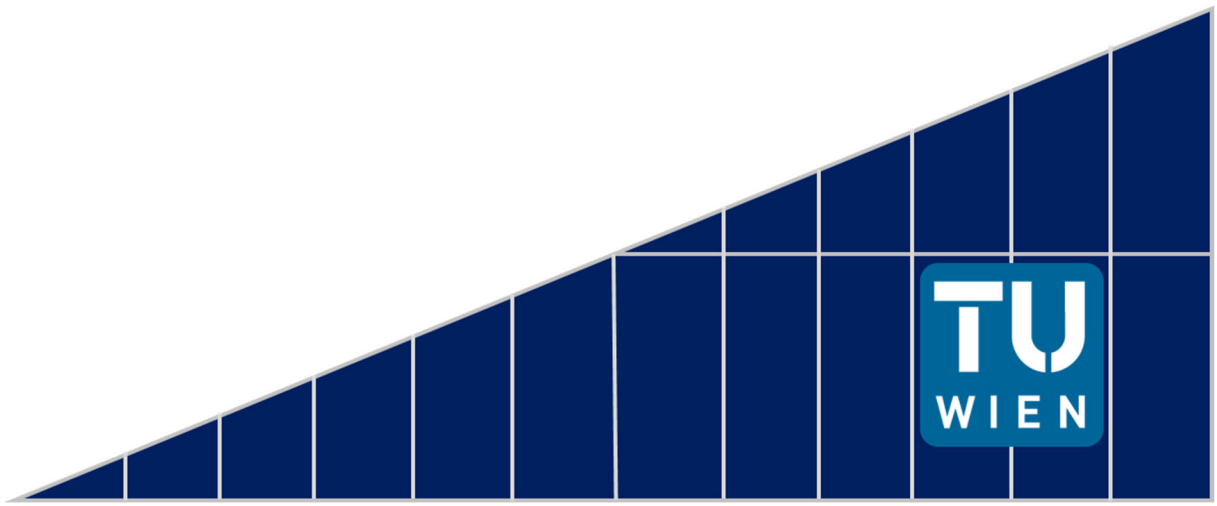
Joint TACO-NanoCat Conference 2023:

TAming COmplexity in Materials: Synergies between Experiment and Modeling

Program and Book of Abstracts

Place: TUtheSky, Getreidemarkt 9, 1060 Vienna

Date: 24-27 September 2023



“Die Tiefe muss man verstecken. Wo? An der Oberfläche.”

“You have to hide the depth. Where? On the surface.”

Hugo von Hofmannsthal (1874-1929)

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European Research Council

Established by the European Commission

Funded by
the European Union

4. Program

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 In0teractions*
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

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Morning

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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

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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**

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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

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Tuesday, 26 September 2023

Afternoon

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Exploring Catalytic Reaction Networks with Machine Learning

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Structure and Reactivity of Bismuth Vanadate-Water Interfaces

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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

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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

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Electrochemical Ionic Synapses for Analog Deep Learning and Beyond

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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)**

5. Talk Abstracts

(in chronological order)

Symmetry constraints in machine learning models of electronic and atomic interactions*

Boris Kozinsky

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Discovery and understanding of next-generation materials requires a challenging combination of the high accuracy of first-principles calculations with the ability to reach large size and time scales. We pursue a multi-tier method development strategy in which machine learning (ML) algorithms are combined with exact physical symmetries and constraints to significantly accelerate computations of electronic structure and atomistic dynamics. First, density functional theory (DFT) is the cornerstone of modern computational materials science, but its current approximations fall short of the required accuracy and efficiency for predictive calculations of defect properties, band gaps, stability, and electrochemical potentials of materials for energy storage and conversion. To advance the capability of DFT we introduce non-local charge density descriptors that satisfy exact scaling constraints and learn exchange functionals called CIDER [1]. These models are orders of magnitude faster in self-consistent calculations for solids than hybrid functionals but similar in accuracy. On a different level, we accelerate molecular dynamics (MD) simulations by using machine learning to capture the potential energy surfaces obtained from quantum calculations. We developed NequIP [2] and Allegro [3], the first deep equivariant neural network interatomic potential models, whose Euclidean symmetry-preserving layer architecture achieves state-of-the-art data efficiency and accuracy for simulating dynamics of molecules and materials. In parallel, we implement autonomous active learning of interactions in reactive systems, with the FLARE algorithm that constructs accurate and uncertainty-aware Bayesian force fields on-the-fly from a molecular dynamics simulation, using Gaussian process regression [4]. These MD simulations are used to explore long-time dynamics of phase transformations and heterogeneous reactions.

References

[1] K. Bystrom, B. Kozinsky, arXiv:2303.00682 (2023)
[2] S. Batzner et al., *Nature Comm.* 13 (1), 2453 (2022)
[3] A. Musaelian, S. Batzner et al., *Nature Comm.* 14, 579 (2023)
[4] J. Vandermause et al., *Nature Comm.* 13 (1), 5183 (2022)

* invited

Learning Differences and Derivatives: Efficient ML for Materials*

Georg Kresse, Bernhard Schmiedmayer,
Carla Verdi, Caroline Faller, Peitao Liu

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I will present two key developments from SFB TACO, Δ-learning and learning of vectorial quantities, in particular, the polarisation in periodic materials.

Δ-learning is an efficient approach to construct a machine-learned force field for density functionals or correlated wavefunction methods that are expensive to evaluate. We have now used this approach for many materials, including zirconia [1], SrTiO3 [3] and CO adsorbed on Rh(111) [2], as well as water. For the first three applications, we have learned the difference between a semi-local functional and the random phase approximation. Typically, we find that the number of computations for the expensive method can be reduced by one to almost two orders of magnitude using Δ -learning. The final machine-learned force field has the same speed and convenience as any other force field and can be used to make finite temperature predictions or exhaustive searches of the configuration space as for any other MLFF. For water, we have learned the difference between expensive hybrid functionals and a semi-local functional. Remarkable as few as 20 hybrid functional calculations suffice to determine a MLFF that has comparable accuracy as conventional DFT based MLFF.

The second development is aimed at simulating infrared spectra for complex periodic systems at finite temperature. The IR spectrum is related to the Fourier transform of the autocorrelation function of the polarization. So determining the IR spectrum requires efficient predictions of the polarisation, ideally for millions of configurations to obtain statistically accurate results. The main problem to be solved is that the polarisation is difficult to determine accurately from first principles for periodic structures. We address this by calculating and learning the derivative of the polarisation, the Born effective charges from first-principles calculations. Remarkably, the anti-derivative (Stamm-function) can be unambiguously determined using machine learning techniques. Armed with this, we calculate the IR spectrum for water and MAPbI3 for different phases at finite temperature. Very good agreement with experiment is found. Our approach paves the way for accurate simulations of IR spectra for complex materials typically found under operating conditions in catalytic converters.

References

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2. Liu, Wang, Avargues, Verdi, Singraber, Karsai, Chen, and Kresse, Phys. Rev. Lett. 130, 078001 (2023)
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* TACO P03

Treating Strain Effects in Large-Scale Reconstructions*

F. Libisch, L. Linhart, C. Schattauer

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Accurately simulating the quantum properties of surface reconstructions or defects requires large supercells (on the atomic scale) as well as a precise treatment of the underlying physics. A particular challenge here is the correct treatment of strain, which often extends far beyond the immediate defect or surface. We use parametrized approaches such as tight binding to directly simulate large-scale systems containing many thousands of atoms. We directly parametrize our models from density functional theory to correctly describe the underlying physics. I focus on two applications: strain effects in the optical response of defect centers in 2D semiconductors [1], as well as moiré superstructures that emerge due to finite twist angles or lattice mismatches at interfaces [2]. In both cases, our predictions agree well with experimental observations.

Mechanical strain is a powerful tuning knob for excitons, Coulomb-bound electron–hole complexes dominating optical properties of two-dimensional semiconductors. We use defect-bound excitons in WSe2, a two-dimensional semiconductor to study the strain behavior of these fragile many-body states [1]. Strain brings dark and localized excitons in monolayer WSe2 into energetic resonance, forming a new hybrid state that inherits the properties of the constituent species. Our tight-binding model correctly describes the essential characteristics of the hybridized state, including an order-of-magnitude enhanced light/matter coupling, avoided-crossing energy shifts, and strain tunability of many-body interactions.

In moiré crystals formed by stacking van der Waals materials, surprisingly diverse correlated electronic phases and optical properties can be realized by a subtle change in twist angle. As a second example for the importance of strain, we investigate the change in phonon spectra in twisted bilayers, adding an insight to moiré physics [2]. Over a range of small twist angles, the phonon spectra evolve rapidly owing to ultra-strong coupling between different phonon modes and atomic reconstructions of the moiré pattern. We develop a low-energy continuum model for phonons that predicts the properties of large moiré supercells and successfully captures the essential experimental observations. Our model promotes a comprehensive and unified understanding of the structural, optical and electronic properties of moiré superlattices.

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2. J. Quan, L. Linhart, M.-L. Lin, D. Lee. J. Zhu, C-Y. Wang, W-T. Hsu, J. Choi, J. Embley, C. Young, T. Taniguchi, K. Watanabe, C-K. Shih, K. Lai, A. MacDonald, P-H. Tan, F. Libisch, and X. Li, Nature Materials **20** (2021) 1100

* contributed

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

Viktor Zaverkin,[1,2] Johannes Kästner[1]

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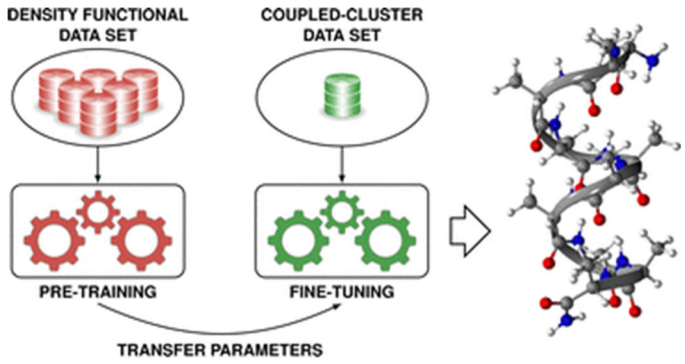
The development of machine-learned interatomic potentials requires generating sufficiently expressive atomistic data sets. Active learning algorithms select data points on which labels, *i.e.*, energies and forces, are calculated for inclusion in the training set. However, for batch mode active learning, *i.e.*, when multiple data points are selected at once, conventional active-learning algorithms can perform poorly. Therefore, we investigate algorithms specifically designed for this setting and show that they can outperform traditional algorithms. We investigate selection based on the resulting training set's informativeness, diversity, and representativeness. We propose using gradient features specific to atomistic neural networks to evaluate the informativeness of queried samples, including several approximations allowing for their efficient evaluation. To avoid selecting similar structures, we present several methods that enforce the diversity and representativeness of the selected batch. Furthermore, we use transfer learning to improve the quality of the resulting potential, use training data from cluster calculations to predict bulk properties, and present a scheme to learn tensorial quantities, like the magnetic anisotropy.



Scheme of our transfer-learning approach.

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2. Zaverkin, V., Holzmüller, D., Bonfirraro, L., & Kästner, J. "Transfer learning for chemically accurate interatomic neural network potentials." *Phys. Chem. Chem. Phys.* **25**, 5383–5396 (2023)
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4. Zaverkin, V., Netz, J., Zills, F., Köhn, A., & Kästner, J. "Thermally Averaged Magnetic Anisotropy Tensors via Machine Learning Based on Gaussian Moments." *J. Chem. Theory Comput.* **18**, 1-12 (2022)
5. Zaverkin, V., & Kästner, J. "Gaussian Moments as Physically Inspired Molecular Descriptors for Accurate and Scalable Machine Learning Potentials." *J. Chem. Theory Comput*. **16**, 5410-5421 (2020)

* invited

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

Jesús Carrete

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Understanding and exploiting the properties of complex material systems like surfaces requires exploring their configurational landscapes in search of plausible structures characterized by their low energies and/or by agreement with experimental spectroscopic measurements. In both cases, direct first-principles calculations fall short on account of the many evaluations of basic dynamical quantities (like energies and forces) or features of the charge distribution (such as its polarizability) necessary. The problem is compounded by the numbers of atoms that must be included in those evaluations. Machine-learning dynamical models offer the ability to overcome this limitation by combining great accuracy and performance. However, the flexibility of their functional form is a double-edged sword, and they can likewise introduce dramatic artifacts. Therefore, a reliable uncertainty estimator is a key ingredient in the successful use of machine-learning force fields for predictive calculations. Important considerations are correlation with error, overhead during training and inference, and efficient workflows to systematically improve the force field. For descriptor-based neural-network force fields,[1] simple committees are often the only option considered due to their easy implementation. This contribution will discuss how to generalize the deep-ensemble design based on multiheaded neural networks and a heteroscedastic loss, which can efficiently deal with uncertainties in both energy and forces and take sources of aleatoric uncertainty affecting the training data into account.[2] A comparison between uncertainty metrics based on deep ensembles, committees, and bootstrap-aggregation ensembles will be illustrated based on realistic data sets. Building on those metrics and using an algorithmically differentiable implementation, an adversarial approach to active learning can be readily deployed to progressively refine the force fields. The final part of the presentation will deal with several important practical lessons learned while applying this kind of workflow.

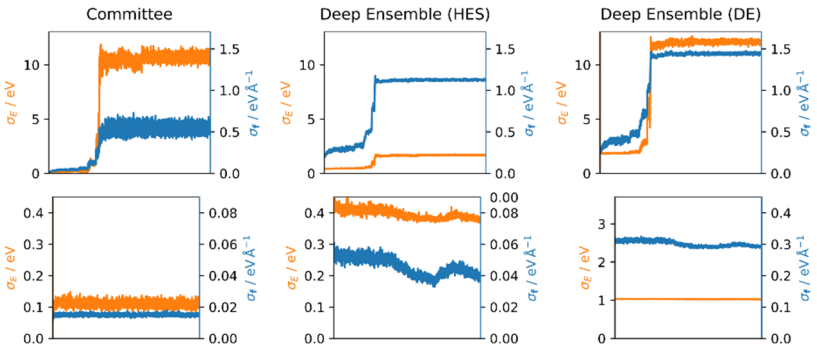

Figure: Evolution of several uncertainty metrics along a molecular-dynamics trajectory using two different generations of a machine-learning force field (top and bottom) separated by a round of active learning. The explosion in the value of those metrics accurately predicts the point where the simulation is entering unphysical territory.

References

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* TACO P09

Towards Chemical Accuracy for Surface Chemistry Using Coupled-Cluster Theory*

A. Grüneis, A. Irmler, T. Schäfer, F. Hummel, N. Masios, A. Gallo

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Coupled-cluster theory is widely used in high-accuracy ab initio calculations in the field of molecular quantum chemistry to produce reliable benchmark energies and related properties. Reliable benchmark results can be used to resolve existing discrepancies between theory and experiment or to improve more approximate methods, such as density functional theory using approximate functionals. Recent methodological developments have significantly expanded the scope of periodic coupled-cluster theory to study solids and surfaces. This talk will review recent methodological developments, such as its extension to the study of metallic systems[1]. The discussed applications will cover a wide range of materials science problems including the study of defects in alkaline earth oxides[2], CO adsorption on MgO[3] and CO_2 adsorption in porous materials[4]. These calculations and the comparison to experiment and other theories including quantum Monte Carlo and approximate density functionals often enables to reach consensus for important materials properties.

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2. A. Gallo, F. Hummel, A. Irmler, A. Grüneis, *Journal of Chemical Physics* **154** (2021) 064106
3. B. X. Shi, A. Zen, V. Kapil, P. R. Nagy, A. Grüneis and A. Michaelides, https://doi.org/10.26434/chemrxiv-2023-h4czl-v2 (2023)
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* invited

Spatial Distribution of Interacting Defects using Machine Learning*

Cesare Franchini

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The rich and tunable physics of oxides depends on their precise chemical composition and the presence of impurities. Point defects, such as atomic vacancies, interstitial atoms, or dopants, are often accompanied by the formation of polarons, manifested by the spatial localization of charge carriers due to the coupling between excess charge and lattice phonons [1]. Determining the spatial arrangement of a system composed of many interacting polarons and defects is a challenging task that is difficult to achieve with traditional first-principles simulations and spectroscopy techniques but can be conducted more efficiently using machine learning and computer vision algorithms [2,3]. Here, we use a variety of machine learning schemes to analyze the distribution of surface oxygen vacancies and induced small polarons on rutile TiO_2(110), taking into account polaron-polaron and polaron-vacancies interactions.

By quantifying single-defect virtual energies with a feed-forward neural network and modeling the annealing process through a global optimization scheme, we obtained a ground-state large-scale configuration that explains the inhomogeneous oxygen vacancy distribution observed in atomic force microscopy images. The proposed methodology enables the study of defect distribution at previously inaccessible tens of nm scales.

References

1. C. Franchini, M. Reticcioli, M. Setvin, U. Diebold, Polarons in materials, Nature Reviews Materials (2021).
2. V.C. Birschitzky, F. Ellinger, U. Diebold, M. Reticcioli, C. Franchini, Machine learning for exploring small polaron configurational space. npj Computational Materials (2022).
3. M. Corrias, et al., Automated real-space lattice extraction for atomic force microscopy images, Machine Learning: Science and Technology (2022)

* TACO P07

Machine Learning Density Functionals from the Random-Phase Approximation*

S. Riemelmoser[1,2], C. Verdi[1,3], M. Kaltak[4], G. Kresse[1,4]

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We have recently developed a machine learning (ML) method that substitutes the random-phase approximation (RPA) with a non-local density functional [1]. For our ML-RPA scheme, we use interesting parallels to ML interatomic potentials. On the one hand, we adapt the power spectrum representation of atomic environments [2] to construct two- and three-body descriptors from the electronic density. Fig. 1 shows how these descriptors can be understood as non-local generalizations of the electronic density and its gradient, respectively. On the other hand, we use the optimized effective potential method to obtain RPA exchange-correlation potentials [3]. Similar to the atomic forces in ML interatomic potential methods, this provides derivative information for ML-RPA. Further, ML-RPA can be applied self-consistently, and ML-RPA forces can be calculated at large scale. In this talk, we discuss the ML-RPA formalism in detail and present its application to diamond surfaces and liquid water [1].

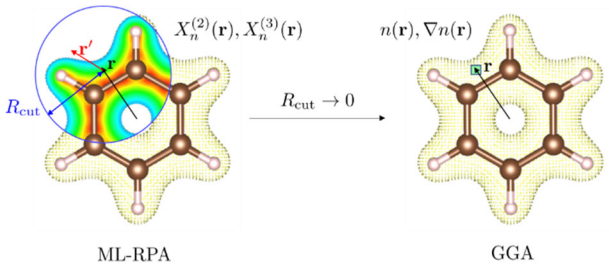

Figure 1: The ML-RPA density functional is a non-local extension of the generalized gradient approximation (GGA). In the limit of small cutoffs, the two- and three-body descriptors reduce to the local density and its gradient, respectively.

References

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* contributed

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

Ralf Drautz

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Efficient Density Functional Theory (DFT) codes made high-throughput calculations for tens of thousands of atomic configurations a routine task. The availability of large DFT datasets drove the development of different flavors of machine learning potentials. The Atomic Cluster Expansion (ACE) [1] unifies many of the different machine learning potentials, from classical approaches based on empirical descriptors to current graph neural network architectures, without requiring explicit machine learning strategies like neural networks or Gaussian process regression.

In my talk I will introduce ACE and relate it to other descriptors. I will also briefly discuss the implementation of ACE and highlight its efficiency [2,3]. I will then show the application of ACE to pipe diffusion in tungsten and the prediction of structure formation in carbon (Fig. 1) [4]. I will further discuss generalizations of ACE to multi-component materials, magnetism [5,6], charge transfer and semi-local interactions [7,8] and highlight an initial application to the representation of many-electron wavefunctions [9]. Before concluding, I will show extensions of ACE software for efficient phase space exploration [10] and large-scale simulations.

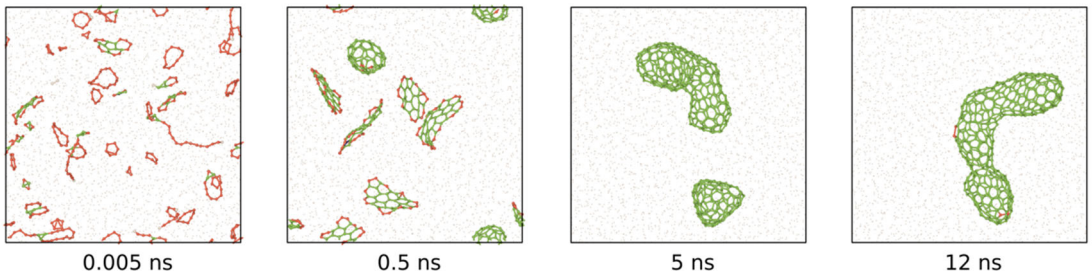

Fig. 1: Snapshots from high-temperature molecular dynamics simulations of carbon in argon atmosphere.

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10. Y. Lysogorskiy, A. Bochkarev, M. Mrovec, R. Drautz, *Phys. Rev. Materials* **7** (2023) 043801

* invited

Boltzmann Generators*

Jonas Köhler[1,2]

[1]*Microsoft Research AI4Science*

[2]*Freie Universität Berlin*

Boltzmann Generators offer a compelling approach to sample from complex molecular distributions, providing a bridge between statistical mechanics and machine learning. This talk aims to introduce the fundamentals of Boltzmann Generators, highlight the latest advancements that improve sampling efficiency and accuracy, and explore its application in the realm of coarse-graining.

* invited

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

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Transition metal carbides feature high hardness and phase stability, but suffer from inherent brittleness. The properties of these carbides can be tuned by combining different carbides in solid solutions, giving rise to multinary or compositionally complex carbides. But the vast combinatorial space of these carbides present a new challenge for materials design. To tackle this problem, we used ab initio calculations to screen the mechanical properties of the multinary carbides of the 9 IVb-VIb metals and Al. The chosen compunds encompass all equimolar combinations of solid solutions with 1 to 5 metals, amounting to 637 individual compositions. The simulation cells were set up as 2x2x2 supercells of the TiC prototype (SG Fm-3m) with 64 atoms, the metals were distributed on the metal-sublattice by the special quasi-random structure algorithm. The cells were then relaxed using VASP, and the mechanical properties were calculated from the equilibrium structure with the stress-strain method. This high-throughput exploration still requires significant computational expense, we therefore use machine-learning (ML) algorithms trained on the ab initio data to predict the properties of the full desired phase space from a small representative subset. The efficacy of these ML models depends strongly on expressive co-variates. Here, we explore the impact of the electronic density of states (DoS) as co-variate to improve the prediction efficacy. We have calculated the DoS from the relaxed structures in the range from -10 to +5 eV around the Fermi level. To implement the DoS in the ML algorithm efficiently, we extracted the salient information by two procedures. First, we fitted the DoS with a simple mathematical function, describing the DoS with a double triangle fit. One of the triangle functions is fitted to the states forming the covalent bonds in the region around -10 to -4 eV, the second triangle to the metallic states around the Fermi-level. We thus express the DoS with 6 variables: the position, height, and width of the triangles. The second route represents an integrative binning of the DoS in certain regions. Here, we found that bins in the regions from -2 to 0 and 0 to +2 eV offer the best prediction improvement. With both methods we can improve the absolute R2 prediction scores of mechanical properties like bulk, shear, Young's modulus, and Cauchy pressure by up to 30%, thus allowing a decent property prediction from a very small subset of the phase space.

* contributed

Liquid-Phase Catalytic Oxidation of Alcohols over Spinel Oxides*

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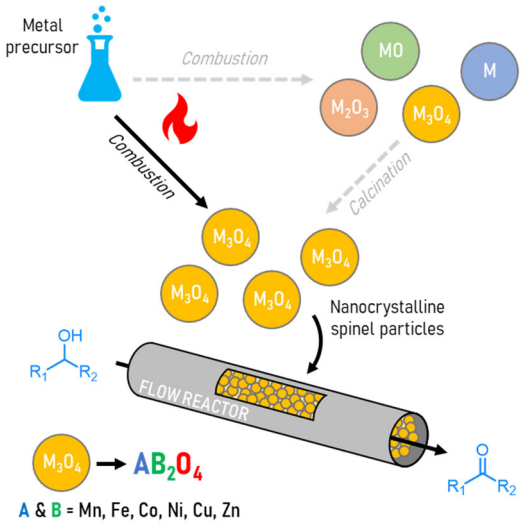

Figure 1. Catalyst synthesis and testing of oxidation of alcohols over spinel oxides.

The selective oxidation of alcohols is an important synthetic tool in the portfolio of the chemical industry. Even though the oxidation of small alcohols such as methanol to formaldehyde are established processes, the selective transformation of higher alcohols is more challenging; moreover, the mechanistic understanding of these reactions over heterogeneous catalysts is still poor, especially about the phenomena taking place at the solid-liquid interface [1]. Besides, the most active catalysts are based on noble metals [2]; metal oxide catalysts are more complex and comprise less defined active sites, but they are based on more earth-abundant metals and are less susceptible to leaching. Therefore, the surface study and design of more active and selective oxide catalysts are important matters in light of the green transition. In this regard, oxides of the spinel type proved to be outstanding catalysts in liquid-phase aerobic oxidations [3]. A library of nanocrystalline spinels based on Mn, Fe, Co, Ni, Cu and Zn was prepared using the combustion method followed by calcination. The obtained solids were characterised by XRD, FT-IR, SEM-EDX, N_2-physisorption, and XPS. The catalysts were tested in the liquid-phase oxidation of 2-butanol in a flow reactor, and the collected liquid and gas samples were analysed by GC-FID. Every spinel with a different elemental composition produces a different type of combustion, which is reflected in the different morphology and phase composition of the solids. While the as-synthesised Mn, Co and Ni ferrites are pure, the rest of the combinations required calcination, each with a different temperature, atmosphere and cooling. The temperature stability of each material was tested to assess the suitability of different pretreatments, as well as the crystal growth during those. The catalysts were tested in a flow reactor, in the presence of water and O_2, to study the effect of the catalyst composition on the activity and selectivity. Finally, the stability of the catalyst to water and to the reaction conditions was also assessed.

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* TACO P10

Surface Hydroxylation of an Ultrathin Co_3O_4(111) Film Grown on Ir(100): *In Situ* Near Ambient Pressure XPS and DFT Studies*

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Cobalt oxides are promising inexpensive functional materials for many applications including heterogeneous oxidation catalysis (low-temperature CO oxidation[1-4], preferential oxidation of CO (PROX)[5], oxidation of hydrocarbons[1,6], Ostwald synthesis of nitric acid by oxidation of ammonia[7], etc.), and Li-based rechargeable batteries (electrode materials[8,9], electrocatalysis[10]). Despite their outstanding performance in both areas, atomic-level structure-function relationships still need to be better developed.

In the present study, the interaction of spinel Co_3O_4 with H_2O vapor is reported, which is assumed to cause catalytic deactivation through surface hydroxylation. As a suitable model system, a Co_3O_4(111) thin film was grown in ultrahigh vacuum (UHV) on a bulk-truncated Ir(100)-surface *via* physical vapor deposition (PVD), and was characterized in UHV as well. Subsequently, synchrotron-based *in situ* near ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) was carried out while the oxide thin film was exposed to 0.5 mbar H_2O vapor at room temperature, with hydroxylation monitored in the O 1s region. Based on density functional theory (DFT) modeling, employing a PBE+U method implemented in the Vienna *ab initio* simulation package (VASP)[11,12], the OH surface coverage was determined and its evolution with time described by kinetic modeling. The obtained fundamental insights may enable to counteract H_2O-induced deactivation and improve performance in H_2O-related reactions.

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* TACO P08

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

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Climate change concerns have spurred a growing interest in developing environmentally friendly technologies for energy generation and to re-utilize CO_2 in thermal catalysis applications where it is reacted with green H_2 from electrolysis to produce methanol or high-order hydrocarbons. Moreover, the electrochemical reduction of CO_2 (CO2RR) into value-added chemicals and fuels offers an additional possibility to store renewable energy into chemical bonds. It is therefore of particular interest to develop efficient, selective and durable (electro)-catalysts that can operate under mild reaction conditions (lower pressures and temperatures, lower overpotentials). Nonetheless, in order to tailor the chemical reactivity of nanocatalysts, fundamental understanding of their structure and surface composition under reaction conditions must be obtained. It should be kept in mind that even morphologically and chemically well-defined pre-catalysts will be susceptible to drastic modifications under operando conditions, especially when the reaction conditions themselves change dynamically.

This talk will offer new insights into the thermal and electrocatalytic reduction of CO_2 as well as the oxygen evolution reaction (OER) using model pre-catalysts ranging from single atoms to small clusters, large nanoparticles and thin films. Some of the aspects that will be discussed include: (i) the stabilization of high-loadings of single atoms on oxide supports and their enhanced reactivity, (ii) the design of size- and shape-controlled pre-catalysts (Cu_2O cubes, ZnO-Cu_2O cubes, CoOx NPs) and differently-oriented thin films (Ga/Cu, Co_3O_4, $Co_{1+\delta}Fe_{2-\delta}O_4$), (iii) the role of the support (C, CeO_2, SiO_2, ZnO, Al_2O_3, ZnOAl) on the catalytic stability and performance, (iv) the understanding of the active state formation and the correlation between the dynamically evolving structure and composition of the (electro-)catalysts under operando reaction conditions and their activity and selectivity.

These results are expected to open up new routes for the reutilization of CO2 through its direct conversion into industrially valuable chemicals and fuels such as ethylene, methanol and ethanol and the generation of green H_2 through water splitting.

* invited

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

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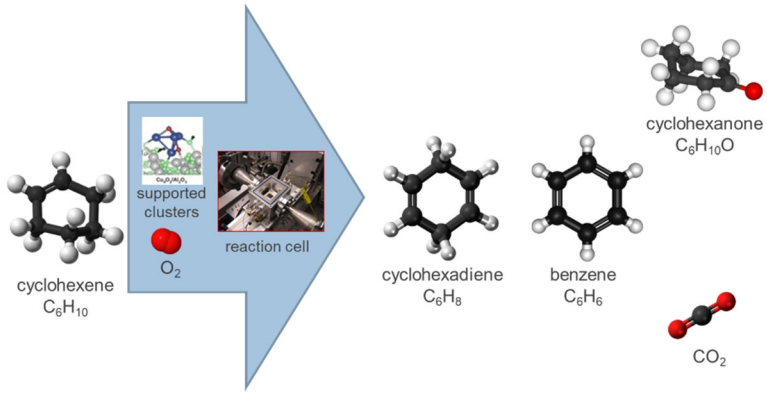
The focus of the presentation will be on catalysts by supported monodisperse subnanometer clusters made of a handful of atoms, supported on technologically relevant oxide- and model carbon-based supports. The performance of Co, Cu, Pd and CuPd clusters on the example of oxidative dehydrogenation reactions where an atomic precision fabrication of mono- and bimetallic clusters allows for the fine-tuning of their activity and selectivity by varying the size and composition of the clusters in an atom-by-atom fashion and by support effects.

In the second part of the presentation, as time will allow the conversion of CO2 on copper cluster-based catalysts to methane vs. methanol or longer chain hydrocarbons will be discussed in the dependency of cluster size and the support used.



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* NanoCat

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

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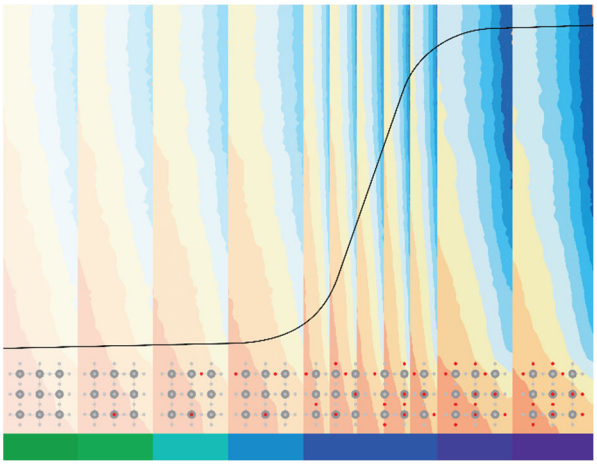

Figure 1. The time-resolved optical data (vertical axis) as a function of pH (horizontal axis) generates a reaction isotherm (black trace). The emission (in blue) counts the intermediate population created by the first proton and electron transfer from an absorbed water species.

Computationally, often the energetics of intermediate reaction steps differentiate the efficiency of heterogeneous catalysts for product evolution. Yet, when compared to experiment, kinetic models are applied. For example, a material's activity measured by one rate of product evolution is plotted as a function of the calculated formation energies of intermediate chemical forms. A critically important reaction for which this dichotomy between experiment and theory exists is the oxygen evolution reaction (OER) from water. In the laboratory group, we employ time-resolved optical and vibrational spectroscopy to deconstruct OER into its individual reaction steps on an electrode surface. In the presentation, I will describe the experimental methodology and the chosen model system, the n-doped $SrTiO_3$/aqueous interface. I'll show how these experiments identify both the rates and energetics of the first reaction step, the release of a proton and electron from an absorbed water species, denoted by OH* or O*. A recent success was to isolate a Langmuir isotherm of the intermediate population arising within < 2 ps on the $SrTiO_3$ surface (Figure 1)[1]. The intermediate population is of trapped holes measured by emission from the conduction band into unoccupied states in the middle of the semi-conductor bandgap. The isotherm is tuned by the pH of the electrolyte. Current work connects the decay of these intermediates at microsecond timescales, presumably related to later reaction steps of OER, to their pH-dependent formation. A growing area is to apply the particular experimental methodology to a surface of similar electronic structure but diverse crystal geometries, namely rutile TiO_2.

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* invited

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

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Our research focused on understanding the dynamic behavior of electrocatalytic systems under operating conditions [1,2]. We developed the ReaxFF reactive force field to simulate the atomic and molecular interactions within these systems to study a range of surface phenomena such as adsorption, diffusion, and catalytic reactions.

We have investigated catalytic performance in processes such as the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER) on different surfaces. Our results highlight the role of surface structure, kinetics, and environmental factors such as pH and temperature in determining system behavior and stability.

In addition, we used density functional theory (DFT) to investigate the electronic structure of clusters on graphene substrates, which are commonly used as catalyst supports in fuel cells [3]. Our analyzes revealed that the size, shape, and symmetry of the clusters, as well as the nature of the graphene support, significantly affect the stability and activity of the clusters, with bonding considerations being crucial.

In summary, our research, supported by the ReaxFF force field, provided fundamental insights into the behavior of catalytic systems on surfaces, including adsorption, diffusion, and catalytic reactions. These findings underscore the importance of understanding surface properties and electronic structures for developing efficient and stable catalysts for practical applications.

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* NanoCat

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

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More than 50 years ago, it has been proposed that hydrogen can be generated at the interface between TiO_2 and water by photocatalytic dissociation using sunlight. However, despite extensive work in this area, an experimental view on the fundamentals of the process is still missing, mainly due to the lack of a proper tool to explore specifically the interface between water and TiO_2 on an ultrafast timescale. Sum frequency generation spectroscopy (SFG), is an inherently surface sensitive tool, allowing the study of the water-TiO_2 interface without monitoring the bulk water present. From the intensity and frequency of the static SFG signal, we extract information about the different water species binding to the TiO_2.[1] To obtain information on the mechanism of the water splitting process, time-resolved SFG experiments have been performed. In these experiments, the TiO_2 thin film is excited with a short UV pulse mimicking the sun light. Subsequently, the O-H stretch vibrations of the interfacial species are monitored on a sub-picosecond timescale. Our data show that the surface charge changes on ultrafast timescales upon excitation resulting in restructuring and partly dissociation of the water molecules of 10s of ps timescales. For the first time experimentally, the light-induced reaction at the TiO_2-water interface has been monitored under realistic conditions at the timescale the reaction takes place.[2]

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* TACO P11

Exploring Catalytic Reaction Networks with Machine Learning*

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Chemical reaction networks form the heart of microkinetic models, which are one of the key tools available for gaining detailed mechanistic insight into heterogeneous catalytic processes. The exploration of complex chemical reaction networks is therefore a central task in current catalysis research. Unfortunately, microscopic experimental information about which elementary reaction steps are relevant to a given process is almost always sparse, making the inference of networks from experiments alone almost impossible. While first-principles computational approaches provide important complementary insights to this end, their predictions also come with substantial uncertainties related to the underlying approximations and, crucially, the use of idealized structure models. In this talk, I will review our approaches in this context, aiding both the inference of effective kinetic rate laws from experiment and the computational exploration of chemical reaction networks. We thereby aim at maximum agility and data efficiency, relying on active learning that only queries data on demand.

* invited

Structure and Reactivity of Bismuth Vanadate-Water Interfaces*

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Bismuth vanadate (BVO) is a promising photoanode for photoelectrochemical cells, due to its tunable band gap (~2.4 – 2.6 eV), favorable alignment of its valence band with the water oxidation potential, stability in aqueous environments, and its relative easiness of preparation [1]. In a recent study [2], we showed that tuning surface termination/composition and hence surface energetics is critical to improve the efficiency of the oxygen evolution reaction (OER) [2]. In addition, we highlighted [3] the importance of surface defects in altering the reactivity of BVO toward water, concomitant to water modifications to the electronic structure of the photoanode. However, a complete atomistic description of the interface between defective facets of BVO and water is not yet available, and yet it is necessary for the optimization of the OER efficiency. Here we carry out first principles molecular dynamics simulations with the Qbox code (http://qboxcode.org/) of BVO-water interfaces with different composition, as well as measurements of the electronic (XPS) and vibrational (IRRAS) spectra of water-covered BVO thin films. We combine theoretical and experimental results on spectra and computed electronic properties to characterize the interplay between surface hydroxylation and metal oxidation states at the surface, and to understand their impact on surface reactivity.

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* contributed

Synthesis and Catalytic Activity of Atomically Precise Model Catalysts*

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Surface science studies serve as a unique platform for studies of atomically precise materials; exploring their structure, stability, and activity. These precisely defined systems, often homotopic, are crucial for validating theoretical methods and uncovering structure-activity relationships in more complex environments. The challenge lies in approaching the complexity of real-world catalysts. In this talk, I will demonstrate the preparation and characterization of complex models composed of metal adatoms and monodispersed oxide clusters supported on oxides, as well as of mixed oxide surfaces. A combination of high-resolution imaging, spectroscopic characterization, reactivity measurements, and density functional calculations are essential to attain mechanistic insights into surface structure, adsorbate binding, diffusion, clustering, and product formation. The presented studies focus on $(MoO_3)_n$ oligomer deposition on anatase TiO_2(101) and Rh atoms on Fe_3O_4(001), revealing their temperature and coverage-dependent behavior and stability. Catalytic reactions of carboxylic acids are used to assess the structure-activity relationships. Monomolecular acetic acid dehydration on TiO_2(101) is contrasted with bimolecular carbon-carbon coupling on nano-faceted TiO_2(101). Well-defined ultra-high vacuum conditions provide key conditions to attain insights into the role of ketene in acetone formation. For Rh-Fe_3O_4(001), formate and hydroxyl intermediates are shown to destabilize in-surface Rh and converting it to highly active Rh adatoms. These studies provide mechanistic insight into model catalytic reactions, essential for understanding complex high-surface-area catalysts.

* invited

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

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Infrared reflection absorption spectroscopy (IRAS) is a wide-spread technique in heterogenous catalysis, and it is an ideal tool for the comparison of real and model catalysts [1]. Most surface science groups perform IRAS studies either directly on metal single crystals, or on (ultra-)thin metal oxide films grown on such samples [2]. Achieving high-quality data from metal-oxide single crystal surfaces is difficult because their low reflectivity necessitates averaging many individual measurements with long acquisition times [3]. The goal of this work was to develop an IRAS setup for studying the adsorption of molecules on model "single-atom" catalysts. Here, the problem of low intensity due to the low reflectivity of the oxide support is exacerbated by the sub-monolayer coverage of adsorbates on single adatoms. In the contribution, I will present the novel IRAS system we have developed to overcome these two challenges.

The main improvements over commonly used setups are a high numerical aperture, an optimized optical path, control of the incidence angle range, and high mechanical stability. The high numerical aperture of the optical system leads to an increase in the amount of light reflected from a small single crystal sample. This is achieved by placing both the illumination and collector mirrors inside the UHV chamber close to the sample. To minimize the loss of signal, optimization of the optical path was performed using a ray tracing program. The other limit is the small area on the sample that is covered with adsorbates: in our setup, a molecular beam delivers adsorbates with a spot diameter of 3.5 mm [4]. Infrared light contributing to the signal is reflected only from this area.

The differential reflectivity of non-metallic samples varies strongly with incidence angle, and can even change a sign, leading to cancellation. The optimum angle ranges are different for every material. As our setup has a large range of incident angles, we can use this to our advantage: Using two adjustable aperture plates, we can vary the minimum and maximum incidence angle from 49° to 85° to maximize the signal for every material. Angle control also allows us to optimize the signal for both p-polarized and s-polarized light independently.

We successfully executed and compared D_2O and CO absorbance measurements on a rutile $TiO_2(110)$ surface, and our results agree with the established literature [3]. By properly selecting the incidence angle range, we achieved a signal-to-noise ratio of ~68 for 1 ML CO adsorbed on TiO_2 with only 150 seconds of measurement time. As our first IRAS study focusing on a "single-atom" model catalyst, measurements of CO adsorbed on Rh-decorated $TiO_2(110)$ will be presented.

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* TACO P04

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

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Water has been extensively studied through computer simulations. Empirical force fields and first-principles calculations have provided valuable knowledge about different properties of water. Until recently, the accuracy of the latter had not been available for phenomena involving large systems and long timescales, where empirical force fields had to be applied. The development of machine learning potentials has allowed us to accurately explore these systems at a similar cost to simple models. Here, we investigate bulk liquid water by applying two prominent approaches, i.e., neural-network and kernel-based potentials, for different functionals. In particular, we compute the maximum in the density, the diffusion constant, and the radial distribution functions. We also compare the computational cost and accuracy of these machine-learning methods. Then, we use neural-network potentials to study two cases of water at the interface. We start with the interface between water and its most common crystalline counterpart, ice Ih. In this case, we focus on the melting and growth of ice [1]. Finally, we study the interface between magnetite(001) and water. For this interface, we use the subsurface cation vacancy (SCV) model, which has been validated experimentally and in ab initio calculations [2]. By means of molecular dynamics simulations, we study the kinetics of single water molecules, the formation of water clusters, and the stability of the SCV surface under full water coverage.

References

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* TACO P12

Electrochemical Ionic Synapses for Analog Deep Learning and Beyond*

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Deep learning is a powerful algorithm for machine learning applications such as computer vision and natural language processing. However, the training of these neural networks is limited by the traditional von Neumann architecture of our current CPUs and GPUs. Shuttling data back and forth between the separate memory and computation units in such architecture results in significant energy consumption; many orders of magnitude greater than the energy consumption in human brain. In our research, we aim to reduce the energy consumption in analog, brain-inspired computing, by focusing on designing materials and devices that use ions to perform data storage and computation in a single architecture. In this talk, I will share our work on the ionic electrochemical synapses, whose electronic conductivity we can control deterministically by electrochemical insertion/extraction of dopant ions across the active device layer. We are exploring protons and magnesium ions, which bring different advantages to the operation of the device. The protons present very low energy consumption, on par with biological synapses in the brain. Magnesium ions present with better stability without the need for encapsulation. The modeling results indicate the desirable material properties, such as ion conductivity and interface charge transfer kinetics, that we must achieve for fast (ns), low energy (< fJ) and low voltage (1V) performance of these devices. We are also exploring ion dynamics in these materials to emulate bio-realistic learning rules deduced from neuroscience studies. Our findings provide pathways towards brain-inspired hardware that has high yield and consistency and uses significantly lesser energy as compared to current computing architectures.

* invited

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

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The surfaces of multicomponent perovskite oxides play a crucial role in many established and emerging technologies [1]. Yet, little is known about their atomic-scale details. The few systems that have been systematically investigated have shown a mindbogglingly rich structural variety on their surfaces [2, 3].

Here, we focus on the lowest-energy orientation of lanthanum strontium manganite ($La_{0.8}Sr_{0.2}MnO_3$, LSMO). We grow (001)-oriented epitaxial thin films by pulsed-laser deposition (PLD) and characterize its surfaces using a variety of surface-science tools, most prominently scanning tunneling microscopy (STM).

The films display two types of surface terminations over a broad range of parameters: one is rich in Mn, the other in La and Sr. This apparent simplicity is in striking contrast with the rich variety that we have witnessed on LSMO(110) [4]. The Mn-rich structure is particularly intriguing. In low-energy electron diffraction (LEED), it shows a 4-fold-symmetric pattern that cannot be explained by a set of two basis vectors as expected for a crystalline termination. A set of four, four-dimensional reciprocal-space vectors is needed instead – reminiscent of quasi-crystalline order. STM reveals an aperiodic real-space structure with an FFT consistent with the LEED pattern.

References

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* TACO P02

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

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Resolving the exact arrangement of atoms at surfaces is one of the key tasks of surface science. The surface atomic structure translates into chemical, catalytic and electronic properties of materials, yet its understanding is a nontrivial problem. Here I will illustrate novel options that emerge thanks to the development of combined STM/AFM on the experimental side, and machine-learning methods on the theory side. A peculiar system of copper oxide on Cu(111) will be used to demonstrate the approach: Various structures will be solved, starting from an amorphous layer, through complex reconstructions such as so called "29" or "44", up to the formation of bulk oxide. Possible future directions of this approach will be discussed.

* invited

Atomic Structure of Reconstructed Alumina*

Johanna Hütner, Andrea Conti, David Kugler, Florian Mittendorfer, Ulrike Diebold, Michael Schmid, Jan Balajka

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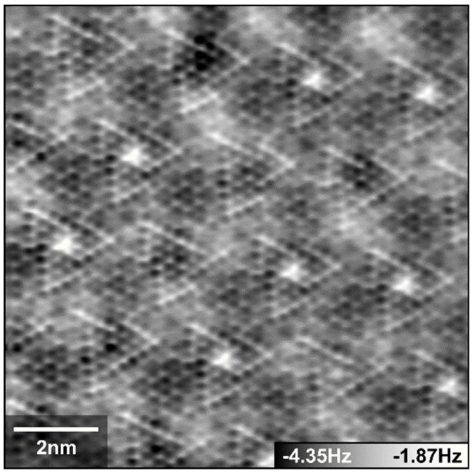
Corundum α-Al_2O_3 is an important ceramic widely used in electronics, optical applications, or as catalyst support. Despite its importance, the atomic structure of the most stable (0001) termination has not been conclusively determined. Detailed studies of Al_2O_3 surfaces have been stymied by its insulating nature, preventing the use of many surface science methods.

Structural models based on surface X-ray diffraction (SXRD) [1] and atomic force microscopy (AFM) [2] concluded the (√31 × √31)R±9°-reconstructed Al_2O_3(0001) surface formed upon high-temperature annealing is terminated by one or two layers of metallic Al strained to lattice-match the oxide substrate.

We imaged the reconstructed Al_2O_3(0001) surface with noncontact AFM (nc-AFM) using specifically functionalized tips for chemically-sensitive contrast. In particular, CuO_x terminated tips [3] enabled us to directly identify oxygen and aluminum atoms in the topmost layer.

With the aid of ab-initio calculations, we propose a structural model of the (√31 × √31)R±9°-reconstructed Al_2O_3(0001) surface consistent with atomically resolved nc-AFM images and area-averaging spectroscopic data. Unlike prior models, the surface does not contain a metallic Al layer but consists of oxygen and aluminum atoms arranged in similar structural units as reported in thin AlO_x films [4,5].



NC-AFM image of (√31 × √31)R±9°-reconstructed Al_2O_3(0001) acquired with a CuO_x-terminated tip (qPlus, 4 K)

References

1. G. Renaud, et al., Phys. Rev. Lett. 73, 13 (1994)
2. J. V. Lauritsen, et al., Phys. Rev. Lett. 103, 076103 (2009)
3. B. Shulze Lammers, et al., Nanoscale 13, 13617 (2021)
4. G. Kresse, et al., Science 308, 1440 (2005)
5. M. Schmid, et al., Phys. Rev. Lett. 99, 196104 (2007)

* contributed

6. Poster Titles

(in alphabetical order by first author's surname)

1. **Gustavo Andrade Silva Alves, Institute of Materials Chemistry, TU Wien**
   Enabling Methanol Selectivity in MoS_2 Catalysts for CO_2 Hydrogenation: The Role of the ZnO Support

2. **Viktor Birschitzky, Computational Materials Physics , University of Vienna (TACO P07)**
   Machine Learning the Mutual Polaron-Defect Interaction: Oxygen Vacancies on Rutile TiO_2(110)

3. **Lukas Bogner, Department of Physical Chemistry, University of Vienna (TACO P11)**
   Molecular Structure of Polymer Photocatalyst-Water Interfaces

4. **Florian Buchner, Institute of Materials Chemistry, TU Wien (TACO P09)**
   Long-Range Electrostatics in the JAX-MD Ecosystem Using the Multilevel Summation Method

5. **Llorenç Albons Caldentey, Universita Karlova**
   Characterization of $BaTiO_3$ at the Atomic Scale: Surface Structure and its Ferroelectric Behaviour

6. **Andrea Conti, Institute of Applied Physics, TU Wien**
   Ab-Initio Derived Force Fields for the Prediction of Surface Reconstructions of Al_2O_3(0001)

7. **Alessandro Coretti, Computational and Soft Matter Physics, University of Vienna (TACO P12)**
   Normalizing Flows for Statistical Mechanics

8. **Marco Corrias, Computational Materials Physics, University of Vienna (TACO P07)**
   Automated Real-Space Lattice Extraction and Atom Counting for Atomic Force Microscopy Images

9. **Sebastian Falkner, Computational and Soft Matter Physics, University of Vienna (TACO P12)**
   Learning Dynamics from Trajectories

10. **Carolin Faller, Computational Materials Physics, University of Vienna (TACO P03)**
    Long-Range Electrostatic Descriptors for Machine Learning Force Fields

11. **Giada Franceschi, Institute of Applied Physics, TU Wien**
    Imaging Feldspar Microcline and the First Stages of Ice Nucleation at the Atomic Scale

12. **Alexander Gorfer, Computational and Soft Matter Physics, University of Vienna**
    A Machine Learning Force Field for Albite and the Diffusion Mechanisms of its Defects

13. **Christopher Heard, Charles University Prague**
    Machine Learning Framework for Operando Simulations of (Zeolitic) Materials with Quantitative Accuracy

14. **Esther Heid, TU Wien, Institute of Materials Chemistry, TU Wien**
    Errors and Uncertainty in Machine Learning Models

15. **Harsharan Kaur, Department of Physical Chemistry, University of Vienna (TACO P11)**
    Fabrication and Characterization of Fe_2O_3 on Glass Substrates

16. **Federico Loi, J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences (NanoCat)**
    Oxidation of Size-Selected Agn Clusters on Graphene: A Combined Experimental and Theoretical XPS Study

17. **Rajesh Mandal, Technion - Israel Institute of Technology**
    New Insight into the Phase Transition in $BaTiO_3$

18. **Qaisar Maqbool, Institute of Materials Chemistry, TU Wien (TACO P08)**
    Operando Spectroscopy of Working VOC Nanocomposite Sensors

19. **Joanna Olszówka, J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences (NanoCat)**
    Preparation and In-Situ Characterization of the Semi-Model Catalytic Systems as a Key to Understanding Structure-Function Relationships in Dry Methane Reforming

20. **Aykut Aytekin Öztürk, Institute of Materials Science and Technology, TU Berlin**
    Benchmarking electrical conductivity of metal oxides using DFT

21. **Michael Pittenauer, Institute of Materials Chemistry, TU Wien (TACO P10)**
    Insights in the Water-Gas Shift Reaction over $CoFe_2O_4$ and $NiFe_2O_4$ Based on Operando Spectroscopy Techniques

22. **Christoph Rameshan, Chair of Physical Chemistry, Montanuni Leoben (TACO P10)**
    Combining Lab-Based NAP-XPS with Impedance Spectroscopy: Characterizing Oxide Catalysts for CO_2 Activation

23. **Paul Ryan, Institute of Applied Physics, TU Wien**
    The True Surface Tension of Pure-Water in Its Pure-Vapour

24. **Muhammad Zubair Saleem, University of Agriculture Faisalabad, Pakistan**
    Use of Heterogeneous Catalysts for Wastewater Treatment

25. **Pankaj Kumar Samal, Charles University Prague**
    Structure-Property Relationships in Model Electrocatalysis: How Do Ceria Nanoparticles Behave under Potential?

26. **Johannes Schörghuber, Institute of Materials Chemistry, TU Wien**
    Electron-Passing Neural Networks

27. **Abdul Selim, J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences (NanoCat)**
    Highly Selective Oxidation of Biomass to Glucaric Acid over the ZrO_2 Supported Au/Pt Nanocatalyst

28. **Karolína Simkovičová, J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences (NanoCat)**
    The Effect of Morphology and Copper Loading on Catalytic Activity of Nanostructured Cu/FeO_x Catalysts in CO_2 Hydrogenation

29. **Panukorn Sombut, Institute of Applied Physics, TU Wien**
    Two Can Be Better Than One: CO-Induced Dimer Decay Responsible for Gem-Dicarbonyl Formation on a Model Single-Atom Catalyst

30. **Parinya Tangpakonsab, Institute of Materials Chemistry, TU Wien (TACO P08)**
    Modeling Copper Oxide and Cobalt Oxide Catalyst: Adsorption and Reactions

31. **Nico Unglert, Institute of Materials Chemistry, TU Wien (TACO P09)**
    Neural-Network Force Field Backed Nested Sampling: Study of the Silicon p-T Phase Diagram

32. **Mykhailo Vaidulych, J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences (NanoCat)**
    Titania-Supported Pd, Pt, and Pt-Pd Catalysts for Low-Temperature Selective Oxidative Dehydrogenation of Cyclohexene

33. **Francesco Valentini, Institute of Materials Chemistry, TU Wien**
    Alternative Approach to Zeolite-Carbon Composites Synthesis with Enhanced CO_2 Adsorption Properties

34. **Stanislav Valtera, J. Heyrovský Institute of Physical Chemistry (NanoCat)**
    Switching Selectivity in the Oxidative Dehydrogenation of Cyclohexene by Atomic-Precision Control of Catalyst Composition

35. **Ivonne Elizabeth Ventura Rosales, Computational and Soft Matter Physics, University of Vienna**
    Elasticity Behavior of Amphiphilic Diblock Copolymer Brushes under Confined Geometry

36. **Chunlei Wang, Institute of Applied Physics, TU Wien (TACO P04)**
    C_2H_4 Adsorption on Rh-Decorated $Fe_3O_4(001)$ Surface

37. **Ralf Wanzenböck, Institute of Materials Chemistry, TU Wien (TACO P09)**
    Accelerated Search for Surface Reconstructions

38. **Thomas Wicht, Institute of Materials Chemistry, TU Wien (TACO P08)**
    Methane Partial Oxidation on Ni Nanoparticles Supported by MgO-ZrO_2 Mixed Oxides

39. **Johannes Zeininger, Institute of Materials Chemistry, TU Wien (TACO P08)**
    Resolving Single Particle Catalysis by In Situ Microscopy: Complexity in Catalytic H_2 Oxidation

40. **Moritz Zelenka, Department of Physical Chemistry, University of Vienna (TACO P11)**
    Laser Spectroscopy and the Interfacial Structure at the Spinel-Water Interface

7. Restaurant Suggestions

Gasthaus “Zur Eisernen Zeit“: Typical Viennese Restaurant
Am Naschmarkt, Stand 316-320

NENI am Naschmarkt: Modern & international cuisine
Am Naschmarkt, Stand 510

La Scala: Italian cuisine in Vienna

Elisabethstraße 13

Glacis-Beisl: Typical Viennese Heurigen (closed on Mondays)

Museumsquartier, Breite Gasse 4

Addicted to Rock, Gin, and Burger: Burger restaurant

Getreidemarkt 11

Ebi Mini: Fine Japanese restaurant

Gumpendorfer Straße 3

Tofu and Chili: Authentic Chinese restaurant (only few places!)

Linke Wienzeile 18

8. Conference Dinner: Practical Information

We will have the conference dinner at a typical Viennese wine tavern ("Heurigen"), the **Feuerwehr Wagner**. It is located in the vineyards on the outskirts of Vienna. The address is **Grinzinger Straße 53, 1190 Vienna**.

Here is how to get there:

- By public means of transport: Get on line U4 at *Karlsplatz* until the end stop *Heiligenstadt*. There, change to bus line 38A heading toward *Kahlenberg* until stop *Neugebauerweg* (six stops). The bus stop is 45 m from the entrance to the Heurigen. The ride takes about 35 minutes.

- Grab a taxi (there is a taxi stand at Linke Wienzeile 4 or call, e.g., +43 1 31300 or +43 1 40100) or Uber. The ride takes about 20 minutes.

We ordered a free buffet (including vegetarian and vegan options) for all conference participants. Drinks have to be paid individually!

Below the nano cat, there is plenty of room at the bottom of this page for your notes.

Sunday, 24.9.

Start	End	Speaker / Event
16:00	17:00	Registration
17:00	17:10	Welcome words by Ulrike Diebold
17:10	17:50	Boris Kozinsky
17:50	18:15	Georg Kresse
18:15	18:40	Florian Libisch
18:40	19:00	Poster Speed Talks I.
19:00	21:30	**Welcome Reception & Poster Session I.**

Monday, 25.9.

Start	End	Speaker / Event
09:00	09:40	Johannes Kästner
09:40	10:05	Jesus Carrete
10:05	10:45	Coffee Break
10:45	11:25	Andreas Grüneis
11:25	11:50	Cesare Franchini
11:50	12:15	Stefan Riemelmoser
12:15	13:45	Lunch Break
13:45	14:25	Ralf Drautz
14:25	15:05	Jonas Köhler
15:05	15:45	Coffee Break
15:45	16:10	Andreas Kretschmer
16:10	16:35	Alberto Tampieri
16:35	17:00	Thomas Haunold
17:00	17:20	Poster Speed Talks II.
17:20	20:30	**Poster Session II.**

Tuesday, 26.9.

Start	End	Speaker / Event
09:00	09:40	Beatriz Roldan
09:40	10:05	Stefan Vajda
10:05	10:45	Coffee Break
10:45	11:25	Tanja Cuk
11:25	11:50	Christoph Jung
11:50	12:15	Ellen Backus
12:15	13:45	Lunch Break
13:45	14:25	Karsten Reuter
14:25	14:50	Giacomo Melani
14:50	15:30	Coffee Break
15:30	16:10	Zdenek Dohnalek
16:10	16:35	Jiri Pavelec
16:35	17:00	Pablo Montero
19:00		**Conference Dinner**

Wednesday, 27.9.

Start	End	Speaker / Event
09:00	09:40	Bilge Yildiz
09:40	10:05	Michele Riva
10:05	10:45	Coffee Break
10:45	11:25	Martin Setvin
11:25	11:50	Jan Balajka
		END