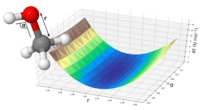
Mario Öeren gave this presentation at the ACS Fall 2018 National Meeting & Exposition held in Boston, USA.

Abstract

Non-covalent, electrostatic interactions play a significant role in many chemical applications and evaluating their strength is crucial for progress in fields such as drug design and material science. In most cases, due to the nature of these interactions, ab initio calculations are required to accurately assess their strength. However, due to their computational cost, *ab initio* methods are not suitable for screening datasets with large numbers of structures.

We will present a method based on Gaussian approximation potentials (GAPs), which are interatomic potentials trained on ab initio data using machine learning. While GAPs could be applied to any interaction, we chose hydrogen bonds as an example for this presentation. We will describe the workflow to prepare the GAP training set, how to generate GAPs from density functional theory data using the software QUIP and how to calculate the hydrogen bond energies for a structure from the resulting model. Such an approach allows us to achieve results close to *ab initio* accuracy, but with significantly lower computational costs. The results are validated against the *ab initio* calculations and quantum theory of atoms in molecules results.

While GAPs have been mostly used for molecular dynamics simulations of bulk crystals, they can be applied to a variety of problems which require the exploration of a complex potential energy surface (PES); for example, the hydrogen bond energy model described herein can be used in scoring functions for protein-ligand interactions.



You can download this presentation as a PDF .