The Same Number Of Optimized Parameters (SNOOP) scheme for determining intermolecular interaction energies

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The determination of intermolecular interaction energies remains one of the central tasks of computational chemistry with applications in diverse fields such as molecular biology and material sciences. We propose the *Same Number Of Optimized Parameters* (SNOOP) scheme as an alternative to the counterpoise method for treating basis set superposition errors in calculations of intermolecular interaction energies with focus on the coupled-cluster hierarchy of electronic structure models. The key point of the SNOOP scheme is to enforce that the number of optimized wave function parameters for the noninteracting system is the same as for the interacting system to ensure a delicate balance between the quality of the monomer and dimer finite basis set calculations. Numerical MP2 and CCSD(T) results for small test systems, such as the water and benzene dimers, show that the SNOOP scheme in general outperforms the uncorrected and counterpoise approaches. Furthermore, SNOOP interaction energies calculated using a finite basis are of similar quality as interaction energies obtained by extrapolating counterpoise-corrected interaction energies obtained at a similar computational cost.

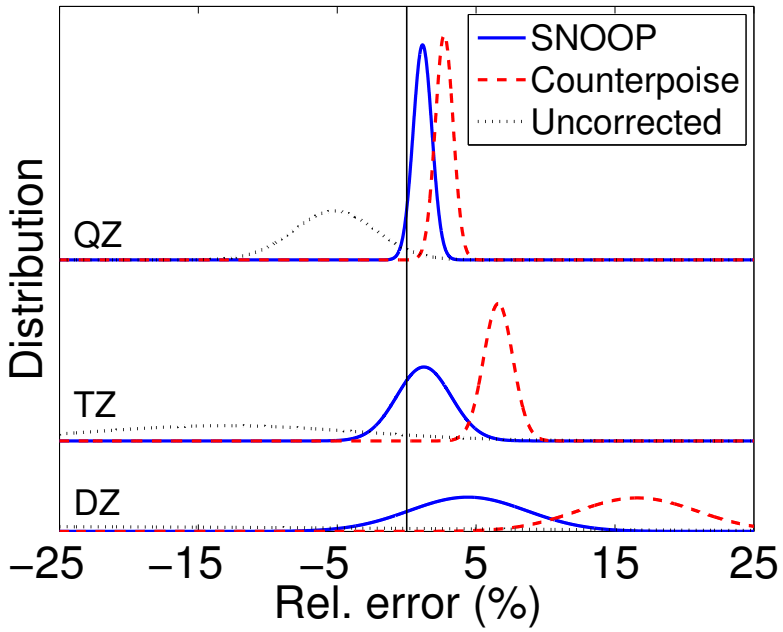

Figure 1: Normal distributions of MP2 errors for uncorrected, counterpoise-corrected, and SNOOP interaction energies for the aug-cc-pVDZ (bottom), aug-cc-pVTZ (middle), and aug-cc-pVQZ (top) basis sets.