The Effect of Base Density Functional on the Performance of the Many-Body Dispersion Correction

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The use of post-self-consistent dispersion corrections is now standard practice when applying density-functional theory to systems where non-covalent interactions are important. To this end, there exist a few popular dispersion corrections in the literature, including the Tkatchenko-Scheffler (TS) and subsequent many-body dispersion (MBD) methods. For both TS and MBD, it is common to pair these methods with the PBE and PBE0 functionals. However, we have previously shown that improved performance can be obtained using functionals based on B86b, rather than PBE, exchange for the particular case of the exchange-hole dipole moment (XDM) dispersion correction [1]. Here we opine on how the choice of base functional affects the accuracy obtainable with TS and MBD for a suite of benchmark test sets. Statistics comparing the use of PBE and B86bPBE, as well as the PBE0 and B86bPBE-25X hybrid functionals, are reported.

[1] AJA Price, KR Bryenton, ER Johnson, Requirements for an accurate dispersion-corrected density functional. *J. Chem. Phys.* **154**, 230902 (2021).