TACO Retreat 2025

Program

Date: September 22 – 24, 2025

Place: Steinschaler Dörfl, 3213 Frankenfels

Monday, September 22

11:00 – 12:00	Arrival, Check-in, Get Together
12:00 – 13:15	Lunch
	Session 1, Chair: Gareth Parkinson
13:15 – 13:25	**Ulrike Diebold**: Welcome Address
13:25 – 14:10	Keynote I: **Hannes Jónsson**, University of Iceland *Towards Improved Methodology for Photocatalysis Simulations*
14:10 – 14:35	**Christian Schäfer**, TU Wien *Taming Polaritonics*
14:35 – 15:00	**Cesare Franchini**, University of Vienna (P07) *Nanosecond Machine Learning Polaron Dynamics*
15:00 – 15:30	Coffee Break
	Session 2, Chair: Karin Föttinger
15:30 – 16:15	Keynote II: **Gregory A. Kimmel**, Pacific Northwest National Laboratory *The Structure and Reactivity of Water and Carboxylic Acids on Model TiO_2 Catalysts*
16:15 – 16:40	**Florian Kraushofer**, TU Wien (P04) *Unravelling the Nature of Realistic 'Single Atom' Active Sites*
16:40 – 17:05	**Alexander Genest**, TU Wien (P08) *$LaCoO_3$ and $LaNiO_3$ – Exploring CO Oxidation from Experiment and Theory*
17:05 – 17:30	**Silvio Bellomi**, TU Wien (P10) *Low-Temperature Alcohol Oxidation in Cobalt-Based Catalysis: Redox States and Transient Acetate Blocking*
17:30 – 18:00	Poster Speed Talks (Chair: Stefan Uttenthaler)
18:00 – 19:30	Dinner
19:30 – Open-End	Poster Session / Executive Board Meeting (PIs, Co-PIs, & Student Representatives)

Tuesday, September 23

07:30 – 09:00	Breakfast
	Session 3, Chair: Johanna Carbone
09:00 – 09:45	Keynote III: **Lorenzo Monacelli**, University La Sapienza *A Unified Quantum Framework for Electrons and Ions: The Self-Consistent Harmonic Approximation on a Neural Network Curved Manifold*
09:45 – 10:10	**Georg Kresse**, University of Vienna (P03) *Auxiliary Field Quantum Monte Carlo: Towards Reference Results for Molecules, Solids, and their Surfaces?*
10:10 – 10:35	**Florian Libisch**, TU Wien *Machine Learning for Defects in 2D Semiconductors*
10:35 – 11:05	Coffee Break & Poster Session
	Session 4, Chair: Christoph Dellago
11:05 – 11:50	Keynote IV: **Benjamin Rotenberg**, Sorbonne University *Making Sense of Electrical Noise by Simulating Electrolyte Solutions*
11:50 – 12:15	**Ellen Backus**, University of Vienna (P11) *Photopolymers: Interfacial Structure and Hydrogen Production Efficiency*
12:15 – 12:30	Workshop Photo
12:30 – 13:45	Lunch
	Session 5
13:45 – 18:00	Outdoor Discussions
18:00 – 19:30	Dinner
19:30 – 20:00	General Assembly
20:00 – Open-End	Poster Session

TACO

TAMING COMPLEXITY TOGETHER

Wednesday, September 24

07:30 – 09:00	Breakfast
	Session 7, Chair: Günther Rupprechter
09:00 – 09:45	Keynote V: **Alexander Ganose**, Imperial College London *Electron and Thermal Transport at Database Scale*
09:45 – 10:10	**Esther Heid**, TU Wien (P09) *Uncertain Foundation Models for Complex Surface Reconstructions*
10:10 – 10:35	**Pablo Montero de Hijes**, University of Vienna (P12) *Recent Progress in Ice Nucleation Studies*
10:35 – 11:05	Coffee Break & Poster Session
	Session 8, Chair: Georg Madsen
11:05 – 11:50	Keynote VI: **Johannes Margraf**, University of Bayreuth *How Foundation Models for Atomistic Modelling are Changing Materials Discovery*
11:50 – 12:15	**Ulrike Diebold**, TU Wien (P02) *Quantitative Surface Structure of Multi-Component Oxides: Progress & Plans*
12:15 – 12:25	Ulrike Diebold Concluding Remarks
12:25 – 13:45	Lunch, End of Workshop
13:45	Pick up by bus to St. Pölten Main Station

Posters

Gustavo Alves (P10)	*MoS_2 Catalysts for CO_2 Hydrogenation to Methanol: Investigating the Interplay between Oxides and Sulfides via In-situ X-Ray Absorption Spectroscopy*
Andrea Conti (P02)	*The Unreconstructed α-Al_2O_3(0001) Surface is Inhomogeneous and Rough*
Alessandro Coretti (P12)	*Normalizing Flows for Nested Sampling of Condensed Matter Systems*
Tobias Dickbreder (P11)	*Does Water Form Surface Hydroxyls on Calcite (10.4) at High pH?*
Eva Doloszeski (P09)	*Neural-Network-Backed Evolutionary Search for Novel (2×4) $SrTiO_3$ (110) Surface Reconstructions*
Florian Dörr (P02)	*ViPErLEED: Automated Magnetic-Field Compensation in LEED I(V)*
Susanne Gross (P08)	*La-Modified Cobalt Oxide Thin Films: A Surface Science Study*
Maosheng Hao	*On the Role of Electronic Doorway States in the Secondary Electron Emission from Solids*
David Kugler (P04)	*Stabilization of the Polar Spinel $MgAl_2O_4$(001) Surface by an Al-rich Reconstruction*
Luca Leoni (P07)	*Machine Learning Potentials for Localized Charge Dynamics in Materials*
Sita Schönbauer	*Machine-Learned Force Fields for Lattice Dynamics at Coupled-Cluster Level Accuracy*
Deborah Steiner (P10)	*Flow Hydrogenation of Aldol Condensation Products from Bio-Derived Aldehydes over Cu–Mg–Al Catalysts*
Parinya Tangpakonsab (P08)	*Selective CO oxidation over Cu1/CeO_2 single atom catalysts*
Chunlei Wang (P04)	*H_2 Adsorption on a Single-Atom Rh/Fe_3O_4(001) Catalyst*
Sophie Zeilinger (P11)	*SAXS Analysis of Fluorinated Acid-Induced Microheterogeneties in HFIP Water Binary Mixtures*

Talk Abstracts

Keynote I

Towards Improved Methodology for Photocatalysis Simulations

Hannes Jónsson

Faculty of Physical Sciences and Science Institute, University of Iceland

Several ongoing methodology developments for improved photocatalysis simulations will be introduced, including:

(1) a new method for calculating excited electronic states by finding saddle points on the electronic energy surface,

(2) explicit self-interaction correction to density functionals for improved band gaps and balance between localized and delocalized states,

(3) neural network-assisted selective configuration interaction calculations with DFT embedding for obtaining benchmark data,

(4) semi-infinite solid (instead of slab) calculations to represent surfaces,

(5) hybrid simulation method where a liquid phase is described with the SCME polarisable potential energy function while the solid and nearby molecules are described using DFT.

A brief introduction to an upcoming Solar-to-X pathfinder project involving, in particular, photochemical reduction on Cu doped TiO_2 surfaces will be given.

Keynote II

The Structure and Reactivity of Water and Carboxylic Acids on Model TiO_2 Catalysts

Gregory A. Kimmel

Physical and Computational Science Directorate, Pacific Northwest National Laboratory, P.O. Box 999, Richland, WA 99352, USA

Polarization- and angle-resolved infrared reflection absorption spectroscopy (IRAS) is a powerful tool for investigating the bonding geometry of molecules on anisotropic dielectric substrates such as rutile $TiO_2(110)$ and anatase $TiO_2(101)$. This talk will highlight how we have used IRAS in combination with temperature-programmed desorption (TPD) and theory to investigate two topics that are relevant for catalysis. First, experiments investigating the structure of water adlayers on r-$TiO_2(110)$ and a-$TiO_2(101)$ show that subtle differences in the spatial arrangement of 5-fold coordinated Ti, Ti5c, on these two surfaces lead to substantial differences in the structure of the water adlayer. In particular, the strong bond between water and Ti5c produces "anchor points" whose spatial arrangement impacts the subsequent development of the hydrogen bond network in the water layer. The second part of the talk will describe experiments investigating the reactions of acetic acid on single crystal a-$TiO_2(101)$ and faceted a-$TiO_2(101)$ nanoparticles. Understanding the adsorption and reactivity of carboxylic acids on oxide surfaces is of great interest in catalysis for biomass upgrading via ketonization, a carbon–carbon coupling reaction. On single crystals in ultrahigh vacuum (UHV), our experiments show that acetic acid reacts to form ketene, which desorbs without subsequent reactions. In contrast, when acetic acid is deposited on layers of nanoparticles in the same UHV system, acetone is also produced along with ketene. The results suggest that ketene, which desorbs from one nanoparticle and subsequently reacts with acetic acid on another nanoparticle, is key intermediate in the reactions to produce acetone. Density functional theory calculations support ketene's reactivity via low-barrier coupling pathways that converge on a common β-ketoacid intermediate.

Keynote III

A Unified Quantum Framework for Electrons and Ions: The Self-Consistent Harmonic Approximation on a Neural Network Curved Manifold

Lorenzo Monacelli

Dipartimento di Fisica, Università di Roma Sapienza, Rome, Italy

The numerical solution of the many-body problem of interacting electrons and ions beyond the adiabatic approximation is a key challenge in condensed matter physics, chemistry, and materials science. Efficient strategies that simultaneously address the thermal fluctuations of ions at ambient temperature without struggling to describe the electronic quantum state from first principles are missing. Here, we devise a novel approach that minimizes the total (electronic and ionic) free energy by optimizing an ansatz Gaussian quantum density matrix on a curved manifold parameterized through a neural network. The curved manifold hybridizes the degrees of freedom introducing electronic correlation and electron-phonon coupling in the quantum state. This approach, originally designed for a flat Cartesian space to study quantum nuclei at finite temperatures, can efficiently tackle both the ground and excited state properties of electronic systems, thus paving the way to a unified quantum description for electrons and atomic nuclei.

Keynote IV

Making Sense of Electrical Noise by Simulating Electrolyte Solutions

Benjamin Rotenberg

Sorbonne University, Paris, France

Seemingly unrelated experiments such as electrolyte transport through nanotubes, nano-scale electrochemistry, NMR relaxometry and Surface Force Balance measurements, all probe electrical fluctuations: of the electric current, the charge and polarization, the field gradient (for quadrupolar nuclei) and the coupled mass/charge densities. Using molecular and mesoscopic simulations, it is possible to predict the fluctuations of these observables from the dynamics of ions and solvent molecules, thereby enabling experimentalists to decipher the microscopic properties encoded in the measured electrical noise. In this presentation, I will illustrate this idea, focusing on the link between the electrode charge fluctuations in nanocapacitors, the electrochemical response, and the properties of the interfacial electrolyte.

Keynote V

Electron and Thermal Transport at Database Scale

Alexander Ganose

Imperial College London, UK

Automated ab initio calculations have emerged as a powerful tool for computational materials science. Such workflows offer many benefits over traditional manual approaches, including the ability to create large datasets for machine learning; however, complex materials properties, such as electronic and thermal transport, have proved difficult to perform high-throughput. Here, I introduce our latest work developing automation tools that are easy to use and enable interoperability between density functional theory packages. I introduce our workflows for obtaining electronic and thermal transport and their role in materials discovery efforts.

Keynote VI

How Foundation Models for Atomistic Modelling are Changing Materials Discovery

Johannes Margraf

Physical Chemistry V: Theory and Machine Learning, University of Bayreuth, Germany

The design and discovery of new materials from first principles has been a tantalizing prospect for computational chemistry for the past decades. Realizing this promise has been highly challenging due to several factors, including the vastness of chemical space and the discrepancy between idealized crystal structures and real (potentially disordered) materials. In this context, machine learning interatomic potentials (MLIPs) have become an important tool, as they allow a more realistic description of materials due to their high computational efficiency. Until recently, MLIPs had to be developed from scratch for each class of materials, however, which is impractical for exploring large composition spaces. This has changed with the emergence of foundation models for atomistic materials chemistry, which are pre-trained for materials across the periodic table. In this talk, I will discuss how these foundation models are changing computational materials discovery, focusing on their potential for structure prediction in large composition spaces. We will also consider the remaining limitations of the models and computational materials discovery more generally. For the former, we will discuss the need for electrostatics-aware and non-local models; for the latter, we will discuss the role of crystallographic disorder when predicting new materials.

Photopolymers: Interfacial Structure and Hydrogen Production Efficiency

Ellen Backus

Faculty of Chemistry, Department of Physical Chemistry, University of Vienna, Vienna, Austria

Conjugated polymers have proven to be efficient, earth-abundant catalysts for the production of green hydrogen from just water and sunlight. Here, we discuss the molecular structure of different polymer-water interfaces and link structural motifs to observed trends of the hydrogen evolution rate. Three polymer catalysts were compared: Two polymers with a fluorene-co-dibenzo[b,d]thiophene sulfone backbone, where one polymer had dodecyl sidechains and the other one more hydrophilic ether sidechains and one polymer with a fluorene co-phenyl backbone and dodecyl sidechains. Sum frequency generation spectroscopy revealed that the interfacial water structure was qualitatively similar for the three probed polymers. A pH dependence indicates a negative surface charge for all polymer films. The similarity of the water structure at the different polymer surfaces evidenced that variations in hydrogen production cannot be solely attributed to polymer-water interactions but rather selective interactions with sacrificial electron donors, so-called scavengers. Ascorbic acid as a scavenger had only a little effect on the interfacial structure. Contrary, triethylamine strongly adsorbed on the hydrophobic dodecyl side chains, which decreased the polymer surface charge and water orientation. Such interactions were not observed with ether sidechains and likely relate to the higher hydrogen evolution rate. These insights aid a rational further enhancement of polymer catalysts.

Unravelling the Nature of Realistic 'Single Atom' Active Sites

Florian Kraushofer

Faculty of Physics, Institute of Applied Physics, TU Wien, Vienna, Austria

Despite many successes in synthesizing single-atom catalysts, there is a fundamental mismatch between most experimental work and the theoretical modelling of these systems. Applied catalysts are based on complex powder supports and are fabricated and used in environments containing various potential ligands and contaminants, whereas theoretical treatment is generally based on density functional theory (DFT) calculations assuming low-index facets on idealized supports, often placing the single catalyst atom in a bulk continuation site. Single-crystal supports prepared in UHV provide a direct experimental analogue to DFT and a bridge to more complex systems, enabling validation of the sites assumed by theory.

Using the iron oxide α-Fe2O3 as an example, I will show that simple adatom or substitutional models are generally not representative of the structures found in surface-science experiments. Stabilization requires added complexity, such as dynamic surface restructuring and stabilizing ligands from the gas phase. These factors must be taken into account to explain the experimental data. I will summarize recent results on dispersed Rh and Pt atoms on the α-Fe2O3($1\bar{1}02$) facet, outline our current theoretical picture, and highlight preliminary findings and open challenges for both experiment and modelling.

P 04

Taming Polaritonics

Christian Schäfer

Faculty of Physics, Institute of Applied Physics, TU Wien, Vienna, Austria

Sufficient confinement of electromagnetic modes leads to a frequent exchange of energy between a material and light, resulting in the creation of hybrid light-matter states, called polaritons. Here, I illustrate how spectral design with polaritons is utilized to reach mode- and enantiomer-selective catalysis. We discuss that strong interaction between optical and vibrational modes leads to changes in chemical rate constants [1-2]. Machine learning is critical to tame the computational complexity of experimentally relevant systems. Furthermore, a proof-of-concept work demonstrates that meta-material design can be used to boost charge transfer at plasmonic surfaces [3] -- promising a bright future for polaritonically driven catalysis guided by machine learning.

[1] C. Schäfer, J. Flick, E. Ronca, P. Narang, and A. Rubio, Nature Communications, (2022) 13:7817.

[2] C. Schäfer, J. Fojt, E. Lindgren, and P. Erhart, J. Am. Chem. Soc. 2024, 146, 8, 5402-5413.

[3] J. Fojt, P. Erhart, C. Schäfer, Nano Lett. 2024, 24, 38, 11913–11920.