BSSE correction for N-body clusters within an approximate treatment of the Site-Site Function Counterpoise Scheme

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The accurate quantum chemical evaluation of intermolecular interactions is a highly demanding task, especially for weak interactions and for large interacting systems. The supermolecular approach suffers from the so-called basis set superposition error (BSSE), which arises due to the more significant incompleteness of the basis sets used for the calculation on the monomers than for the one of the N-mers. The most widely used prescription to correct for BSSE effects is the counterpoise (CP) correction of Boys and Bernardi. In the framework of the counterpoise method Wells and Wilson proposed the so called site-site function CP (SSFC) approach, which corrects for BSSE in aggregates with various subunits.

In this work we present a simplification of the SSFC scheme, which aims at a reduction of the size of the one-particle basis set. The accuracy of the proposed approach is investigated for the water cluster series: $(H_20)_n$ with n=10,12,14,16,18 and 20 at SCF, MP2, CCSD and CCSD(T) level of theory. Additionally we present MP2, CCSD and CCSD(T) correlation energies of the water series (up to n=18) obtained with the incremental scheme using the domain-specific basis set approach.

Literature:

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