Efficient calculations of accurate interaction energies for nano-scale systems

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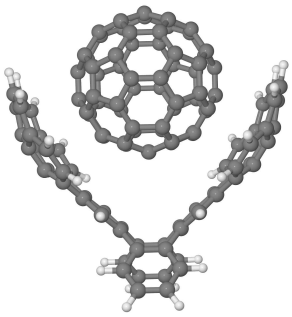
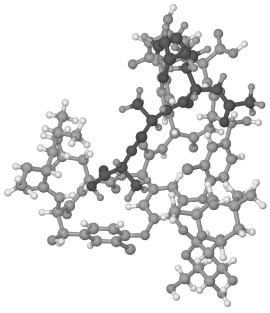
Calculations of interaction energies for nano-scale systems containing a few hundred atoms are currently beyond the reach of wave-function based *ab initio* methods. A commonly applied remedy for this problem is to use "density functional theory plus dispersion" (DFT-D) approaches but these methods are inherently limited due to the approximate character of the atom-atom type dispersion. Symmetry-adapted perturbation theory based on the DFT description of the monomers [SAPT(DFT)] provides high-quality interaction energies. Dispersion energies computed from the coupled Kohn-Sham dynamic density-density response functions used within the SAPT(DFT) method are very accurate and can solve the above-mentioned problem. We present a new highly-efficient implementation of the algorithm [1] that removes several computational barriers present in available implementations and enables calculations of dispersion energies for systems as large as 230 atoms and 5000 basis functions with modest computational resources. We applied this new code to two systems: the buckycatcher ($C_{60}H_{24}$) complex with fullerene (C_{60}) and the vancomycin ($C_{66}H_{75}Cl_2N_9O_{24}$) complex with di-acetyl-Lys-D-Ala-D-Ala ($C_{16}H_{28}N_4O_6$) bacterial wall precursor, both calculations performed with triple-zeta quality basis sets. Our implementation makes it possible to finally use *ab initio* computed dispersion energies in DFT-D schemes. We made also improvements in other interaction energy components, including the most time consuming exchange-dispersion term opening the full SAPT(DFT) capabilities to the nano-scale systems.



buckycatcher–fullerene



vancomycin–peptide

[1] Podeszwa, R., Cencek, W., Szalewicz, K., *J. Chem. Theory Comput.*, **8**, 1963, 2012.