DFT-SAPT based on *ab initio* potentials

A. Daniel Boese and Georg Jansen

Department of Organic Chemistry, University of Duisburg-Essen

D-45137 Essen, Germany

Symmetry Adapted Perturbation Theory (SAPT) is one of the main tools for calculating intermolecular interactions. The scaling of SAPT is very dependent on the fragment method used; whereas SAPT based on post-Hartree-Fock methods has a scaling of at least N^7 (with N the number of electrons), DFT-SAPT only scales as N^5. With the use of DFT, however, some not necessarily warranted empiricism enters the method. For this, the exchange-correlation potential is calculated via a functional of choice, and enters as such into the framework of SAPT. It is well known, however, that *ab initio* exchange correlation potentials can be calculated via the Zhao-Morrison-Parr (ZMP) and related methods. There are technical difficulties with this method, since the underlying fragments will have to be calculated with the DFT grid of the ghost calculation. These have been resolved using a versatile, elaborate 3D moving-weighted least-squares algorithm. Finally, we are able to report some first results using BD(ZMP)-SAPT for some model systems.