Sunday, 24 September 2023

16:00 – 17:00	**Registration**

Chair: Ulrike Diebold

17:00 – 17:10	**Welcome address by Ulrike Diebold, TU Wien**
17:10 – 17:50	**Boris Kozinsky, Harvard University (invited)** *Symmetry constraints in machine learning models of electronic and atomic interactions*
17:50 – 18:15	**Georg Kresse, University of Vienna (TACO P03)** *Learning Differences and Derivatives: Efficient ML for Materials*
18:15 – 18:40	**Florian Libisch, TU Wien (contributed)** *Treating Strain Effects in Large-Scale Reconstructions*
18:40 – 19:00	**Poster Speed Talks**
19:00 – 21:30	**Welcome Reception and Poster Session** Catering by BRoK Catering Company

Monday, 25 September 2023

Morning

Chair: Georg Madsen

09:00 – 09:40 **Johannes Kästner, University of Stuttgart (invited)**

Gaussian-Moment Neural Networks Provide Transferable and Uniformly Accurate Interatomic Potentials

09:40 – 10:05 **Jesus Carrete, TU Wien (TACO P09)**

Uncertainty Quantification and Adversarial Learning Strategies for Neural-Network Force Fields

10:05 – 10:45 **Coffee Break**

Chair: Matthias Meier

10:45 – 11:25 **Andreas Grüneis, TU Wien (invited)**

Towards Chemical Accuracy for Surface Chemistry Using Coupled-Cluster Theory

11:25 – 11:50 **Cesare Franchini, University of Vienna (TACO P07)**

Spatial Distribution of Interacting Defects Using Machine Learning

11:50 – 12:15 **Stefan Riemelmoser, University of Vienna (contributed)**

Machine Learning Density Functionals for the Random-Phase Approximation

12:15 – 13:45 **Lunch Break**

Monday, 25 September 2023

Afternoon

Chair: Christoph Dellago

13:45 – 14:25 **Ralf Drautz, Ruhr University Bochum (invited)**

Atomic Cluster Expansion for a Unified Approach to Machine Learning Interatomic Potentials

14:25 – 15:05 **Jonas Köhler, Microsoft / Freie Universität Berlin (invited)**

Boltzmann Generators

15:05 – 15:45 **Coffee Break**

Chair: Michael Schmid

15:45 – 16:10 **Andreas Kretschmer, TU Wien (contributed)**

Encoding the Electronic Density of States for Machine Learning of Mechanical Properties in Transition Metal Carbides

16:10 – 16:35 **Alberto Tampieri, TU Wien (TACO P10)**

Liquid-Phase Catalytic Oxidation of Alcohols over Spinel Oxides

16:35 – 17:00 **Thomas Haunold, TU Wien (TACO P08)**

Surface Hydroxylation of Ultrathin Co_3O_4(111) Films: In Situ NAP-XPS and DFT Studies

17:00 – 17:20 **Poster Speed Talks**

17:20 – 20:30 **Poster Session**

Tuesday, 26 September 2023

Morning

Chair: Günther Rupprechter

09:00 – 09:40 **Beatriz Roldán Cuenya, Fritz Haber Institute Berlin (invited)**

From Single Atoms to Clusters, Nanoparticle and Thin Film Catalysts in Energy Conversion

09:40 – 10:05 **Štefan Vajda, J. Heyrovský Institute of Physical Chemistry (NanoCat)**

Size- and Composition-Selected Subnanometer Clusters in Catalysis: Controlling Selectivity

10:05 – 10:45 **Coffee Break**

Chair: Karin Föttinger

10:45 – 11:25 **Tanja Cuk, University of Colorado, Boulder (invited)**

Resolving Catalytic Mechanism at an Electrode Surface: Thermodynamics and Kinetics of Reaction Steps

11:25 – 11:50 **Christoph Jung, Universität Ulm (NanoCat)**

Catalysis at Electrode/Electrolyte Interfaces: Insights from DFT and MD

11:50 – 12:15 **Ellen Backus, University of Vienna (TACO P11)**

Ultrafast Surface-Specific Spectroscopy of Water at the TiO_2-Water Interface

12:15 – 13:45 **Lunch Break**

Tuesday, 26 September 2023

Afternoon

Chair: Christoph Rameshan

13:45 – 14:25 **Karsten Reuter, Fritz Haber Institute Berlin (invited)**

Exploring Catalytic Reaction Networks with Machine Learning

14:25 – 14:50 **Giacomo Melani, University of Chicago (contributed)**

Structure and Reactivity of Bismuth Vanadate-Water Interfaces

14:50 – 15:30 **Coffee Break**

Chair: Gareth Parkinson

15:30 – 16:10 **Zdenek Dohnálek, Pacific Northwest National Laboratory (invited)**

Synthesis and Catalytic Activity of Atomically Precise Model Catalysts

16:10 – 16:35 **Jiří Pavelec, TU Wien (TACO P04)**

Optimized Infrared Reflection Absorption Spectroscopy for Metal Oxides: Overcoming Challenges of Low Reflectivity and Sub-Monolayer Coverage

16:35 – 17:00 **Pablo Montero, University of Vienna (TACO P12)**

Ab Initio Machine Learning Simulations of Water: From Bulk to Interfaces

19:00 **Conference Dinner (see Page 55 for practical information – please sign up!)**

Wednesday, 27 September 2023

Morning

Chair: Moritz Eder

09:00 – 09:40 **Bilge Yildiz, Massachusetts Institute of Technology (invited)**

Electrochemical Ionic Synapses for Analog Deep Learning and Beyond

09:40 – 10:05 **Michele Riva, TU Wien (TACO P02)**

Surfaces of $La_{0.8}Sr_{0.2}MnO_3$ at the Atomic Scale

10:05 – 10:45 **Coffee Break**

Chair: Alexander Genest

10:45 – 11:25 **Martin Setvin, Charles University Prague (invited)**

Solving Surface Structures by a Combination of STM/AFM and Machine-Learning Methods

11:25 – 11:50 **Jan Balajka, TU Wien (contributed)**

Atomic Structure of Reconstructed Alumina

END

12:30 – 13:30 **TACO Executive Board Meeting (TACO representatives only)**