The incremental scheme for CCSD(T) and CCSD(T)(F12)

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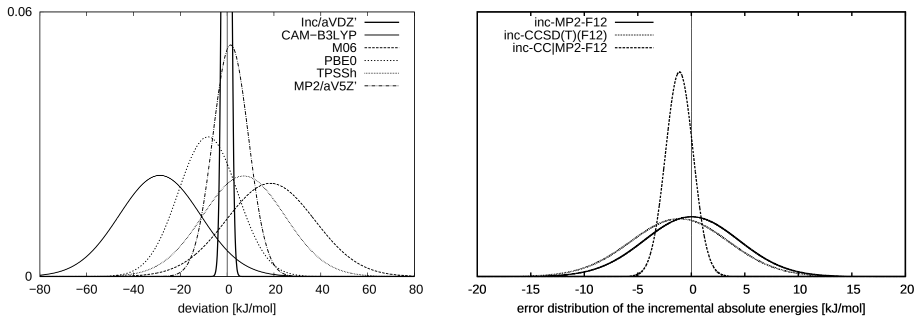
Today DFT based methods provide an optimal balance between accuracy and computational effort. However, for a highly accurate description the accuracy of DFT methods is not sufficient. If a proper basis set is applied, one can yield the required accuracy with wave function based methods such as CCSD(T). In combination with an extrapolation to the basis set limit or explicit correlation the CCSD(T) energies have benchmark quality. The price one has to pay for the high accuracy is a huge computational effort and the standard CCSD(T) computations become quickly infeasible. Therefore it is necessary to introduce approximations to the CCSD(T) model, without significant loss of accuracy. We apply the incremental scheme [1] to exploit the local character of the electron correlation and obtain the CCSD(T) energy at reduced computational effort [2]. It was recently shown, that the errors due to the local approximations can be reduced with MP2-theory [3]. Finally we demonstrate the applicability of our approach for a CCSD(T)/aV5Z' calculation on $\mathrm{Al(H_2O)_{25}^{3+}}$ (76 atoms and 6106 AOs [4]).



a b

a: Error distributions of different state of the art quantum chemical methods with respect to a CCSD(T)/aV5Z reference for the binding energies of 45 metal solvent complexes [4]. b: Error in the absolute energies for the third order inc-CCSD(T)(F12)|MP2/cc-pVDZ-F12 method using 27 molecules [5].

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