CHARGE DISTRIBUTION DEFORMATION IN VAN DER WAALS COMPLEXES INVOLVING ATOMS WITH LOW IONIZATION POTENTIALS

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The semi-empirical method of Hartree-Fock plus damped Dispersion (HFD) has been shown to give accurate potential energy surfaces for noble gas dimers. The two parts to the potentials are the Hartree-Fock energy and the intermolecular correlation energy (obtained from a damped multipolar expansion). For the spin-polarized (triplet) alkali dimers this over- estimates the interaction energy. As the ionization energy decreases, the error increases.

We have modified the HFD method to include the effects of charge deformation, which increases with the polarizability of the atoms. As the atoms approach, the electron clouds repel each other. Because the atoms have a large polarizability, the charge distributions no longer remain centered on their respective nuclei but are pushed away from the other atom. We incorporate this increased distance between the electron clouds into the multipole expansion, resulting in a decreased correlation energy.

Results will be shown for Li, Na, and Mg oligomers.