O 55: Poster Session IV: Poster to Mini-Symposium: Machine learning applications in surface science II

Time: Tuesday 13:30–15:30 Location: P

O 55.1 Tue 13:30 P

Gaussian Approximation Potentials for Surface Catalysis — •Sina Stocker[1,2], Gábor Csányi[3], Karsten Reuter[1,2], and Johannes T. Margraf[1,2] — [1]Technische Universität München, Germany — [2]Fritz Haber Institut der Max Planck Gesellschaft, Berlin, Germany — [3]University of Cambridge, United Kingdom

Predictive-quality first-principles based microkinetic models are increasingly used to analyze (and subsequently optimize) reaction mechanisms in heterogeneous catalysis. In full rigor, such models require the knowledge of all possible elementary reaction steps and their corresponding reaction barriers. Unfortunately, for complex catalytic processes (such as the generation of ethanol from syngas) the number of possible steps is so large that an exhaustive first-principles calculation of all barriers becomes prohibitively expensive.

To overcome this limitation, we develop a machine learned (ML) interatomic potential to model syngas conversion on Rhodium. This ML potential can be used to determine adsorption energies, geometries and reaction barriers for a large number of adsorbates at a fraction of the computational cost of the underlying first-principles method. Specifically, we use the Gaussian Approximation Potential (GAP) framework and explore iterative training and active learning to minimize the number of reference calculations. Here, the particular challenge lies in selecting representative configurations that adequately characterize the reactivity of molecules on a surface. Different training approaches will be compared.

O 55.2 Tue 13:30 P

Materials genes of heterogeneous catalysis from clean experiments and AI — •Lucas Foppa[1,2], Luca M. Ghiringhelli[1,2], Frank Rosowski[3], Robert Schloegl[1,4], Annette Trunschke[1], and Matthias Scheffler[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft — [2]Humboldt-Universität zu Berlin — [3]BASF SE — [4]Max-Planck-Institut für Chemische Energiekonversion

Heterogeneous catalysis is an example of a complex materials function, governed by an intricate interplay of several processes, e.g. the dynamic re-structuring of the catalyst material at reaction conditions and different surface chemical reactions. Modelling the full catalytic progression via first-principles statistical mechanics is impractical, if not impossible. Instead, we show here how an artificial-intelligence approach can be applied, even to an extremely small number of materials, to model catalysis and determine the key descriptive parameters (materials genes) reflecting the processes that trigger, facilitate, or hinder the catalyst performance. We start from a consistent, unparalleled experimental set of "clean data", containing nine vanadium-based oxidation catalysts which were carefully synthesized, fully characterized, and tested according to standardized protocols.[1] By applying the symbolic-regression SISSO approach,[2,3] we identify correlations between the few most relevant materials properties and their reactivity. This approach highlights the underlying physico-chemical processes, and accelerates catalyst design. [1] A. Trunschke, et al., Top. Catal. 63, 1683 (2020). [2] R. Ouyang et al., Phys. Rev. Mater. 2, 083802 (2018). [3] R. Ouyang et al., J. Phys. Mater. 2, 024002 (2019).

O 55.3 Tue 13:30 P

Artificial Intelligence controlls Nanocars across a racetrack — •Bernhard R. Ramsauer[1], Oliver T. Hofmann[1], Grant J. Simpson[2], and Leonhard Grill[2] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institute of Chemistry, University of Graz, Austria

At the world's first nanocar race at CEMES-CNRS, in France, participants had to direct a nanocar across a "racetrack" [1]. In order to control their nanocar, they had to move it using the tip of a STM, albeit without making direct contact with the nanocar.

The physics that govern the molecule's movement and rotation is complex and involves the interaction between the molecule and the tip as well as the molecule and the substrate [2]. Thus, it requires some expertise from humans to manoeuvre the nanocar and predict the outcome of a performed action.

Here, we show how an artificial intelligence (AI) based on reinforcement learning (RL) can be implemented to manipulate single molecules. The AI is implemented in the form of an off-policy RL algorithm, known as the Q-Learning. In a prime example, the AI manoeuvres the nanocar with a success rate of 89%.

Our results can be the basis for more sophisticated techniques of molecular manipulations which allow identification and relocation of single molecules at will, building the basis for future bottom-up constructions of nanotechnology.

[1] Nature Rev. Mater. 2, 17040 (2017)
[2] Nature Nanotech. 12, 604 (2017)

O 55.4 Tue 13:30 P

Configurational polaron energies using machine learning — •Viktor Birschitzky, Michele Reticcioli, and Cesare Franchini — University of Vienna, Faculty of Physics

Polarons are quasiparticles formed by the coupling of excess charge carriers with the phonon field. Polarons form preferentially at surfaces and have a wide range of effects on the chemical and physical properties of the hosting material.[1] First principles calculations of polarons conformational energies typically require large supercells and long molecular dynamics (MD) simulations, making the modeling of multipolaron system within reasonable timescales very challenging. Here, we propose a supervised machine learning scheme based on kernel-regression to solve this problem by learning single polaron energies for the prototypical oxygen-defective rutile TiO_{2-x}(110) surface, where each oxygen vacancy provides two excess electrons. To achieve accurate predictions on an ab initio MD database of polaronic energies[2] a descriptor has been developed, which embodies the interactions between polarons with defects and other localized charge carriers. Our results show that the proposed ML method is able to expand the DFT database with energetically more favorable polaron configurations – improving the convex hull construction – and that generalization at arbitrary polaron concentration and defect types is possible.

[1] C. Franchini et al., Polarons in Material, Nature Review Materials, (2021)
[2] M. Reticcioli et al., Formation and dynamics of small polarons on the rutile TiO_2 surface, Physical Review B, (2018)

O 55.5 Tue 13:30 P

Image-to-graph translation of atomic force microscopy images using graph neural networks — •Niko Oinonen[1], Fedor Urtev[1,2], Alexander Ilin[2], Juho Kannala[2], and Adam Foster[1,3,4] — [1]Department of Applied Physics, Aalto University, Finland — [2]Department of Computer Science, Aalto University, Finland — [3]Graduate School Materials Science in Mainz, Germany — [4]WPI Nano Life Science Institute, Kanazawa University, Japan

The atomic force microscope (AFM) is an important tool in nanoscale science for imaging surfaces and molecules on surfaces. State-of-the-art AFM setups operating in vacuum at low temperatures are able to resolve features on the scale of individual atoms in molecules. However, the process of interpreting the resulting AFM images in some cases can be very challenging even for highly trained experts in the field. We are working towards greater interpretability and greater automation of the processing of AFM images using machine learning methods [1]. We are currently exploring the possibility of directly predicting the atomic structure of the sample as a graph using graph neural networks (GNN) [2]. We propose a GNN model which, conditioned on an AFM image, iteratively constructs the graph of the sample molecule present in the AFM image, following similar work by Li et al. [3]. This is still a work-in-progress, but our initial results are showing promise.

[1] B. Alldritt et al. Sci. Adv. 6(9), eaay6913, 2020.
[2] P. W. Battaglia et al. arXiv:1806.01261.
[3] Y. Li et al. arXiv:1803.03324.

O 55.6 Tue 13:30 P

Inverse problem to AFM imaging with iterative correction loop — •Prokop Hapala[1], Lauri Kurki[2], Niko Oinonen[2], Fedor Urtev[2], Filippo Federici Canova[2], Juho Kannala[2], and Adam S. Foster[2] — [1]Department of Condensed Matter Theory, FZÚ AV ČR, v.v.i. — [2]Department of Applied Physics, Aalto University Espoo, Finland

In the last year we pioneered machine-learning methods for reconstruction of molecular structure from high-resolution AFM images of non-

planar organic molecules [1], which opens the way to broader application of this experimental technique for single-molecule analysis [2] e.g. in the pharmaceutical industry. Nevertheless, the robustness of one-shot scheme relying on general-purpose convolutional neural networks (CNN) seems limited as it discards physical insight. We attempt to improve our method by integrating the CNN module together with an image simulation module and interatomic force-field into an iterative feedback loop, which gradually improves the match between reference and simulated image. Such a scheme, with a machine-learned model providing educated trial-move within a global optimization algorithm, can be possibly useful also for solving other difficult inverse problems. [1] Alldritt B., et al., Sci. Adv., vol. 6, no. 9, p. Eaay6913. (2020) [2] Schuler, B., et.al. JACS, 137(31), 9870-9876. (2015)

O 55.7 Tue 13:30 P

Single-Atom Alloy Catalysts Designed by First-Principles Calculations and Artificial Intelligence — Zhong-Kang Han[1], Debalaya Sarker[1], Runhai Ouyang[2], Aliaksei Mazheika[3], Yi Gao[4], and •Sergey V. Levchenko[1] — [1]Skoltech, Moscow, RU — [2]Shanghai University, CN — [3]Technische Universitaet Berlin, DE — [4]Shanghai Advanced Research Institute, Chinese Academy of Sciences, CN

Single-atom metal alloy catalysts (SAACs) have recently become a very active new frontier in catalysis research. However, discovery of new SAACs is hindered by the lack of fast yet reliable prediction of the catalytic properties of the sheer number of candidate materials. In this work, we address this problem by applying a compressed-sensing data-analytics approach parameterized with density-functional inputs. Besides consistently predicting high efficiency of the experimentally studied SAACs, we identify more than two hundred yet unreported promising candidates. Some of these new candidates are predicted to exhibit even higher stability and efficiency than the reported ones. Our study demonstrates the importance of breaking linear relationships to avoid bias in catalysis design, as well as provides a recipe for selecting best candidate materials from hundreds of thousands of transition-metal SAACs for various applications. In addition, we demosntrate how the data-mining approach subgroup discovery can be used to obtain a qualitative understanding of complex symbolic regression models.

O 55.8 Tue 13:30 P

Automated Tip Functionalization and Image interpretation with Machine Learning in Atomic Force Microscopy — Benjamin Alldritt[1], Chen Xu[1], Prokop Hapala[2], Ondrej Krejci[1], •Fedor Urtev[1], Filippo Federici Canova[1,3], Juho Kannala[1], Peter Liljeroth[1], and Adam Foster[1,4,5] — [1]Aalto University, Espoo, Finland — [2]Czech Academy of Sciences, Prague, Czechia — [3]Nanolayers Research Computing Ltd., London, UK — [4]Graduate School Materials Science in Mainz, Germany — [5]WPI Nano Life Science Institute, Kanazawa, Japan

Atomic force microscopy (AFM) is ubiquitous nanoscale characterisation technique to measure a 3D map of surface roughness at atomic resolutions [1]. AFM data interpretation and quantitative analysis for complex mixtures of molecules and bulky 3D molecules can be difficult [2], due to the complex nature of contrast in AFM images, and need significant acceleration and automation to make AFM technique available to a wide range of laboratories and clinics. Here, we introduce a machine learning (ML) approach both for the preparation of AFM experiments and for data interpretation in AFM. For the first objective our method involves a convolutional neural network (CNN) that has been trained to analyse the quality of a CO-terminated tip. For the interpretation of AFM images, we introduce ML image descriptors characterising the molecular configuration, allowing us to predict the molecular structure directly. [1] L. Gross et al., Science, vol. 325, no. 5944, (2009). [2] O. M. Gordon and P. J. Moriarty, Mach. Learn. Sci. Technol., vol. 1, no. 2, (2020).