TACO Retreat 2022

Program

Date: September 14 – 16, 2022

Place: Steinschaler Dörfl, 3213 Frankenfels

Wednesday, September 14

11:00 – 12:00	Arrival, Check-in, Get Together
12:00 – 13:15	Lunch

Session 1, Chair: Moritz Eder

13:15 – 13:25	**Ulrike Diebold**: Welcome Address
13:25 – 14:10	Keynote I: **Annabella Seloni**, Princeton University *Water-Titania Interfaces from Ab Initio Deep Neural Network Simulations*
14:10 – 14:35	**Ellen Backus**, University of Vienna (P11) *Towards Water Splitting at Oxide Water Interfaces*
14:35 – 15:00	**Gareth Parkinson**, TU Wien (P04) *Ethylene Adsorption at Clean and Rh-Decorated Fe_3O_4 Surfaces*
15:00 – 15:30	Coffee Break

Session 2, Chair: Alessandro Coretti

15:30 – 16:15	Keynote II: **Roberto Car**, Princeton University *Multiscale Modeling of Materials with Deep Neural Networks trained on First-Principles Quantum Mechanical Data*
16:15 – 16:40	**Christoph Dellago**, University of Vienna (P12) *Machine Learning for Rare Events*
16:40 – 17:05	**Cesare Franchini**, University of Vienna (P07) *P0laron7: Types, Patterns, and Dynamics*
17:05 – 18:00	Poster Speed Talks
18:00 – 19:30	Dinner
19:30 – Open End	Poster Session

Thursday, September 15

07:30 – 09:00	Breakfast

Session 3, Chair: Alexander Genest

09:00 – 09:45	Keynote III: **Rossitza Pentcheva**, University Duisburg-Essen *Designing Electronic Phases at Oxide Interfaces for Energy Conversion Applications*
09:45 – 10:10	**Georg Madsen**, TU Wien (P09) *Transferability of Neural Network Force Fields for Evolutionary Structure Searches*
10:10 – 10:35	**Georg Kresse**, University of Vienna (P03) *Machine Learning Density Functionals and the Polarization Using Derivative Information*
10:35 – 11:05	Coffee Break & Poster Viewing

Session 4, Chair: Michele Riva

11:05 – 11:50	Keynote IV: **Claus Ropers**, MPI for Multidisciplinary Sciences *Probing Ultrafast Dynamics at Surfaces with Low-Energy Electron Pulses*
11:50 – 12:15	**Ulrike Diebold**, TU Wien (P02) *Surface Structure and Reactivity at the Atomic Scale: Progress, Plans, Ideas*
12:15 – 13:45	Lunch

Session 5, Chair: Alberto Tampieri

13:45 – 14:30	Keynote V: **Jan-Dierk Grunwaldt**, Karlsruhe Institute of Technology *Probing of Structural Dynamics of Single Sites, Clusters and Noble Metal Particles Using X-Ray and Microscopic Techniques*
14:30 – 14:55	**Günther Rupprechter**, TU Wien (P08) *Catalysis by Cobalt-Based Perovskites*
14:55 – 15:35	Coffee Break & Workshop Photo

Session 6, Chair: Chunlei Wang

15:35 – 16:00	**Karin Föttinger**, TU Wien (P10) *Structure and Reactivity of Mixed Oxide Nanoparticles: Progress and Next Steps*
16:00 – 16:25	**Carla Verdi**, University of Vienna (P03) *Δ-Machine Learning Beyond DFT: From Quantum Paraelectricity to CO Adsorption*
16:25 – 18:15	Poster Session
18:15 – 19:45	Dinner
19:45 – 20:45	Executive Board Meeting / Poster discussions

Friday, September 16

07:30 – 09:00	Breakfast
	Session 7, Chair: Pablo Montero de Hijes
09:00 – 09:45	**Ralph Claessen**, University Würzburg Keynote VI: *Orbital Engineering of Atomic Monolayers as Quantum Spin Hall Insulators*
09:45 – 10:10	**Michael Schmid**, TU Wien (P02) *Thermodynamic Analysis of Temperature-Programmed Desorption for Complex Surfaces*
10:10 – 10:35	Coffee Break & Poster Viewing
	Session 8, Chair: Xia Li
10:35 – 11:05	**Michele Reticcioli**, University of Vienna (P07) *Novel Polaron Effects on Perovskite Surfaces*
11:05 – 11:30	**Jesús Carrete Montaña**, TU Wien (P09) *Uncertainty Quantification and Multi-Objective Optimization in a Neural-Network Force Field*
11:30 – 11:55	Final discussion
11:55 – 12:00	**Ulrike Diebold**: Closing Remarks
12:00 – 13:30	Lunch
13:30	End of Workshop