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Many-Body Molecular Dynamics: Chemical and Spectroscopic Accuracy from the Gas to the Condensed Phase

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Two of the most challenging problems at the intersection of electronic structure theory and molecular dynamics simulations are the accurate representation of intermolecular interactions and the development of reduced-scaling algorithms applicable to large systems. To some extent, these two problems are antithetical, since the accurate calculation of non-covalent interactions typically requires correlated, post-Hartree-Fock methods whose computational scaling with respect to system size precludes the application of these methods to large systems. Our many-body molecular dynamics (MB-MD) methodology for aqueous systems that overcomes these limitations and enables computer simulations from the gas to the condensed phase, with chemical and spectroscopic accuracy. MB-MD is a unified molecular dynamics framework that combines many-body representations for potential energy, dipole moment, and polarizability surfaces, derived entirely from correlated electronic structure data using supervised learning techniques, with quantum dynamics methods that explicitly account for nuclear quantum effects. The accuracy of the MB-MD methodology is assessed through the analysis of several properties of aqueous systems across different phases with a particular focus on nuclear quantum effects and vibrational spectra.