O 1: Overview Talk Johannes T. Margraf

Time: Monday 9:30–10:15 Location: HE 101

Invited Talk O 1.1 Mon 9:30 HE 101

(Surface-)science-driven machine learning — •Johannes T. Margraf — University of Bayreuth

This talk discusses research towards the establishment of a science-driven approach to machine learning (ML) for surface science and chemistry.[1] In many fields, ML is a fundamentally data-driven endeavor, meaning that specific databases and benchmark problems (i.e. big data) are at the center of methodological development. While this has certainly led to tremendous advances in recent years (e.g. in image generation and natural language processing), the full diversity and complexity of surface chemistry cannot be adequately represented by static predefined databases. We therefore aim to build accurate data-efficient models which do not require enormous reference datasets for training. This way, our methods can be applied to a wide range of problems of scientific interest and not just to those for which big data happens to be available. To this end, we explicitly incorporate chemical and physical information into the ML models[2] and integrate the data generation or selection process with the model training[3]. Several examples of this in the context of the atomistic simulation of catalytic processes on surfaces will be discussed.

[1] J.T. Margraf, Angew. Chemie, 62, e202219170 (2023). [2] K. Chen et al. Chem. Sci., 14, 4913-4922 (2023). [3] H. Jung et al. NPJ Comput. Mater., 9, 114 (2023).