

Quantum Simulations of Condensed Matter at Coupled Cluster Accuracy

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Traditionally, molecular simulations have been based on parameterized interaction models. Such Force Field Molecular Dynamics (FFMD) follows a hierarchy from simple pair potentials to sophisticated many-body expansions. Later, Ab Initio Molecular Dynamics (AIMD) such as Car-Parrinello simulations came on stage where the interactions are computed on-the-fly from concurrent density functional theory calculations. I will speak about our recent advances that add a new direction: Coupled Cluster Molecular Dynamics (CCMD). The key idea is to incorporate "quantum-chemical accuracy", namely the CCSD(T) coupled cluster method, in efficient simulations that also include nuclear quantum effects via path integrals. This has been achieved by intertwining a quasi-linear scaling CCSD(T) electron correlation method developed for static calculations of finite gas phase systems with machine learning potentials to enable dynamical simulations of condensed phase systems at finite temperatures. The CCMD approach breaks new ground which I will showcase with applications to isotope effects on key structural and dynamical properties of liquid water, thereby resolving ongoing controversies.