Uncertainty Quantification of Atomistic Partial Charges in Liquid Phase Molecular Dynamics

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Abstract: Molecular dynamics (MD) simulation is an important tool for the in silico characterization of a large variety of materials properties and phenomena at the nanoscale. However, MD simulations involve many input parameters that are rarely reported with an associated uncertainty. For example, accurate MD simulations of soft matter rely on careful parametrization of atomistic partial charges. In this work, we look to quantify the uncertainty associated with solvent properties (responses, υ) as predicted from atomistic MD simulations as a result of inherently uncertain partial charges (parameters, q). Liquid-phase systems of the common solvent acetonitrile (ACN) are chosen as test cases. We report the results of 500 simulations with partial charges naively sampled from distributions assumed based on literature values. Additionally, we have performed both local and global sensitivity analysis utilizing a Morris screening procedure. Our results highlight the importance of careful choice of partial charges for accurate prediction of materials properties, as well as the necessity to investigate multiple macroscopic properties when validating a given set of MD parameters.

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