

# TAming COmplexity in Materials Modeling (TACO) 3<sup>rd</sup> Annual Ph.D. Workshop

Date:	February 11–14, 2024
Place:	JUFA Hotel, Coburgstraße 253, 8970 Schladming

# Sunday, February 11

08:00 - 12:00	Bus transfer from Vienna (Wiedner Hauptstr./Resselg.) to Schladming
12:00 - 16:00	Outdoor discussions
16:00 – 16:25	Check-in

### Chair: Johannes Zeininger (P08)

16:25 – 16:30	Ulrike Diebold, TU Wien (P01): Welcome address
16:30 – 17:30	<b>Elisabeth Schrattenholzer</b> Words, Voice, and Attitude: How they Enhance or Hinder Success
17:30 – 17:50	Break
17:50 – 18:30	<b>Marc Georg Willinger, TU Munich (invited)</b> Observing while it Happens: Operando Electron Microscopy in Catalysis Research
18:30 – 19:00	<b>Chunlei Wang, TU Wien (P04)</b> CO-Induced Dimer Decay Responsible for Gem-Dicarbonyl Formation on a Model Single-Atom Catalyst
19:00 – 20:00	Dinner
20:00 - 20:20	Poster Speed Talks (chair: Thomas Ruh, P01)
20:20 – open-end	Poster session

# Monday, February 12

08:00 - 09:00	Breakfast
09:00 - 15:00	Outdoor discussions



Chair: Parinya "Lewis" Tangpakonsab (P08)

15:00 – 15:40	<b>Liliana Lukashuk, Johnson Matthey (invited)</b> Steel Industry Decarbonisation via Valorising Emissions from Steel Making into Sustainable Products
15:40 – 16:10	<b>Michael Pittenauer, TU Wien (P10)</b> Insights in the Gas Phase Oxidation of 2-Propanol over CoFe <sub>2</sub> O <sub>4</sub> and NiFe <sub>2</sub> O <sub>4</sub>
16:10 – 16:40	<b>Thomas Wicht, TU Wien (P08)</b> Ethylene Hydrogenation on HOPG-Supported Ag, Au, and Cu: Surface Science and Model Catalysis
16:40 – 17:00	Break

## Chair: Ralf Wanzenböck (P09)

17:00 – 17:40	<b>Zachary Ulissi, Meta &amp; Carnegie Mellon (invited, remote via <u>Zoom</u>)</b> Open Datasets and Deep Learning Interatomic Potentials for Catalyst Discovery
17:40 - 18:10	<b>Nico Unglert, TU Wien (P09)</b> Neural-Network Force Field Backed Nested Sampling: Study of the Silicon p–T Phase Diagram
18:10 - 18:40	<b>Alexander Gorfer, University of Vienna (P12)</b> Frenkel Pair Energetics in Disordered Solid Solutions Applied on Alkali Feldspar
19:00 - 20:00	Dinner
20:00 - 20:30	General Assembly
20:30 – open-end	Poster session

# Tuesday, February 13

08.00 - 09.00	Breakfast
00.00 - 09.00	DICANIASL

09:00 – 15:00 Outdoor discussions



## Chair: Carolin Faller (P03)

15:00 – 15:40	Markus Valtiner, TU Wien (invited) Energy Transition
15:40 – 16:10	<b>Viktor Birschitzky, University of Vienna (P07)</b> Unraveling the Interplay of Polarons and Defects Through Machine Learning
16:10 – 16:40	<b>Payal Wadhwa, University of Vienna (P03)</b> Machine-Learning-Aided Studies of Absorption of D <sub>2</sub> O Molecules on TiO <sub>2</sub> (110) and Nano-Pyramidal Reconstruction of the Cu <sub>2</sub> O (111) Surface

16:40 – 17:00 Break

## Chair: Moritz Zelenka (P11)

17:00 – 17:40	<b>Davide Ferri, Paul Scherrer Institute (invited)</b> Diving with Spectroscopy – Exploring Catalytic Solid-Liquid Interfaces
17:40 – 18:10	<b>Harsharan Kaur, University of Vienna (P11)</b> Exploring the Interfacial Water Molecular Behaviour in the Vicinity of Iron Oxide Thin Films at the Solid-Liquid Interface
18:10 – 18:40	<b>Alexander Imre, TU Wien (P02)</b> ViPErLEED and Structure Elucidation: Progress and Challenges
19:00 - 20:00	Dinner
20:00 - 21:00	Executive Board meeting (PI, Co-PIs & student representatives)
21:00 – open-end	Poster Session

# Wednesday, February 14

07:00 – 07:45	Breakfast, Check-out
8:00 – ca. 12:00	Bus transfer to Vienna

## Posters

Florian Buchner (P09)	msmJAX: Fast Electrostatics in Python with the Multilevel
Marco Corrias (P07)	Total-Variation-Based Image Decomposition and Denoising for Microscopy Images
Florian Dörr (P02)	ViPErLEED: Measurement package
Moritz Eder (P04)	Multitechnique Characterization of Rhodium Gem- Dicarbonyls on TiO2(110)
Sebastian Falkner (P12)	Learning Dynamics from Trajectories
Thomas Haunold (P08)	Surface Hydroxylation of an Ultrathin Co₃O₄(111) Film Grown on Ir(100): Near-Ambient Pressure XPS and DFT Studies Summation Method
Michael Ketter (P09)	Batch-Mode Active Learning a Neural-Network Force Field with Nested Sampling: A Case Study on Silicon
Marie Kienzer (P02)	Quantitative LEED of Oxide Surfaces
Jessica Michalke (P10)	Pyrolytic Syntheses Of Solid Base Metal Hydrogenation Catalysts
Jiri Pavelec (P04)	Infrared Reflection Absorption Spectroscopy of CO and D <sub>2</sub> O adsorbed on TiO <sub>2</sub> (110)
Thomas Plaikner	Ground and Excited Many-Electron States Using Coupled- Cluster Theory
Christoph Rameshan (P10)	Doping of Perovskite Oxide Catalysts - Unravelling the Complex Exsolution Behaviour
Erik Rheinfrank (P02)	The Incommensurately Modulated Structure of La <sub>0.8</sub> Sr <sub>0.2</sub> MnO <sub>3</sub> (001)
Sita Schönbauer	Machine-Learned Force Fields Using Coupled-Cluster Theory
Alberto Tampieri (P10)	A Bizarre Cubic/Tetragonal Phase Transition Behaviour in Copper Ferrite
Parinya Tangpakonsab (P08)	CO Oxidation at the Perovskite LaCoO <sub>3</sub> Surface vs. $Co_3O_4$ and CuO: A Comparative DFT Study
Ralf Wanzenböck (P09)	Exploring Ti-rich STO(110) Reconstructions: Active-Learned, Transferable Neural Networks Driving Evolutionary Searches
Johannes Zeininger (P08)	Cooperative Catalytic Behaviour on the Nanoscale: Chemical Interactions on a Single Particle Exposed
Moritz Zelenka (P11)	Metal Oxide Interfaces

#### **Observing while it happens: Operando Electron Microscopy in Catalysis Research**

Marc Willinger

Chair of Electron Microscopy with Research Emphasis on Energy Materials, Department of Chemistry, TUM School of Natural Sciences, TU Munich, Lichtenbergstasse 4, 85748 Garching e-mail: marc.willinger@tum.de

#### Abstract:

Our aim is to understand processes that lead to the emergence of catalytic function. Using a combination of operando scanning and transmission electron microscopy, we study the dynamic interplay between reactive gas-phase and active catalyst at different length- and time-scales. Starting with simple model catalysts, such as polycrystalline metal foils, we observe the propagation of chemical waves and reveal how catalytic activity depends on grain orientation, coupling mechanisms, and reaction conditions [1]. In the case of redox-reactions on non-noble metals, we find that the active catalyst is operating near a phase-boundary where metallic and oxidized phases coexist [2]. Real-time imaging reveals fascinating oscillatory redox dynamics that increase in complexity with the increasing chemical potential of the gas phase. When moving from simple model catalysts to industrially relevant metal nanoparticles supported on reducible oxide carriers, we find different manifestations of strong metal-support interactions and structural dynamics due to redox processes that can be related to catalytic function [3,4]. The aim of the presentation is to demonstrate that active catalysts are dynamically adapting to the reaction environment and that catalytic function is related to the catalysts ability to participate in the reaction through reversible changes in its structure and/or (local) composition.



**Left:** Propagating reaction fronts observed by *in situ* SEM during NO<sub>2</sub> hydrogenation on polycrystalline Pt. **Right:** Pt particle supported on TiO<sub>2</sub> in an initially SMSI encapsulated state undergoes morphological changes and loss of encapsulating titania overlayer upon exposure to redox-reactive environment. [4].

#### **References:**

Barroo C. et al. Nat Catal 3, 30–39 (2020).
Huang X. et al. Adv. Mater. 2101772 (2021).
Beck A. et al. Nat. Catal 4, 488-497 (2021)
H. Frey et al., Science 376, 982-987 (2022)

## CO-Induced Dimer Decay Responsible for Gem-Dicarbonyl Formation on a Model Single-Atom Catalyst

Chunlei Wang,<sup>1</sup> Panukorn Sombut,<sup>1</sup> Lena Puntscher,<sup>1</sup> Zdenek Jakub,<sup>1,2</sup> Matthias Meier,<sup>1,3</sup> Jiri Pavelec,<sup>1</sup>

Roland Bliem,<sup>5</sup> Michael Schmid,<sup>1</sup> Ulrike Diebold,<sup>1</sup> Cesare Franchini,<sup>3,4</sup> Gareth S. Parkinson<sup>1\*</sup>

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The precise exploration and anticipation of the structure-activity relationship between catalysts and reactants remain crucial endeavors for catalysis scientists. Achieving this requires advanced catalysts and state-of-the-art characterization techniques to offer a thorough understanding of catalytic processes. We will give content of two aspects in the present talk: a recent scientific summary of our work and a brief introduction of our newly designed infrared spectroscopy instrument for future plans. Firstly, we employed a combination of density functional theory (DFT) and time-lapse scanning tunneling microscopy (STM) to study the behavior of CO adsorption on Rh1 single atoms and Rh2 dimers supported by well-defined Fe<sub>3</sub>O<sub>4</sub>(001) single crystal. CO adsorption at Rh<sub>1</sub> sites results exclusively in stable Rh<sub>1</sub>CO monocarbonyls, because the Rh atom adapts its coordination to create a stable pseudosquare planar environment.  $Rh_1(CO)_2$  gem-dicarbonyl species are also observed, but these form exclusively through the breakup of Rh<sub>2</sub> dimers via an unstable Rh<sub>2</sub>(CO)<sub>3</sub> intermediate. Our results clearly show that the adsorption of reactants can have a strong influence on the structure of the system, and that CO exposure can be used to redisperse small clusters that form during reactions. Overall, this work provides new insights into the rational design of novel single-atom catalysts through the synthesis of dimer catalysts. In the second part, we would like to briefly report the progress of our infrared technique and some preliminary collected data on TiO<sub>2</sub> system.

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#### Steel industry decarbonisation via valorising emissions from steel making into sustainable products

Liliana Lukashuk

To reach EU climate targets, the steel and iron producing sectors are looking to decrease their CO2 emissions by up to 90% by 2050. The residual carbon-rich gases from the steel-making processes, such as basic oxygen furnace gas (BOFG) and blast furnace gas (BFG), are considered a valuable feedstock for the chemical sector (hydrogen and ammonia production). In this presentation, an overview of technical solutions for the production of chemicals from BOFG and BFG gas streams will be discussed together with all the steps taken for the evaluation of the suitability of catalytic materials. The results of detailed investigations of functional catalytic materials in this new area of application will be presented, focusing on in-depth catalytic studies with post-characterisation results. In addition, an improved fundamental understanding of catalysts will be discussed, highlighting the approach for underpinning industrial catalysis using synchrotron-based advanced characterisation techniques.

#### Insights in the gas phase oxidation of 2-propanol over CoFe<sub>2</sub>O<sub>4</sub> and NiFe<sub>2</sub>O<sub>4</sub> nanoparticles

#### **Michael Pittenauer**

#### Supervisor: Karin Föttinger

Ferrite spinels as catalysts of various oxidation reactions are widely investigated. One of the most important model reactions in this field is the oxidation of 2-propanol. In the literature ferrites have been reported to be not completely specifically reactive towards 2-propanol resulting in oxidative dehydrogenation (partial oxidation to acetone), subtotal oxidation to carboxylic acids, dehydrogenation, total and subtotal combustion and steam reforming being all relevant in the investigation of 2-propanol oxidation. This talk aims at clarifying the contribution of the reactions mentioned above by temperature programmed 2-propanol oxidation with different ratios of 2-propanol:O<sub>2</sub> as well as temperature programmed acetone oxidation, ex-situ XRD phase analysis and *operando*-DRIFTS-MS studies.

#### Ethylene hydrogenation on HOPG supported Ag, Au and Cu: surface science and model catalysis

Thomas Wicht

Model catalysts of Ag, Au, and Cu nanoparticles supported on graphite were manufactured, characterized, and tested in ethylene hydrogenation. The carbon-supported nanoparticles exhibited improved catalytic performance compared to unsupported metal foils, due to enhanced hydrogen availability, highlighting the support effect of carbon and providing insights for rational catalyst design.

#### Open Datasets and Deep Learning Interatomic Potentials for Catalyst Discovery

Zachary Ulissi

Machine learning accelerated catalyst discovery efforts have seen much progress in the last few years. Datasets of computational calculations have improved, models to connect surface structure with electronic structure or adsorption energies have gotten more sophisticated, and active learning exploration strategies are becoming routine in discovery efforts. Large-scale data and machine learning modeling efforts like the Open Catalyst Project (https://opencatalystproject.org/) have elevated computational catalysis to a first-class problem in the broader machine learning community and led to rapid improvements in accuracy with new state-of-the-art Al/ML models appearing every 3-4 months since 2020. The resulting models are now accurate enough to assist with many day-to-day catalyst simulation efforts (AdsorbML), and to share the capabilities with the community we have released an online demo (https://open-catalyst.metademolab.com/) and representative case studies. I will finally discuss current and future efforts to build similar approaches for other climate-related and materials challenges like direct air capture via the OpenDAC collaboration.

# Neural-network force field backed nested sampling: Study of the silicon *p*-*T* phase diagram

N. Unglert<sup>1</sup>, J. Carrete<sup>2,1</sup>, L. B. Pártay<sup>3</sup>, and G. K. H. Madsen<sup>1</sup>

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Nested sampling is a promising method for calculating phase diagrams of materials [1]. However, the computational cost limits its applicability if ab-initio accuracy is required. In the present work [2], we report on the efficient use of a neural-network force field [3] in conjunction with the nested-sampling algorithm. We train our force fields on a recently reported database of silicon structures and demonstrate our approach on the low-pressure region of the silicon pressure-temperature phase diagram between 0 and 16 GPa. The simulated phase diagram shows a good agreement with experimental results, closely reproducing the melting line. Furthermore, all of the experimentally stable structures within the investigated pressure range are also observed in our simulations. We point out the importance of the choice of exchange-correlation functional for the training data and show how the r2SCAN meta-GGA plays a pivotal role in achieving accurate thermodynamic behaviour. We furthermore perform a detailed analysis of the potential energy surface exploration and highlight the critical role of a diverse and representative training data set.

#### References

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- 2. Unglert N., Carrete J., Pártay L. B., and Madsen G. K. H. Phys. Rev. Mater. 2023, 7, 123804.
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#### Unraveling the interplay of polarons and defects through machine learning

Viktor Birschitzky

Oxide materials play a pivotal role in various technological applications and their intricate physics is governed by their composition, the presence of defects, and the formation of polarons. However, the complex interplay between polarons and defects poses significant challenges for first-principles simulations.

In recent years, machine learning (ML) has revolutionized materials modeling, enabling simulations at ab initio accuracy at a fraction of the computational cost. Despite these advancements, ML-based simulations face two major obstacles when dealing with defects and their associated localized charges.

In the presence of multiple point-like defects, the sampling problem leads to a combinatorial explosion of possible defect arrangements, making it computationally infeasible to explore the full range of configurations. We propose a combination of ML and global optimization strategies to overcome this challenge [1,2].

The second problem is the dynamic evolution of polaronic charge, which has not been adequately addressed in ML-based simulations. Here, we give an outlook on future developments based on deep learning, which explicitly model the temporal behavior of polaronic charges.

[1] Birschitzky, V. C., Ellinger, F., Diebold, U., Reticcioli, M. & Franchini, C. Machine learning for exploring small polaron configurational space. npj Comput Mater 8, 1–9 (2022).

[2] Birschitzky, V. C., et al. Machine Learning Based Prediction of Polaron-Vacancy Patterns on the  $TiO_2(110)$  Surface, in preparation (2024).

# Machine learning aided studies of absorption of $D_2O$ molecules on TiO<sub>2</sub> (110), and nano-pyramidal reconstruction of Cu<sub>2</sub>O (111) surface

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The recent developments in machine learning have greatly increased its demand in the field of material science because of its ability to address a myriad of challenging problems with exceptional accuracy and minimum human intervention. However, accurate force field generation needs proper training data. Recently developed "on-the-fly learning" technique in VASP, has provided a simplified and efficient approach to address this issue [1, 2]. In this talk, we will discuss two problems addressed by machinelearned force fields (MLFF) based on on-the-fly learning. Firstly, we will discuss the absorption of 1 Monolayer (ML) and 2 ML  $D_2O$  molecules on the TiO<sub>2</sub>(110) surface, where the generated MLFF provided the same reconstructed surfaces as observed in experiments. We also calculated the absorption spectra for 1ML and 2ML  $D_2O$  molecules at TiO<sub>2</sub>(110) surface, where the asymmetric stretch is observed at 2622 cm $^{-1}$  and 2629 cm $^{-1}$ , respectively, while the symmetric stretch is observed at 2480 cm<sup>-1</sup> and 2389 cm<sup>-1</sup>, respectively. The second part of my talk will be based upon the long-standing problem of the most stable reconstruction of Copper Oxide (Cu<sub>2</sub>O) (111) surface. Here, we started with a stoichiometric  $(\sqrt{3} \times \sqrt{3})$ R30° supercell, and found a new pyramidal reconstruction using MLFF compared to previous theoretical reports. We also calculated the phase diagram of the various models of  $(\sqrt{3} \times \sqrt{3})$ R30° reconstructions using PBE and HSE06 functionals. Both studies indicate on-the-fly learning to be a fast and efficient way to find the most stable reconstructed surfaces.

- Jinnouchi, R.; Lahnsteiner, J.; Karsai, F.; Kresse, G.; Bokdam, M. Phys. Rev. Lett. 2019, 122, 225701.
- (2) Jinnouchi, R.; Karsai, F.; Kresse, G. Phys. Rev. B 2019, 100, 014105.

## Diving with spectroscopy – exploring catalytic solid-liquid interfaces

Davide Ferri

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Various heterogeneous catalytic processes involved in the production of pharmaceuticals and fine chemicals, in the biomass valorization chain and in water purification occur in a liquid environment. Despite its ubiquity, the molecular processes taking place at the solid-liquid interface, the contact between the liquid environment and the surface of the catalyst, are still largely approximated by gas phase



experiments exploiting in situ and operando approaches. However, the same spectroscopy and diffraction methods that contributed to develop the vast understanding on catalytic solid-gas interfaces also appropriate are to

characterize the structure of catalysts in the presence of a liquid, often irrespective of temperature and pressure. In this contribution, I will present methods that we use to examine solid-liquid interfaces and will show examples of studies from my own experience aiming at understanding the catalytic solid-liquid interface from a molecular perspective and at developing tools to interrogate it. I will discuss especially the behavior of supported precious metal nanoparticles.

# Exploring the interfacial water molecular behaviour in the vicinity of iron oxide thin films at the solid-liquid interface

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Iron oxides are considered a relevant class of materials that display unique crystal compositions, distinct morphologies, and remarkable magnetic properties [1-4]. They are of great environmental importance owing to their efficient recycling ability [2,3]. As a consequence, iron oxides are being widely employed in various scientific domains ranging from optoelectronics, catalysis, medicinal industry, energy conversions, molecular sensing, corrosion prevention, and developing purification technologies [1-4]. Hematite (Fe<sub>2</sub>O<sub>3</sub>) and magnetite (Fe<sub>3</sub>O<sub>4</sub>) are the two most widely applied iron oxide materials especially as thin films. Hematite emerged as a promising anode material because of its suitable band gap of about 2.2 eV, excellent chemical stability in a broad pH range, natural abundance, non-toxicity, and low cost [5]. On the contrary, magnetite is a completely oxidized version of iron oxide which provides a smaller band gap of ~0.1 eV and is a relevant precursor for the formation of hematite [5]. Both of the iron oxide polymorphs are known to demonstrate exceptional photocatalytic properties and are in principle suitable for water splitting [2,3,5]. However, their water oxidation efficiency is limited by certain factors which include short lifetime and low mobility of charge carriers, which ultimately relies on the thickness of the film and structural homogeneity in order to support the mobility of the charges within the device [2,3]. Hence, it would be of great interest to conduct thin film fabrication of iron oxides on the substrate and evaluate their morphological and optical properties for the designing of optimal coatings for water-splitting applications.

In the present work, we aim to investigate the fabricated hematite and magnetite thin films onto a calcium fluoride (CaF<sub>2</sub>) substrates for their potential application towards understanding the photocatalytic splitting of water molecules. The fabrication of iron oxides on a CaF<sub>2</sub> substrates is performed using radio-frequency (RF) sputtering of iron oxide targets. The sputter-coated CaF<sub>2</sub> substrates were characterized for their film thickness, surface morphology, and spectroscopic properties by using a variety of techniques which include ellipsometry, and UV-visible absorption spectroscopy. The film thickness was found to lie in range of ~47-54 nm. The UV-visible profile of both the iron oxide films showcased >80% of the transmission in the visible region of the spectrum. The raman micro-spectroscopic data demonstrated that both the fabricated films were crystalline and nearly homogeneous and surprisingly depict similar Raman features. Subsequently, the iron oxide-coated substrates were examined at the solid-liquid interface to understand their interfacial molecular-level behaviour with the introduction of water molecules in their vicinity by using the interface-specific sum frequency generation vibrational spectroscopy (SFG VS) [7]. The experiments were performed in a solid-liquid geometry with the variation of solution pH and ionic strength. We observed a differential OH-stretching vibrational pattern for the hematite and magnetite films respectively, which provided us the information about the relative hydrogen bonding environment and the probable orientation of the water molecules at the solid-liquid interface. The pH-dependent studies showcased that the weakly coordinated water molecules dominate for Fe<sub>2</sub>O<sub>3</sub>) while strongly coordinated water molecules dominate in for Fe<sub>3</sub>O<sub>4</sub> films interfacing the aqueous media with rising pH value. The ionic strength-dependent studies were conducted to rule out the contribution from the bulk water molecular ordering. The observations depicted that the weakly coordinated water molecules represent the true interfacial feature. Through preliminary work, we intend to contribute towards the fundamental insights about the catalytic splitting of water molecules at the molecular-scale. Further results will be discussed in details at the conference.

#### References

- [1] Kefeni, K. K., Mamba, B. B., & Msagati, T. A. (2017). Application of spinel ferrite nanoparticles in water and waste water treatment: a review. *Separation and Purification Technology*, 188, 399-422.
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## **ViPErLEED and Structure Elucidation: Progress and Challenges**

TACO subproject PO2 is focused on determining and understanding the surface structures of complex materials. For this purpose, we employ a large toolbox of ultra-high vacuum (UHV) and computational techniques. Among these, we have placed a particular emphasis on low energy electron diffraction (LEED). LEED is sensitive to the topmost atomic layers and as such provides quick, qualitative insight into surface structure and ordering.

Additionally, by studying the diffraction intensities as a function of incident electron energy (LEED-I(V)), it is possible to quantitatively compare experimentally observed surfaces with structural models.

Despite the powerful possibility of direct experiment-to-theory comparison, LEED-I(V) is only regularly used by few specialized groups around the world. A main obstacle for widespread adoption is that existing solutions for LEED-I(V) analysis and simulation are hard to use for scientists who are not already experts in the field.

To resolve this issue, we have developed the Vienna Package for Erlangen LEED (ViPErLEED) – a package of three independent but complementary tools for easy LEED-I(V) acquisition and analysis. All parts of ViPErLEED will be released as open source at the time of publishing:

- Electronics: We provide schematics and control software for electronics, which allows users to easily and cheaply upgrade existing retail LEED setups for acquiring high fidelity LEED-I(V) data. These ViPErLEED electronics are based on an Arduino and can be home built from off-the-shelf components.
- **Spot-tracker:** ViPErLEED provides a modern ImageJ plugin for spot tracking and extraction of LEED-I(V) spectra from raw diffraction images. The automatically extracted curves can be used for further analysis or as a fingerprint of the prepared surface.
- **Software:** For modern LEED-I(V) analysis, we introduce a Python package for calculation and optimization of theoretical LEED-I(V) spectra. The ViPErLEED software is developed based on, and as an extension to, the established TensErLEED package. It further uses standard file formats, enables automated symmetry detection, and can set up calculations with just a handful of parameters.

At this occasion, we present an overview of the current state of all parts of ViPErLEED, the ongoing developments and remaining challenges.







Fig. 1. Screenshot and example input of the ViPErLEED package. (a) The spot tracker evaluates the beam intensities with minimal user intervention. (b) The input for the structure search requires a file with initial coordinates and only a handful of other parameters.