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## TAming COmplexity in Materials Modeling (TACO)

### 1<sup>st</sup> Annual PhD Workshop

**Date:** April 3–6, 2022

**Place:** JUFA Hotel, Coburgstraße 253, 8970 Schladming

#### Sunday, April 3

07:30 – 11:30	Bus transfer from Vienna (Wiedner Hauptstr./Resselg.) to Schladming
11:30 – 12:30	Check-in, Get-together
12:30 – 13:00	Lunch
13:00 – 19:00	Outdoor discussions
19:00 – 19:30	Dinner
19:30 – 20:10	<b>Andreas Nening, TU Wien</b> <i>Cation Segregation in Perovskite Oxides and its Effect on Oxygen Exchange Kinetics</i>
20:10 – 20:40	<b>Florian Buchner, TU Wien (P09, <a href="#">via Zoom</a>)</b> <i>Studies on the <math>Fe_2O_3(1-102)</math> Surface Using Evolutionary Search</i>
20:40 – 21:10	<b>Jiri Pavelec, TU Wien (P04)</b> <i>Progress in IRAS Development and Structure of <math>Fe_3O_4(111)</math></i>
21:10 – 23:00	<b>Poster session</b>

## Monday, April 4

08:00 – 08:30	Breakfast
8:30 – 12:30	Outdoor discussions
12:30 – 13:00	Lunch
14:50 – 15:30	<b>Marco Eckhoff, Georg-August-Universität Göttingen</b> <i>Insights into Lithium Manganese Oxide–Water Interfaces Using High-Dimensional Neural Networks</i>
15:30 – 16:00	<b>Thomas Haunold, TU Wien (P08)</b> <i>LiO<sub>x</sub>-Modification of Ni and Co<sub>3</sub>O<sub>4</sub> Surfaces</i>
16:00 – 16:30	Break
16:30 – 17:00	<b>Viktor Birschtzky, University of Vienna (P07)</b> <i>Machine Learning for Exploring Small Polaron Configurational Space</i>
17:00 – 17:30	<b>Moritz Zelenka, University of Vienna (P11)</b> <i>MgO and Spinel Skiing on the Interface</i>
19:00 – 19:30	Dinner
19:30 – 20:00	<b>Sebastian Falkner, University of Vienna (P12)</b> <i>Generative Neural Networks for Efficient Sampling from Complex Distributions</i>
20:00 – 20:40	<b>Maricruz Sanchez, TU Wien</b> <i>Unraveling Structure and Location of Cu-oxo Clusters Hosted by Zeolites for the Direct Methane to Methanol Reaction</i>
20:40 – 21:10	<b>Michael Pittenauer, TU Wien (P10, <a href="#">via Zoom</a>)</b> <i>Characterisation and Water-Gas Shift Reactivity of Co- and Ni-Ferrites</i>
21:10 – 23:00	<b>Poster session</b>



## Tuesday, April 5

08:00 – 08:30	Breakfast
8:30 – 12:30	Outdoor discussions
12:30 – 13:00	Lunch
14:50 – 15:30	<b>Stefan Förster, Martin-Luther-Universität Halle-Wittenberg</b> <i>The Atomic Structure of Oxide Quasicrystals</i>
15:30 – 16:00	<b>Erik Rheinfrank, TU Wien (P02)</b> <i>Surface Structures of <math>\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3(001)</math> Thin Films Grown by Pulsed Laser Deposition</i>
16:00 – 16:30	Break
16:30 – 17:10	<b>Tobias Schäfer, TU Wien</b> <i>Complex Oxides: Accurate First-Principle Benchmarks for Machine-Learning – the Role of Many-Electron Correlation Explained without too many Equations</i>
17:10 – 17:40	<b>Martin Unzog, University of Vienna (P03)</b> <i>Implementing the Bethe-Salpeter Equation for Core-Electron-Hole Bound States</i>
17:40 – 18:30	<b>Executive-board meeting (PI, CO-PIs &amp; student representatives)</b>
19:00 – 19:30	Dinner
20:00 – 21:00	<b>General Assembly</b>



## Wednesday, April 6

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