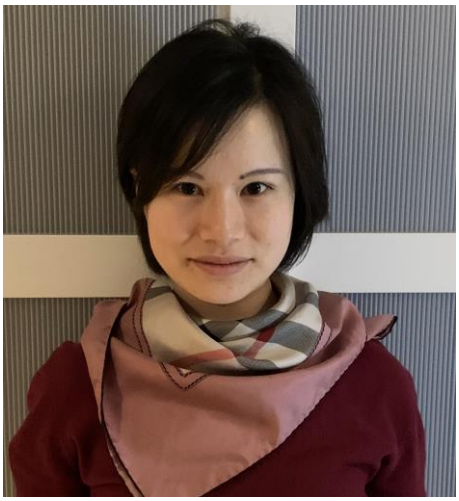
UCLA College | Physical Sciences Chemistry & Biochemistry

THEORETICAL PHYSICAL CHEMISTRY SEMINAR



Dr. Bingqing Cheng

Research Fellow

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Friday, Jan. 22, 2021

12:00 PM PST

Zoom

Predicting material properties with the help of machine learning

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 capacity and 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, for the omnipresent and technologically essential system of water, a first-principles thermodynamic description not only leads to excellent agreement with experiments, but also reveals the crucial role of nuclear quantum fluctuations in modulating the thermodynamic stabilities of different phases of water. As another example, we simulated the high-pressure hydrogen system with converged system size and simulation length, and found, contrary to established beliefs, supercritical behaviour of liquid hydrogen above the melting line. 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.

Please contact nikke@chem.ucla.edu for additional information.