Physics inspired machine learning at the atomic scale

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.

Short bio: Martin Uhrin holds a master's degree in computational physics from the University of Edinburgh (2009), and a PhD in computational condensed matter physics from University College London (2015). He moved to EPFL, Switzerland as a postdoctoral fellow, where he focused on high-throughput screening for accelerated materials discovery and became the lead author of the workflow engine powering AiiDA, a widely used materials informatics platform. In 2019, he moved to the Danish Technical University to develop machine learning methods for the computational design of battery materials. Most recently (2021), he returned to EPFL as a scientist hosted in the group of Nicola Marzari where he carries out independent research on physics-inspired machine learning methods and inverse design of materials and molecules.