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Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals LEEOR KRONIK, Weizmann Institute of Science, Israel, NOA MAROM, University of Texas at Austin, Austin, TX, ALEXANDRE TKATCHENKO, MARIANA ROSSI, VIVEKANAND V. GOBRE, Fritz-Haber-Institut, Germany, ODED HOD, Tel Aviv University, Israel, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, Germany — We present a comparative assessment of the accuracy of two approaches for evaluating dispersion interactions: inter-atomic pair-wise corrections and semi-empirical meta-generalized-gradient-approximation (meta-GGA) based functionals. This is achieved by employing conventional (semi-)local and (screened-)hybrid functionals, as well as semi-empirical hybrid and non-hybrid meta-GGA functionals of the M06 family, with and without pair-wise Tkatchenko-Scheffler corrections. All those are tested against the benchmark S22 set of weakly bound systems, a representative larger molecular complex, and a representative dispersively bound solid. We also compare our results with those obtained from Grimme's pair-wise correction (DFT-D3) and Langreth-Lundqvist functionals (vdW-DF1/2). We find that the semi-empirical kinetic-energy-density dependence of the M06 functionals mimics some of the non-local correlation needed to describe dispersion. However, long-range contributions are still missing. Pair-wise corrections provide for a satisfactory level of accuracy irrespectively of the underlying functional.

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