O 9: Poster Session I: New methods I

Time: Monday 10:30–12:30   Location: P

O 9.1   Mon 10:30   P

Deterministic quantum mechanics: simulation of chemical reactions — •IRMGARD FRANK — Leibniz University Hannover, Hannover, Germany

Roberto Car and Michele Parrinello had the great idea to describe electronic structure using the Schrödinger equation and nuclear motion using Newton dynamics. Over the years it turned out, that with this approach it is possible to describe arbitrary chemical reactions. We observe classical chaos: Starting from identical initial conditions, we will always get the same reaction pathway. If, however, slightly changing the initial conditions, it is possible to observe completely different reactions. Both electronic cloud and nuclear positions are moved using differential equations, hence we have very clearly a deterministic picture. The general idea is similar to Bohm mechanics, with the difference that we use classical Newton dynamics for the nuclei instead of a guiding equation. An apparent difference is that there is no zero-point energy in nuclear motion. This facilitates the description of potential energy surfaces and of motion on these surfaces.

O 9.2   Mon 10:30   P

How to train a Gaussian Approximation Potential for metal oxides: A three stage process towards fast surface sampling — •CARSTEN STAACKE[1,2], JAKOB TIMMERMANN[1,2], YONGYHUK LEE[1,2], CHRISTOPH SCHEURER[1,2], and KARSTEN REUTER[1,2] — [1]Fritz-Haber-Institut der MPG — [2]Technische Universität München

Surface orientation and termination play a decisive role for the chemical and physical behavior of catalysts and functional materials. *Ab initio* thermodynamics comparing the stability of different density-functional theory computed trial structures has emerged as a standard tool to determine surface structures under working conditions. However, limited by the high computational cost, these trial structures are up to now typically derived manually, reflecting the researcher's ability to imagine possible structural models. Efficient and accurate machine-learned (ML) interatomic potentials promise to replace this state-of-the-art by systematic global optimization methods. To this end, we have developed a protocol to train short-ranged ML potentials for metal oxides based on the Gaussian Approximation Potential and Smooth Overlap of Atomic Positions (SOAP) descriptors to capture atomic environments.[1,2] We will present a systematic three-stage training process. For various rutile type metal oxides the role of all three stages will be exemplified and critically evaluated. [1] J. Timmermann *et al.*, Phys. Rev. Lett. **125**, 206101 (2020). [2] A.P. Bartók *et al.*, Phys. Rev. Lett. **104**, 136403 (2010).

O 9.3   Mon 10:30   P

Biaxial atomically resolved force microscopy based on a qPlus sensor operated simultaneously in the first flexural and length extensional modes — •DOMINIK KIRPAL[1], JINGLAN QIU[1,2], KORBINIAN PÜRCKHAUER[1], ALFRED J. WEYMOUTH[1], MICHAEL METZ[1], and FRANZ J. GIESSIBL[1] — [1]Institute of experimental and applied physics, University of Regensburg, Regensburg, Germany — [2]College of Physics and Hebei Key Laboratory of Photophysics Research and Application, Hebei Normal University, Shijiazhuang, Hebei, China

In frequency-modulation atomic force microscopy typically the tip is driven to oscillate vertically, giving a measure of the vertical force component. However, for many systems the lateral force component of force provides valuable information about the sample. Measuring lateral and vertical force components simultaneously by oscillating vertically and laterally has so far only been demonstrated with relatively soft silicon cantilevers and optical detection. Here, we show that the qPlus sensor can be used in biaxial mode with electrical detection by making use of the first flexural mode and the length extension mode. We describe the necessary electrode configuration as well as the electrical detection circuit, and compare the length extension mode to the needle sensor. Finally, we show atomic resolution in ambient conditions of a mica surface and in ultra-high vacuum of a silicon surface. With this, we show how any qPlus AFM setup can be modified to work as a biaxial sensor, allowing two independent force components to be recorded.

O 9.4   Mon 10:30   P

Design of an IRAS Setup to Investigate Adsorbates on Metal-Oxide Single Crystals — •DAVID RATH, JIRI PAVELEC, GARETH PARKINSON, MICHAEL SCHMID, and ULRIKE DIEBOLD — Institut für Angewandte Physik, Technische Universität Wien, A-1040 Wien, Austria

The IRAS system GRISU (**GR**azing incident **I**nfrared absorption **S**pectroscopy **U**nit) was developed for investigations in the research field of single atom catalysis [1]. It combines the commercially available FTIR spectrometer Bruker Vertex 80v with an UHV chamber [2]. GRISU features five mirrors for beam guidance placed in HV and UHV environment. The development was concentrated to optimise the system's performance, flexibility and usability resulting in a small controllable focal-spot diameter (3 mm) on the sample, different optical apertures, and motorised optical components. The simulated system (done with a ray tracing program and a simplified spectrometer model) shows an efficiency of 13 %, i.e. 13 % of the radiation passing through the first aperture (Ø 6 mm) after the IR source in the FTIR spectrometer reaches the detector after being reflected from the molecular beam spot on the sample. Compared to a commercially available system with two parabolic mirrors with a focal length of 500 mm, this is higher by a factor of about 60. All the optical components are mounted precisely in respect to each other to ensure the high performance requirement also after long term use.
[1] G. S. Parkinson, Catal. Lett. 149, 1137 (2019)
[2] J. Pavelec, et al., J. Chem. Phys. 146, 014701 (2017).

O 9.5   Mon 10:30   P

Vienna Package for TensErLEED: A new environment for analysis and calculation of LEED *I(V)* data — •FLORIAN KRAUSHOFER[1], MICHAEL SCHMID[1], TILMAN KISSLINGER[2], ULRIKE DIEBOLD[1], LUTZ HAMMER[2], and MICHELE RIVA[1] — [1]TU Wien, Vienna, Austria — [2]FAU Erlangen-Nürnberg, Erlangen, Germany

Low-Energy Electron Diffraction (LEED) is a structure-sensitive technique commonly available in most surface science laboratories. Beyond the usual application as a tool to determine periodicity and degree of order of a surface phase, the method also gives access to the surface's crystallographic structure via a quantitative analysis of the modulation of beam intensities as a function of electron energy (LEED *I(V)*). This, however, requires complex full-dynamical intensity calculations as well as a time-consuming optimization of structural parameters minimizing the deviation between experimental and calculated *I(V)* curves. The Erlangen program package TensErLEED [1] readily performs this task, but its required user input is almost prohibitively complex.
We show that for most cases, the necessary TensErLEED input can be generated automatically by combining a handful of user parameters and a structure file in a standard format. Based on this, we introduce the new "<u>Vi</u>enna <u>P</u>ackage for Tens<u>ErLEED</u>" (ViPErLEED), which greatly simplifies the code application and substantially reduces the amount of work and potential for errors, even for experienced users. The package is completed by a versatile utility for extracting experimental *I(V)* spectra from a LEED video or stack of images.
[1] V. Blum, and K. Heinz, Comput. Phys. Commun. **134**, 392 (2001).