

Teaching seminar

Physics inspired machine learning at the atomic scale

Speaker: Dr. Martin Uhrin (École polytechnique fédérale de Lausanne - EPFL)

Abstract

Beyond the hype, **machine learning has proven to be an extremely powerful tool to accelerate atomic scale modelling**, opening the door to studying more materials, with a larger quantity of explicit atoms, and with little loss in accuracy compared to the reference model. When coupled with training data from electronic structure calculations, this gives us the ability to accurately probe structure-property relationships at length and time scales scarcely accessible less than a decade ago, and to screen significantly more candidates when searching for materials with specific target properties.

In this talk, I will discuss some of the tools that we have developed that make it trivial to run tens of thousands of ab initio calculations to generate training data, and machine learning methods that efficiently use this data to make predictions. In particular, I will discuss how built-in symmetry awareness and other physically-motivated constraints can make our models more data-efficient and transferable, allowing them to do more with fewer data.

I will use examples from interaction potentials for solid electrolytes, to predicting experimental conductivities of ionic liquids, to accelerating electronic structure calculations themselves. Finally, I will give an outlook on some cutting edge methods that we are developing to invert the structure-property relationship, with the ultimate goal of being able to predict structures given a set of desired properties.

Date: 29/03/2023

At 10:00 a.m

Meeting Room - Building D, First Floor

Zoom: <https://us06web.zoom.us/j/81552404663?pwd=VIRwUzhzRThHR1VSTnVMVlpLcGNPUT09>

