A Journey towards the Heaven of Chemical Fidelity of Intermolecular Force Fields

Alongside the evolution of density functional theory into a new era led by the dispersion-corrected hybrid density functional theory approaches, formulation of a new generation of intermolecular potentials has also taken the center-stage. The Lennard-Jones potential, one of the popular intermolecular pair potentials for performing large-scale simulations fails to capture some of the intricate features of molecular interactions. Woven around the central theme of anisotropy in the nature of intermolecular interactions, I shall describe our quest for chemical fidelity of empirical potential formulations that include (i) incorporation of the anisotropic nature of exchange-repulsion and dispersion contributions, (ii) multipolar description of the dispersion terms, (iii) damping functions to provide an accurate description of the asymptotes, and (iv) transferability of intermolecular interaction terms. I shall illustrate the nuances of intermolecular force field development in the context of modeling the non-covalent interactions governing the binding of atoms and molecules with carbon and boron nitride nanostructures, as well as interlayer interactions in layered nanostructures. Finally, I shall exemplify the hierarchy of empirical potentials by depicting them on the various rungs of the Jacob’s ladder equivalent of density functional theory for the intermolecular force fields.

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