinberger** (TUW)
- 14:15** **Andreas Dürrmann** (University Bayreuth)
Multifunctional molecular switches – Luminescence switching and redox active ligands
- 15:00** **Grace Morgan** (University College Dublin)
Spin state ordering and domain wall dynamics in ferroelastic spin crossover complexes
- 15:30** *Coffee Break*
- 16:00** **Franz Renz** (University of Hanover)
MIMOS Mössbauer spectroscopy in space and daily life
- 16:30** **Karl Kirchner** (TUW)
From iconic stoichiometric textbook reactions to catalytic applications
- 17:00** **End**

For all talks: 5-10 min discussion suggested !!

18:00 **Dinner**

Evening Session

- 19:00** **Meeting of the Program Committee**
- 19:30** **POSTER SHORT PRESENTATIONS AND POSTER SESSION**
(Chair: **Peter Blaha**, TUW)

Please prepare a 3 minutes poster presentation (max 3 slides !) and send it to pblaha@theochem.tuwien.ac.at

Thursday, Feb. 9th, 2023

Topology meets superconductivity

(Chair: **Andrei Pimenov**, TUW)

- 14:00** Introduction by **Andrei Pimenov** (TUW)
- 14:15** **Andrey Chubukov** (University of Minnesota)
Topological quantum-critical point
- 15:00** *Coffee Break*
- 15:30** **Natalia Perkins** (University of Minnesota)
Why are we excited about the Kitaev model?
- 16:00** **Louis Ponet** (EPFL)
Topological switching in a multiferroic material
- 16:30** **End**

18:00 **Dinner**

Evening Session (Chair: **Peter Weinberger**, Science Busters)

- 19:30** **Bertram Batlogg** (ETH Zurich)
New developments in organic electronics
- 20:15** **Anna Pimenov** (TUW)
Art and Science in Dialogue: techArt: „Karlsplatz anders“
- 20:45** **End**

For all talks: 5-10 min discussion suggested !!

Friday, Feb. 10th, 2023

Nanomaterials and SciMix

14:00	Introduction tba
14:15	Pawel Kulesza (University of Warsaw) Progress in catalytic electroreduction of environmentally important inorganic molecules: O ₂ , CO ₂ , and N ₂
14:45	Frieda Kapsamer (TU Wien) Tripodal azole-based ligands for SCO compounds
15:15	<i>Coffee Break</i>
15:45	Closing Remarks
16:00	End

For all talks: 10 min discussion suggested !!

POSTER CONTRIBUTIONS

U. Diebold, G. Franceschi, L. Lezuo, A. Conti, J. Hütner, J. Balajka
TU Wien, Institute of Applied Physics
"Atomically-resolved UHV ncAFM of mineral surfaces"

M. Huber, M. Schöbinger, B. Stöger, P. Weinberger
TU Wien, Institute of Applied Synthetic Chemistry
"Towards a novel meso-tetrazole BODIPY ligand system exhibiting enhanced solid-state emission properties"

M. Schöbinger, M. Huber, B. Stöger, M. Reissner, P. Weinberger
TU Wien, Institute of Applied Synthetic Chemistry
"Tailoring spin transition properties for a series of luminescence active BODIPY-tetrazole Fe(II) complexes"

J. Smith, A. Werner*, P. Weinberger;
TU Wien, Inst. of Applied Synthetic Chemistry
*TU Wien, Inst. of Energy Systems and Thermodynamics
"Mixed Tutton salts in thermochemical energy storage"

D. Wengerowsky, F. Renz
Universität Hannover
„Chemistry and Art“

J. Werner, J. Smith, A. Werner*, P. Weinberger;
TU Wien, Inst. of Applied Synthetic Chemistry
*TU Wien, Inst. of Energy Systems and Thermodynamics
"Synthesis and characterization of novel calcium dicarboxylate hydrates as thermochemical energy storage materials"

S. Mundigler, M. Huber, M. Schöbinger, P. Weinberger
TU Wien, Institute of Applied Synthetic Chemistry
„Design and synthesis of novel tetrazole-BODIPY ligands for luminescence active Fe(II) SCO complexes“

R. A. Talmazan, I. Castillo, T. Hofer, M. Podewitz
TU Wien, Institute of Materials Chemistry
“Evolving towards chemically accurate supramolecular catalyst modelling: A QM/MM/MD study on C-N coupling”

P. Winkler, J. Zeininger M. Raab, Y. Suchorski, G. Rupprechter
TU Wien, Institute of Materials Chemistry
“In situ imaging of multi-states in a catalytic surface reaction”

Iwona A. Rutkowska, Pawel J. Kulesza
University of Warsaw, Faculty of Chemistry
“Multifunctional catalysts composed of bi-metallic nanostructures for electrooxidation of dimethyl ether fuel”

J. Wettstein, D. Szaller, A. Shuvaev, Anna Pimenov, X. Wang, S.-W. Cheong, M. Mostovoy, N. Marzari, S. Artyukhin, L. Ponet, A. Pimenov
TU Wien, Institute of Solid State Physics
"Electric field control of multiple switching regimes in a multiferroic"

Scott Docherty, Christophe Copéret
ETH Zurich
“Structure and role of reducible dopants in bimetallic catalysts for the hydrogenation of CO₂ to methanol”

General Information:

Breakfast: 07.00 – 10.30

Dinner: 18.00 – 20.00