Title: Complete Non-Bonding Force Field Derived From Monomer Electron Densities

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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. To avoid the expensive and daunting refinement of such parameters, it is common to take them from relatively old models, such as UFF or MM3. Recently, it was shown how one can refine such parameters using SAPT computations on a set of model dimers. However, SAPT computations are still expensive and not simply applicable to large molecular systems. In this paper, we propose an efficient protocol to derive reliable nonbonding force fields from DFT computations on isolated monomers. The first step consists of an AIM analysis with the minimal-basis iterative stockholder method, which also yields a model of the valence electron density in terms of atom-centered Slater functions. In the second step, a van der Waals potential (for the Pauli, dispersion and induction interactions) is extracted from the partitioning data. The Slater functions and atomic charges are used directly to model the electrostatic interactions, including the penetration effect. The proposed method was tested on the S66x8 database of intermolecular interaction energies. Our force field shows an RMSD of less than 1kcal/mol when compared to CCSD(T)/CBS reference energies.