Development and application of advanced potentials and QM/MM methods

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Computational simulations to investigate condensed and biological systems have become commonplace. In most cases, the potentials involved make substantial approximations, especially for the non–bonded interactions. We have contributed to the development of the multipolar/polarizable AMOEBA force field and developed a novel force field, called the Gaussian Electrostatic Model (GEM), that employs explicit molecular charge densities. We will present results for the development and application of AMOEBA for water and imidazolium-based ionic liquids using a parametrization paradigm based on Quantum Mechanics, as well as results for an initial water model termed GEM*. We have also developed a new QM/MM package called LICHEM that enables the use of these advanced potentials providing for a significantly more accurate description of the classical environment. This package also includes a new method based on the minimum image convention and a novel smoothing function (QM/MM–LREC) that provides a straightforward way to include long–range electrostatic effects in QM/MM. We will present the latest capabilities of LICHEM including implementation of chain–of–replica methods for path simulations, and the extension of QM/MM–LREC for multipolar/polarizable QM/MM simulations.