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Exchange-correlation functionals for non-covalent interactions

ALBERTO OTERO DE LA ROZA, ERIN JOHNSON, University of California, Merced, GINO DILABIO, National Institute for Nanotechnology, Edmonton — Dispersion, an essential component of non-covalent interactions, is a long-range correlation effect. The non-covalent binding energies calculated using common density functionals vary widely from overly repulsive to spuriously attractive, and there is no a priori clear recipe for choosing any particular functional. Dispersion in DFT is, as a consequence, as much about calculating the dispersion energy accurately as it is about using a base density functional that gives the correct repulsive wall for all interaction types. In the context of pairwise dispersion corrections, this has been addressed by (over)using the dispersion damping function. In this talk, I present a study on the adequacy of different exchange and correlation approximations for non-covalent interactions as well as an analysis of the energy error scaling with system size. I will show, for instance, that cooperative effects in densely hydrogen-bonded systems (e.g. ice) are consistently overestimated by all density-functional approximations. Our results are relevant regarding the accuracy of molecular dynamics simulations, molecular crystal phase transitions, the scaling of non-covalent interactions to systems of biological interest, and the design of new base functionals for non-covalent interactions.

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