Chemical Engineering

Fall 2023 Seminar Series

Unlocking Realism in Molecular Simulations of Aqueous Systems with Data-Driven Many-Body Potentials

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66-110
3:00-4:00pm
2:45pm Reception

Molecular simulations are instrumental in gaining detailed insights into the properties of complex systems, from biomolecules to materials. At the heart of these simulations is the potential energy function (PEF), which maps out the multi-dimensional energy landscape of the system in question. The accuracy of the PEF is crucial, as it dictates the realism and, consequently, the predictive power of any simulation. In principle, correlated wave function (WF) methods, such as coupled cluster with single, double, and perturbative triple excitations, i.e., CCSD(T), can provide an accurate description of molecular interactions from isolated molecules to condensed-phase systems. However, their computational cost limits their applications to systems with only a few tens of atoms. Conversely, conventional force fields (FFs) grounded in empirical parameterizations exhibit limited accuracy and lack predictive power, approximating molecular interactions with simplistic models based on harmonic potentials and classical Coulomb interactions. In this presentation, I will describe our data-driven many-body energy (MB-nrg) formalism, which, exploiting the locality of quantum mechanics, bridges the gap between WF methods and FFs, paving the way for realistic computer simulations from the gas to the condensed phase. MB-nrg seamlessly integrates data-driven machine-learned representations of individual many-body interactions with physics-based many-body models, all derived from CCSD(T) data. I will illustrate the accuracy, transferability, and predictive power of our MB-nrg potentials for various aqueous systems across different thermodynamic states and in different environments.

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