O 35: Poster Solid-Liquid Interfaces: Structure

Time: Tuesday 13:30–15:30 Location: P3

O 35.1 Tue 13:30 P3

Comparision of spin and orbital Rashba effect in Bi_xPb_{1-x}/Ag(111) — •Himanshu Lohani — EP7 University of Wurzburg

Superstructure of heavy elements constructed on the surface of noble metals is one of the most celebrated system in the field of spintronics due to giant Rashba spin splitting found in its surface electronic structure. A new perspective of orbitronics has emerged recently for reinvestigating this system after the uprising of orbital based Rashba effect. Angle resolved photoelectron spectroscopy (ARPES) not only visualizes directly the electronic band dispersion but intensity of the photoemission signal itself carries important information of orbital character of the bands. By using the photoemission intensity calculation which is designed on a tight binding model, we successfully capture evolution of the Rashba surface state bands (SSBs) dispersion and intensity as they are observed in our ARPES data on Bi_xPb_{1-x}/Ag(111). This comparative study hints that buckling of Bi/Pb atoms on Ag(111) surface affects spin polarization of the Rashba SSBs more than their orbital polarization

O 35.2 Tue 13:30 P3

High-Dimensional Neural Network Potentials for Molecular Dynamics Simulations of Mineral-Water Interfaces — •Maite Böhm[1,2], Bernadeta Prus[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

In recent years, High-Dimensional Neural Network Potentials (HDNNP), a frequently used type of machine learning potential, have become a popular tool for simulations of complex systems such as mineral-water interfaces. Here, we present a HDNNP trained to density functional theory energies and forces for tricalcium aluminate ($Ca_3Al_2O_6$, C_3A)-water interfaces, which are of high interest for concrete chemistry. After validation, the obtained HDNNP is applied in large-scale molecular dynamics simulations to unravel the interactions of water with this material by computing a series of structural and dynamical properties.

O 35.3 Tue 13:30 P3

Informed Automated Structure Discovery of Atomic Force Microscopy Images — •Azin Alesafar[1], Joakim Jestilä[1], and Adam Foster[1,2] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan

Atomic Force Microscopy (AFM) enables direct imaging of atomic-level features however, the interpretation of non-planar molecules is challenging due to the fact that only the top layers of these systems interact with the microscope tip. This leads to images deviating from structures familiar to us. Recent Advances in machine learning-based image recognition tools have provided a framework suited to tackle this challenge. However, these methods rely heavily on training data and may produce inaccurate results when faced with unfamiliar structures. An alternative approach is to develop an iterative algorithm that generates realistic 3D structures by comparing simulated and experimental AFM images in a fully automated manner. The final workflow enables the generation of candidate structures using different techniques, such as molecular dynamics, minima hopping, or machine learning models. A deeper understanding of the simulated structural information is achieved through feature detection algorithms and image registration. Furthermore, the simulated structures, and consequently their corresponding AFM images, are automatically evaluated for similarity to reference AFM images using image quality metrics. These approaches are tested on water clusters modeled on gold and copper surfaces using the Neural equivariant interatomic potential (NequIP).

O 35.4 Tue 13:30 P3

In situ electrochemical atomic force microscopy studies of a copper surface during lithium plating and dissolution — •Luca Kaufer[1,2], Daniel Ebeling[1], Thomas Göddenhenrich[1], André Schirmeisen[1], and Jürgen Janek[2] — [1]Institute of Applied Physics, Justus-Liebig-University, Gießen, Germany — [2]Institute of Physical Chemistry, Justus-Liebig-University, Gießen, Germany

This investigation demonstrates the utilisation of atomic force microscopy (AFM) to examine the interactions between liquid electrolytes and copper electrodes. In particular, the focus is on the deposition of lithium on copper surfaces, a crucial process in lithium batteries. Atomic force microscopy (AFM) measurements allow for precise analysis of the surface structure, morphology and dynamic changes during lithium deposition, thereby providing deeper insights into the mechanisms of electrode reactions and the quality of the electrode surface. Such measurements are of great importance to improve the efficiency and lifetime of batteries by helping to understand and control processes such as dendritic growth or non-uniform deposition.[1,2] We will include an examination of the modification of the single-crystal electrode surface, which has been achieved through the utilisation of a bespoke methodology that integrates sputtering, annealing and polishing techniques.

[1] J. Phys. Chem. C 2023, 127, 12492-12501. [2] Faraday Discuss, 2022, 233, 190.