

"Computing and Predicting Properties of Energy Materials"

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Energy materials such as catalysts, battery or solar cell components play a pivotal role in the urgent energy transition. Nowadays, such materials are designed through a combination of experimental and theoretical sampling, with the latter being augmented by machine learned (ML) surrogate models of material properties. The theoretical workflow, thus usually consists of a number of steps ranging from first principle calculations up to large scale sampling potentially employing ML methods.

In my presentation I will discuss two examples of our recent work in these directions. First I will outline our new approach to computing the Newns Anderson chemisorption function in service of estimating ultrafast electron transfer rates between adsorbates and surfaces. I show that using this scheme, the chemisorption function converges both with basis set size and with the size of the surface slab. As a second example, I will discuss our use of ML methods to predict elastic properties of 2D layered perovskites. Through the use of explainable ML algorithms and careful feature selection we can even extract the relationship between a perovskite's structural parameters and its elasticity. Our ML revelations thus can be used as design criteria for future materials.