A Toolkit to Fit Nonbonded Parameters from and for Condensed Phase Simulations

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The quality of atomistic simulations depends decisively on the accuracy of the underlying energy function (force field). Of particular importance for condensed-phase properties are nonbonded interactions, including the electrostatic and Lennard-Jones terms. Permanent atomic multipoles (MTPs) are an extension to common point-charge (PC) representations in atomistic simulations. MTPs are commonly determined from and fitted to an ab initio Electrostatic Potential (ESP), and Lennard-Jones (LJ) parameters are obtained from comparison of experimental and computed observables using molecular dynamics (MD) simulations. For this a set of thermodynamic observables such as density, heat of vaporization, and hydration free energy is chosen, to which the parametrization is fitted. The current work introduces a comprehensive computing environment (Fitting Wizard (FW)) for optimizing nonbonded interactions for atomistic force fields of different qualities. The FW supports fitting of standard PC-based force fields and more physically motivated multipolar (MTP) force fields. A broader study including 20 molecules ranging from N-methyl-acetamide and benzene to halogenated benzenes, phenols, anilines, and pyridines yields a root mean squared deviation for hydration free energies of 0.36 kcal/mol over a range of 8 kcal/mol. It is furthermore shown that PC-based force fields are not necessarily inferior compared to MTP parametrizations depending on the molecule considered.

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