O 109: Poster Session VIII: Poster to Mini-Symposium: Machine learning applications in surface science III

Time: Thursday 13:30–15:30 Location: P

O 109.1 Thu 13:30 P

Development of a Neural Network Potential for Metal-Organic Frameworks — •Marius Herbold and Jörg Behler — Georg-August Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany

Metal-organic frameworks (MOFs) are crystalline porous materials with many applications in chemistry and materials science, from gas separation to heterogeneous catalysis. Computer simulations of chemical processes in MOFs are severely limited by the use of classical force fields (FFs), because most FFs are unable to describe bond formation and breaking. In principle, electronic structure methods, like density-functional theory (DFT), can overcome this problem, but often the required systems are too large for routine applications of DFT. A high-dimensional neural network potential (NNP) combines the advantages of both worlds - the accuracy of first principle methods with the efficiency of simple empirical potentials. Here we present a method to construct a NNP for MOFs using size-converged fragments only.

O 109.2 Thu 13:30 P

Predicting hydration layers on surfaces using deep learning — •Yashasvi S Ranawat[1], Ygor M Jaques[1], and Adam S Foster[1,2] — [1]Department of Applied Physics, Aalto Uiversity, Finland — [2]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Surface characterisation at the nano-scale of a mineral-water interface has applications in understanding many technological and natural processes dominated by the mineral-water interactions, for example biominerelisation, corrosion etc. Atomic Force Microscopy (AFM) has the potential to characterise such surfaces. The image mechanism is governed by the complex interplay of the tip with the hydration layers over the surface and hence high resolution requirements pose a challenge. A direct link between the AFM images and water density over a surface has paved the way for theoretical molecular dynamics methods to simulate the density over a given surface, and therefore the AFM image. The computationally intense theoretical approaches have helped with the surface characterisation. However the search space, given a hydration layer image, is wide and the approach is prohibitively expensive. Here we introduce deep learning methods to swiftly and reliably predict the hydration layer over a given surface. These methods are tested on the polymorphs of calcium carbonate.

O 109.3 Thu 13:30 P

In Silico prediction of antibacterial activity of sesquiterpene lactones using density-functional theory and quantitative structure-activity relationship methods — •Fabian Puga[1], Alicja Mikolajczyk[2], Paola Ordoñez[1], and Henry Pinto[1] — [1]Yachay Tech University, Ecuador — [2]University of Gdansk, Poland

Antibiotic resistance is a problem that involves every humanity. Therefore, the development of new and effective anti-bacterial components is of vital importance. Organic molecules called Sesquiterpene Lactones (STL) have shown a wide spectrum of biological activities especially antibacterial activity against methicillin-resistant staphylococcus aureus (MRSA). Unfortunately, the experimental methods to study the effectiveness of plant-based antibiotics are expensive and time-consuming. In order to tackle these limitations in silico studies can be applied to accelerate the development of more efficient antibiotics. In this study, electronic structure calculations on 21 STL were performed to develop a model capable to predicting the antibacterial activity of new STL molecules. By using an optimal combination of density-functional tight-binding method and ab initio density-functional theory calculations, we were able to calculate the most energetically favorable conformers, their atomic structure and physical-chemical properties. Then using these values QSAR models considering experimental antibacterial activity were developed. Preliminary results suggest that models that includes the HOMO and electronic energy correlates better the antibacterial activity. These results could allow reliable prediction of antibacterial activity for new STL.

O 109.4 Thu 13:30 P

Excitonic Wave Function Reconstruction from Near-Field Spectra Using Machine Learning Techniques — •Fulu Zheng[1], Sidhartha Nayak[2], and Alexander Eisfeld[2] — [1]Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

A general problem in quantum mechanics is the reconstruction of eigenstate wave functions from measured data. In the case of molecular aggregates, information about excitonic eigenstates is vitally important to understand their optical and transport properties. Strong interactions between the transition dipoles of the molecules lead to delocalized excitonic eigenstates where an electronic excitation is coherently shared by many molecules [1]. Here we show that from spatially resolved near field spectra it is possible to reconstruct the underlying delocalized aggregate eigenfunctions [2, 3]. Although this high-dimensional nonlinear problem defies standard numerical or analytical approaches, we have found that it can be solved using a convolutional neural network. For both one-dimensional and two-dimensional aggregates the reconstruction is robust to various types of disorder and noise. The methodology can be easily applied to more complicated cases, promoting information extraction from experimental data in a wide variaty of applications. [1] A. Eisfeld, C. Marquardt, A. Paulheim, and M. Sokolowski, Phys. Rev. Lett. 119, 097402 (2017). [2] X. Gao and A. Eisfeld, J. Phys. Chem. Lett. 9, 6003 (2018). [3] F. Zheng, X. Gao and A. Eisfeld, Phys. Rev. Lett. 123, 163202 (2019).

O 109.5 Thu 13:30 P

Prediction of energetics in nucleation and non-equilibrium growth using machine learning — •Thomas Martynec[1], Sabine H. L. Klapp[1], and Stefan Kowarik[2] — [1]Technische Universität Berlin — [2]Karl-Franzens-Universität Graz

Machine learning is playing an increasing role in the discovery of novel materials and may also facilitate the search for optimum growth conditions of crystals and thin films of these materials. We demonstrate that a convolutional neural network that is trained on snapshots of surface configurations can predict the underlying lateral binding energy and diffusion barrier. Specifically, a single KMC image of the morphology is sufficient to determine the energy barriers with high accuracy for energies in the range of 100 - 550 meV. The CNN can also make correct predictions for images with noise and lower than atomic-scale resolution. We expect our machine learning method to be of use for both, fundamental studies of growth kinetics and for faster optimization of low defect materials growth.

O 109.6 Thu 13:30 P

Predicting the activity and selectivity of bimetallic metal catalysts for ethanol reforming using machine learning — •Nongnuch Artrith — Columbia Center for Computational Electrochemistry, Columbia University, New York, NY, 10027 USA

Machine learning (ML) has proven a powerful tool for accelerating the computational characterization of energy materials. There is a growing number of case studies identifying descriptors of catalytic performance using ML instead of physical intuition. ML is ideally suited for the pattern detection in large uniform data sets, but consistent experimental data sets on catalyst studies are often small. Here we demonstrate how a combination of machine learning and first-principles calculations can be used to extract knowledge from a small set of experimental data.[1] The approach is based on combining a complex ML model trained on a computational library of transition-state energies with simple linear regression models of experimental catalytic activities and selectivities. Using the combined model, we identify the key C-C bond-scission reactions involved in ethanol reforming and perform a computational screening for ethanol reforming on monolayer bimetallic catalysts with architectures TM-Pt-Pt(111) and Pt-TM-Pt(111) (TM = 3d transition metals). The model also predicts four promising catalyst compositions for future experimental studies. The approach is not limited to ethanol reforming but is of general use for the interpretation of experimental observations as well as for the computational discovery of catalytic materials.[2] [1] N. Artrith, Z. Lin, J.G. Chen, *ACS Catal.* **10** (2020) 9438–9444. [2] N. Artrith, *Matter* **3** (2020) 985–986.

O 109.7 Thu 13:30 P

Using Neural Evolution algorithm to generate disordered High Entropy Alloys structures — •Conrard Giresse TETSASSI FEUGMO[1], Kevin Ryczko[2,3], Abu Anand[4], Chandra Singh[4], and Isaac Tamblyn[1,2,3] — [1]National Research Council Canada — [2]Department of Physics , University of Ottawa — [3]Vector Institute for Artificial Intelligence, Toronto, Ontario, Canada — [4]Department of Materials Science and Engineering , University of Toronto

A new inverse design approach using pair distribution functions and atomic properties have been implemented. The generative model combines artificial neural networks (ANNs) and genetic algorithms (GAs) to build high disordered crystal structures. The method was introduced by Ryczko et. al. [J. Phys. Chem. C 124, 26117 (2020).] to optimize the doping of graphene-based three-terminal devices for valleytronic applications. Models have been optimized for multicomponent alloy systems such as High Entropy Alloys (HEAs) and structures have been compared to the Special quasi-random (SQSs). Unlike the SQSs, the average optimization time increase slow with the size of the system (ration 1.4). Moreover, the model is able to generate structures with more than 8000 atoms in a few hundred seconds. Finally selected generated structures have been using to compute properties such as the elastic constants, the bulk modulus, and the Poisson ratio, and the results are similar to the SQSs.

O 109.8 Thu 13:30 P

Automatic image evaluation of aberration-corrected HRTEM images of 2D materials. — •Christopher Leist, Haoyuan Qi, and Ute Kaiser — Central Facility for Electron Microscopy,of Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm, Germany

Aberration-corrected high-resolution transmission electron microscopy (HRTEM) allows for unambiguous elucidation of atomic structures down to sub-Angstrom scale. By determining the positions of each single atom, the distribution and local variation of bond lengths and angles can be evaluated statistically. However, conventional image analysis methods, e.g., handcrafted filter kernels, often requires heavy user supervision and tremendous time cost, posing strong limitations on the data volume for statistical analysis. The incompetence in handling big data volume also incurs the risk of user-induced selection bias, leading to overestimation of low-probability phenomena. Here, we developed a neural network of U-net architecture for automatic analysis of atomic positions in HRTEM images. A combination of networks can be applied to automatically evaluate image series, including automatic exclusion of image regions unusable for evaluation. This method results in large statistics thus reducing the impact of individual errors. The networks are trained with simulated data which reduces user bias and gives a time inexpensive way of generating the required training data. Its implementation on various 2D carbon materials is compared to one another. The distribution of bond angles in CVD graphene, determined by this method, shows excellent agreement with literature.