Predicting material properties with the help of machine learning

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A central goal of computational chemistry is to predict material properties using first-principles methods based on the fundamental laws of quantum mechanics. However, the high computational costs of these methods typically prevent rigorous predictions of macroscopic quantities at finite temperatures.

In this talk, I will demonstrate how to enable such predictions by combining advanced statistical mechanics with machine learning interatomic potentials. I will show toolkits that facilitate the application of machine learning to chemical systems. I will show example applications on computing phase diagrams of matter under high pressures, chemical potentials of liquid mixtures, adsorption isotherms of carbon dioxide in metal-organic frameworks (MOFs), and solubilities of molecular crystals.