Machine Learning and Quantum Mechanics

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Machine learning provides data-driven algorithms for analysis and prediction of experimental and computational observations. It is suited for data-rich settings where many observations are available, but physical or chemical models either do not exist or are too costly to evaluate. In this talk, I will focus on machine learning for results of numerical simulations in quantum physics and chemistry, a topic that has attracted increasing interest over the last years. [1] Examples include accurate energy predictions for molecules and materials for accelerated ab initio molecular dynamics or crystal structure prediction; machine-learned density functionals for (orbital-free) density functional theory, and learning dividing surfaces in the context of transition state theory. I will present key concepts from machine learning, highlight recent examples of its successful application in modeling phenomena at the atomic scale, and discuss aspects such as general representations of atomistic systems and the reliability of predictions.

[1] Matthias Rupp, O. Anatole von Lilienfeld, Kieron Burke: Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry, Journal of Chemical Physics 148(24): 241401, 2018. DOI 10.1063/1.5043213