MB-pol Data-Driven Many-Body Potential: Realistic Simulations of Water Across All Phases

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Despite almost 50 years having passed since the first computer simulations of liquid water, and with numerous computational studies reported since then, achieving a realistic molecular-level picture of water's properties across all phases has remained elusive. In the past decade, the development of efficient algorithms for correlated electronic structure calculations of small molecular complexes, accompanied by tremendous progress in machine-learned representations of multidimensional potential energy surfaces, has opened the doors to the design of highly accurate molecular models. These models are built upon a rigorous representation of the many-body expansion (MBE) of the interaction energies. Here, we provide a comprehensive overview of the performance of the MB-pol data-driven many-body potential that enables realistic simulations of water, ranging from gas-phase clusters to liquid water and ice. Through a systematic analysis of energetic, structural, thermodynamic, and dynamical properties, as well as vibrational spectra, we demonstrate that MB-pol achieves unprecedented accuracy across all phases of water. This is due to its unique ability to quantitatively represent each individual term of the MBE, providing a physically correct description of both short-range and long-range many-body contributions. Comparisons with experimental data probing different regions of the water phase diagram demonstrate that MB-pol effectively represents the long-sought-after "universal model" of water, capable of correctly predicting the molecular properties of water under various conditions and in different environments.