

Charge Transfer Energy in Noncovalent Complexes and Constrained Dipole Moment Density Functional Theory

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The charge transfer energy associated with a non-covalent interaction is a very important quantity to obtain insights about this type of interactions. In general, the approach to this problem has been based on the definition of a charge transfer free state that, in the past, it has been determined through localized molecular orbitals or through the use of charge constrained density functional theory. Although the later has proven to be a very reliable approach because the results are quite independent of the basis set and of the density functional used in the calculation, the charge transfer free state is determined for a specific partition of the space obtained from a population analysis, making the results to depend on the choice of the later. Thus, in this talk we will present a new approach to determine the charge transfer free state by imposing constraints on the dipole moment that do not require from a specific partition of the space, in contrast with the constrained approach based on charges. We will show that this procedure leads to what seem to be more reliable results for the charge transfer energy in non-covalent complexes.

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