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Performance of Common Density Functional Methods for the N-Body Interaction Energies of Water Clusters KENNETH JORDAN, FANG-FANG WANG, University of Pittsburgh — Using an isomer of $(H_2O)_{16}$, which has been the subject of several earlier studies, we demonstrate that, in contrast to the commonly held view, the N-body expansion of the interaction energy evaluated at the MP2 level does not converge monotonically with increasing N. Moreover, comparison of the results of HF and MP2 calculations reveals that this unexpected behavior is primarily due to electron correlation effects. The results of various common density functionals are considered, and the implications of our results for various procedures for correcting DFT for dispersion will be discussed.

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