Dispersion interactions from intermolecular perturbation theory and random phase approximations

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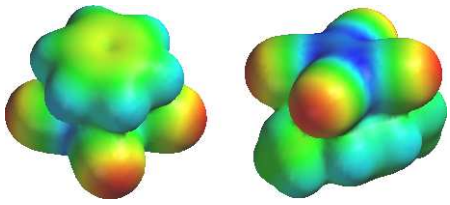
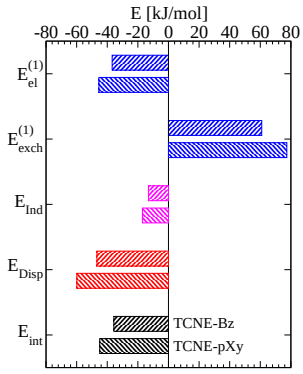
After an overview over the foundations of the DFT-SAPT approach which couples symmetry-adapted intermolecular perturbation theory (SAPT) with a description of the monomers through density functional theory (DFT) a few examples elucidating the role of dispersion interactions will be presented[1, 2, 3]. A modification of the approach avoiding the single-exchange approximation extends its application range to small intermolecular distances[4].





Furthermore, the ability of various expressions linked to the random phase approximation (RPA) to account for dispersion forces within DFT will be discussed[5, 6, 7].

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