An Efficient Protocol to Derive Reliable Additive Nonbonding Force Fields

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Abstract

When atomistic force-field simulations involving new porous materials or new ligands are carried out, carefully tuned nonbonding force-field parameters are not readily available [1,2]. To avoid the expensive and daunting refinement of such parameters, it is common to take them from relatively old models, such as UFF [3] or MM3 [4]. Recently, it was shown how one can refine such parameters using SAPT computations on a set of model dimers [5]. However, SAPT computations are still expensive and not simply applicable to large systems that are commonly encountered in molecular dynamics simulations. In this paper, we propose an efficient protocol to derive reliable nonbonding force fields from DFT computations on isolated monomers.

The first step always consists of a partitioning of the electron density with a recent variant of Stockholder or Hirshfeld partitioning [6,7]. For this work, we applied the newly developed Minimal Basis Iterative Stockholder method. As a side-effect of the partitioning, this method also yields a model of the valence electron density in terms of atom-centered Slater functions. The Slater functions and atomic charges are used to model the electrostatic interactions, including the penetration effect. Also a Buckingham potential (for the Pauli and dispersion interactions) is extracted from the same information. Our methodology reproduces CCSD(T)/CBS reference data on the S66 set with an RMSE below 3 kJ/mol.

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