Constructing, Validating and Using Machine-Learned Potential Energy Surfaces

Markus Meuwly

University of Basel

The potential energy surface (PES) is arguably the most comprehensive description of the energetics of a chemical system. As this object is high-dimensional it is notoriously difficult to parametrize. On the other hand, using brute-force electronic structure techniques is only applicable for the smallest systems, in particular if chemical

reactions are of interest. In this contribution I will discuss the status for constructing, validating and using machine learning for molecular PESs to calculate spectroscopic observables and reaction rates. With the advent of ever more powerful computers the energetics of increasingly large molecules can be described. However, there are

also interesting questions that can be asked for superficially "simple" systems and machine learning-based techniques provide new insights, if combined with experiments.