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Noncovalent interactions in DFT without empirical potentials

Weak non-covalent interactions remain a challenging area for most Density Functional Approximations, and the inclusion of empirical potentials has proven to be an effective way to address their limitations. Recently, we have proposed an alternative approach based on the coupling of a non-empirical double hybrid functional, PBE-QIDH, with a specifically developed basis set named DH-SVPD. This basis set was constructed using a dedicated procedure that does not involve any fitting to external reference data [1]. The results obtained across a wide range of benchmark datasets [2-4] demonstrate that our protocol, PBE-QIDH/DH-SVPD, provides interaction energies that are at least as accurate as those obtained with comparable functionals combined with large triple- or quadruple-ζ basis sets and dispersion corrections. The rationale behind this performance can be attributed to improvements in the description of electronic molecular properties induced by our protocol.

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