

Exploiting Timescale Separation between Energy Contributions to Accelerate Molecular Dynamics in the Effective Fragment Potential

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Capturing the complexity of intermolecular interactions in condensed phases is a challenging task that has relied on both classical and quantum descriptions. However, many classical force fields are not adequate for the study of condensed-phase and biological systems because they overlook non-pairwise-additive effects; and quantum methods are limited to molecular systems of small dimensions. Thus, theoretical methods that can account for various types of intermolecular interactions occurring in condensed phases are required. The effective fragment potential (EFP) method is a systematic approach to describing such interactions in an efficient yet rigorous way. EFP is a quantum mechanical based potential that can be thought of as a non-empirical polarizable force field. In this contribution, we analyze the time evolution of electrostatic, polarization, dispersion, and exchange-repulsion energies in small clusters of water, simulated under the microcanonical ensemble. Based on these results, we propose an approach to accelerate EFP molecular dynamics simulations by exploiting the inherent timescale separation between each of those energy contributions.