New Energy Partitioning Scheme Based on the Self-Consistent Configuration Method for Subsystems

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Abstract

A new scheme for decomposition of interaction energy is proposed. The method is an extension of *self-consistent charge and configuration method for subsystems* (SCCCMS). In SCCCMS atomic charges are used to model mutual interactions between reactants [1-3]. In the proposed formalism interactions are treated rigorously within polarization approximation and a correction that goes beyond this approximation is also proposed. Total interaction energy is partitioned into several components, namely deformation (DEF), electrostatic (ES), polarization (P), charge transfer (CT) and exchange (EX) energies. The CT energy is derived from the energy surface spanned in the population space. Such derivation provides some additional information about molecular system and its charge distribution, e.g. the amount of charge transferred to the other reactant.

The proposed scheme is tested on several illustrative examples and applied to investigate interactions in crown ether complexes. The influence of basis set is examined and the results are compared with those of *Kitaura-Morokuma* and *reduced variational space* analyses.

References

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