Comparisons on several methods of weak interactions

By I_was_a_baby

Abstract: I do some computations for comparing the several methods about describing weak interactions. It can be seen that, if the method of CCSD(T) can be treated as Golden standard, the ability of various methods to describe weak interactions is uneven, where the double hybrid functional, B2PLYP, is the most excellent. The M06-2X, a suitable functional even without DFT-D3 correction, however, make me sad that deviation to the Golden standard is beyond my imagination.

Computational details:
Molecule: $(HF)_3$
Geometry: M06-2X-D3/6-311G* with (99, 590) grid point
Single point: CCSD(T), M06-2X with (99, 590) grid point, MP2, SCS-MP2, MP3, MP2.5, and B2PLYP with the basis set of aug-cc-pVTZ

Results and discussions: The interaction energies between each HF molecules and relative energies to Golden standard, CCSD(T). The unit of energy is Kcal/mol.

Kcal/mol	CCSD(T)	M06-2X-D3	MP2	SCS-MP2	MP3	MP2.5	B2PLYP
E_int	5.02	5.68	4.88	4.43	4.85	4.86	4.95
E_relative	0.00	0.67	-0.14	-0.59	-0.16	-0.15	-0.06

What should I say? B2PLYP is an ancient double hybrid functional, but the result is out of my expectation. Let me take a bold guess, it will be better if the DFT-D3 can be used when we have a computations via B2PLYP.

For M06-2X, I don’t want to say anything anymore.

More? SCS-MP2 is faster on the computations than MP2, however, the accuracy is worse. MP2.5, called a suitable method for hydrogen bonds, is amazing that is surpassed than MP3. Nevertheless, all of them will be recommended, because these are no benefits at the same costs of computations compared with B2PLYP.