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Making machine learning interatomic potentials accurate, efficient, and reliable

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Molecular modeling relies, typically, on two classes of models of interatomic interaction, namely (1) quantum-mechanical (QM) models that are very accurate but very computationally expensive, and (2) empirical interatomic potentials that typically offer only a qualitative accuracy but are very computationally efficient. There have been a number of successful applications of machine learning to constructing interatomic potentials that combine the efficiency of empirical potentials and the accuracy of QM models [Behler and Parrinello, PRL (2007), Bartok et al., PRL (2010)]. A harder challenge, however, is to make such potentials reliable - it requires fitting hundreds to thousands of parameters and making sure that they produce reasonable results in the entire region of interest in the phase space (which could be given only implicitly, e.g., all configurations with energy below a certain threshold).

In my talk I will give a mathematician's perspective on the field of machine learning interatomic potentials. I will then present an example of accurate and computationally efficient machine learning interatomic potentials, and finally I will show how active learning can ensure reliability of such potentials. I will illustrate applications of such potentials in molecular dynamics and crystal structure prediction.