O 71: Mini-Symposium: Machine learning applications in surface science I

Time: Wednesday 13:30–15:30 Location: R1

Opening remarks

Invited Talk O 71.1 Wed 13:45 R1

Machine learning for novel functional materials — •Pascal Friederich — Karlsruhe Institute of Technology, Germany

During the last decade, machine learning (ML) algorithms were increasingly applied to questions in the physical sciences, e.g. to automate labs, to accelerate simulations, and to solve inverse problems such as the design of new materials. This talk will show our recent work on combining ML models with conventional tools to accelerate simulations and to obtain new scientific insight. Firstly, we show that ML enables the analysis of energy disorder in amorphous organic semiconductors which is of high relevance to understand charge transport in devices such as OLEDs.[1] Secondly, we will show how ML models can accelerate ab-initio photodynamics simulations of small molecules to unprecedented simulation times of 10 ns and more.[2] Thirdly, we will show how a combination of graph representations and basic ML regression models can provide scientific insight into organic electronics as well as quantum optical experiments in a highly intuitive and human interpretable way.[3]

[1] The influence of sorbitol doping on aggregation and electronic properties of PEDOT:PSS, P. Friederich, S. Leon, J. D. Perea Ospina, L. Roch and A. Aspuru-Guzik, MLST, 2020. [2] Nanosecond Photodynamics Simulations of a cis-transIsomerization are Enabled by Machine Learning, J. Li, P. Reiser, A. Eberhard, P. Friederich, and S. A. Lopez, DOI: 10.26434/chemrxiv.13047863.v1, 2020. [3] Scientific intuition inspired by machine learning generated hypotheses, P. Friederich, M. Krenn, I. Tamblyn, A. Aspuru-Guzik, arXiv:2010.14236, 2020.

O 71.2 Wed 14:15 R1

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).

O 71.3 Wed 14:30 R1

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.

O 71.4 Wed 14:45 R1

Active Discovery of Organic Semiconductors — •Christian Kunkel[1,2], Johannes T. Margraf[1], Ke Chen[1], Harald Oberhofer[1], and Karsten Reuter[1,2] — [1]Chair for Theoretical Chemistry and Catalysis Research Center — [2]Fritz-Haber Institut der Max-Planck-Gesellschaft

Improving charge-transport of organic semiconductors (OSCs) for electronic applications is usually tackled by empirical structural tuning of promising compounds. Howver, the versatility of organic molecules generates a rich design space whose vastness dictates efficient search strategies. We thus here present an active machine learning (AML) approach that explores this virtually unlimited design space iteratively. Judging suitability of OSC candidates by charge injection and mobility-related descriptors, the AML approach iteratively queries first-principle evaluation on well-selected molecules. We first optimize the approach in a fully characterized, but truncated molecular test space, gaining deep methodological insight about its exploratory behavior. Outperforming a conventional computational funnel, the devised algorithm can thereby successfully leverage its gradually improving knowledge and focus on promising regions of the design space. When subsequently lifting the artificial truncation, high-performance candidates are constantly found while the algorithm meanders ever more deeply through the endless OSC design space. The demonstrated high efficiency in the detection of candidate compounds with superior charge conduction properties highlights the usefulness of autonomously operating systems for a targeted OSC design.

Invited Talk O 71.5 Wed 15:00 R1

Theory-informed Machine Learning for Surface and Interface Structure Reconstruction from Experimental Data — Eric Schwenker[1,2], Chaitanya Kolluru[1,3], Marcel Chlupsa[1], Arun Mannodi Kanakkithodi[1], Richard Hennig[3], Pierre Darancet[1,2], and •Maria Chan[1,2] — [1]Argonne National Laboratory, Lemont, USA — [2]Northwestern University, Evanston, USA — [3]University of Florida, Gainsville, USA

Determining atomistic structure at surfaces and interfaces is challenging because metastable surfaces/interfaces are likely accessible under realistic conditions, rendering energy-only searches insufficient, and experimental data often give incomplete information. Therefore, neither theory nor experimental data alone is sufficient to determine these structures. In this talk, we will discuss how we use machine learning to combine experimental and theory-based data to determine surface and interface structures.