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Predicting material properties with the help of machine learning

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Abstract:

A central goal of computational physics and 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, such as chemical potential, heat capacityand thermal conductivity.

In this talk, I will first discuss how to enable such predictions by combining advanced statistical mechanics with data-driven machine learning interatomic potentials. As an example, we computed the phase diagram of water from density functional theory at the hybrid level, accounting for thermal fluctuations, proton disordering and nuclear quantum effects. As applications in high-pressure physics, we simulated the high-pressure hydrogen system and found supercritical behaviour above the melting line, and mapped the phase diagram of superionic water. Besides thermodynamic properties, I will talk about how to compute the heat conductivities of liquids just from equilibrium molecular dynamics trajectories.

During the second part of the talk, I will rationalize why machine learning potentials work at all, and in particular, the locality argument. I'll show that a machine learning potential trained on liquid water alone can predict the properties of diverse ice phases, because all the local environments characterising the ice phases are found in liquid water.