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Der Wissenschaftsfonds.

TAming COmplexity in Materials Modeling (TACO)

2nd Annual PhD Workshop

Date: February 12–15, 2023

Place: JUFA Hotel, Coburgstraße 253, 8970 Schladming

Sunday, February 12

08:00 – 12:00 Bus transfer from Vienna (Wiedner Hauptstr./Resselg.) to Schladming
12:00 – 13:00 Lunch, Check-in
13:00 – 16:00 Outdoor discussions

Chair: Thomas Ruh (P01)

16:00 – 16:20 **Ulrike Diebold, TU Wien (P01)**
Welcome address

16:20 – 17:00 **Pavel Jelinek, Palacký University (invited)**
On-Surface Chemistry: What Makes it Special?

17:00 – 17:30 **Bernhard Schmiedmayer, University of Vienna (P03)**
Machine Learning Tensorial Quantities: The Infrared Spectrum

17:30 – 17:50 Break

17:50 – 18:30 **Gerhard Mestl, Clariant (invited)**
Successful Joint Industry-Academia Development of the new, innovative EDHOXTM process and catalyst by Linde and Clariant

19:00 – 20:00 Dinner

20:00 – 20:15 **Poster Speed Talks** (chair: Stefan Uttenthaler, P01)

20:15 – open-end **Poster session**

Monday, February 13

08:00 – 08:30	Breakfast
08:30 – 12:00	Outdoor discussions
12:00 – 13:00	Lunch
13:00 – 15:00	Outdoor discussions



Chair: Erik Rheinfrank (P02)

15:00 – 15:40	Lutz Hammer, FAU Erlangen-Nürnberg (invited) <i>Tellurium Structures on Transition Metal Surfaces – Challenges for and Insights from LEED-IV</i>
15:40 – 16:10	Alexander Imre, TU Wien (P02) <i>Accessible LEED-I(V): The Vienna Package for TensErLEED</i>
16:10 – 16:40	Marco Corrias, University of Vienna (P07) <i>Total Variation Denoising and Microscopy Image Analysis</i>
16:40 – 17:00	Break

Chair: Thomas Haunold (P08)

17:00 – 17:40	Jennifer Strunk, LIKAT Rostock (invited) <i>Photocatalysis between High-Purity and Applied Reaction Conditions: Understanding Carbon Dioxide Reduction on the Molecular Level</i>
17:40 – 18:10	Parinya Tangpakonsab, TU Wien (P08) <i>Copper Oxide Catalyst for the Preferential Oxidation of Carbon Monoxide: Experiment and Modeling</i>
18:10 – 18:40	Alberto Tampieri, TU Wien (P10) <i>Nanocrystalline Spinel Oxides and their Use as Catalysts in the Water Gas-Shift Reaction</i>
19:00 – 20:00	Dinner
20:00 – open-end	Poster session

Tuesday, February 14

08:00 – 08:30	Breakfast
08:30 – 12:00	Outdoor discussions
12:00 – 13:00	Lunch
13:00 – 15:00	Outdoor discussions



Chair: Sebastian Falkner (P12)

15:00 – 15:40	Barbara Lechner, TU Munich (invited) <i>A Microscopic View on Nanoscale Structural Dynamics of Oxide-Supported Clusters</i>
15:40 – 16:10	Moritz Eder, TU Wien (P04) <i>Hematite(012) – An Alternative, Water-Stable, Complex Oxide Surface</i>
16:10 – 16:40	Moritz Zelenka, University of Vienna (P11) <i>A Peek at the Spinel-Water Interfacial Structure</i>
16:40 – 17:00	Break

Chair: Pablo Montero de Hijas (P12)

17:00 – 17:40	Livia Bartok-Partay, University of Warwick (invited) <i>Nested Sampling ... What Can We Learn about Interatomic Potentials?</i>
17:40 – 18:10	Ralf Wanzanböck, TU Wien (P09) <i>Accelerated Search for Surface Reconstructions through Chemical and Structural Space</i>
18:10 – 18:40	Salvatore Romano, University of Vienna (P12) <i>Neural Network Potential for the Magnetite-Water Interface</i>
19:00 – 20:00	Dinner
20:00 – 21:00	Executive Board meeting (PI, Co-PIs & student representatives)
20:00 – open-end	Poster Session

Wednesday, February 15

07:00 – 07:45	Breakfast
8:00 – ca. 12:00	Bus transfer to Vienna