Supporting Information for "Energy-Screened Many-Body Expansion: A Practical Yet Accurate Fragmentation Method for Quantum Chemistry"

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(Dated: November 2, 2019)

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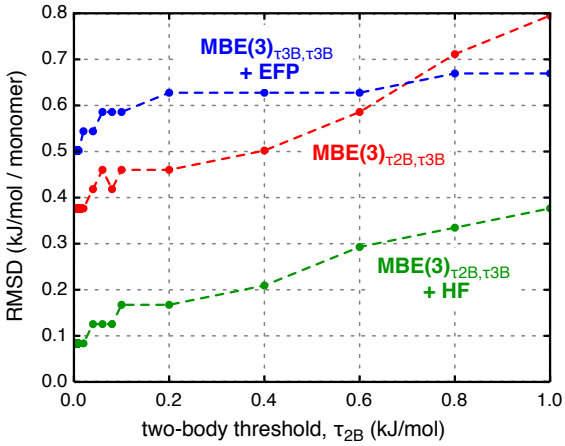

FIG. S1: Errors (with respect to a supersystem calculation) in B3LYP/aDZ calculations on clusters $(H_2O)_{N=6-34}$, as a function of the cutoff τ_{2B} that is applied to the two-body corrections ΔE_{IJ}. The three-body threshold is fixed at $\tau_{3B} = 0.25$ kJ/mol in all calculations. Higher-order induction is recovered by including a HF/aDZ or EFP correction in a two-layer scheme.

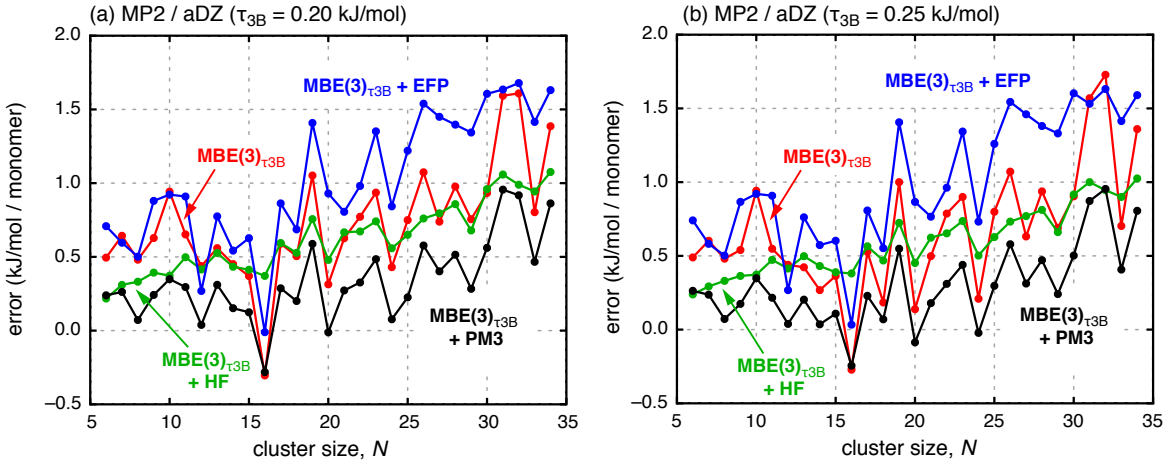

FIG. S2: Signed errors per monomer for MBE(3)$_{\tau 3B}$ approximations at the MP2/aDZ level, using (a) $\tau_{3B} = 0.20$ kJ/mol versus (b) $\tau_{3B} = 0.25$ kJ/mol. The plot in (b) is the same as Fig. 5b, but repeated here to facilitate side-by-side comparison against results in (a) that use the tighter energy threshold. The results demonstrate that there is very little difference in the errors obtained using one threshold versus the other.

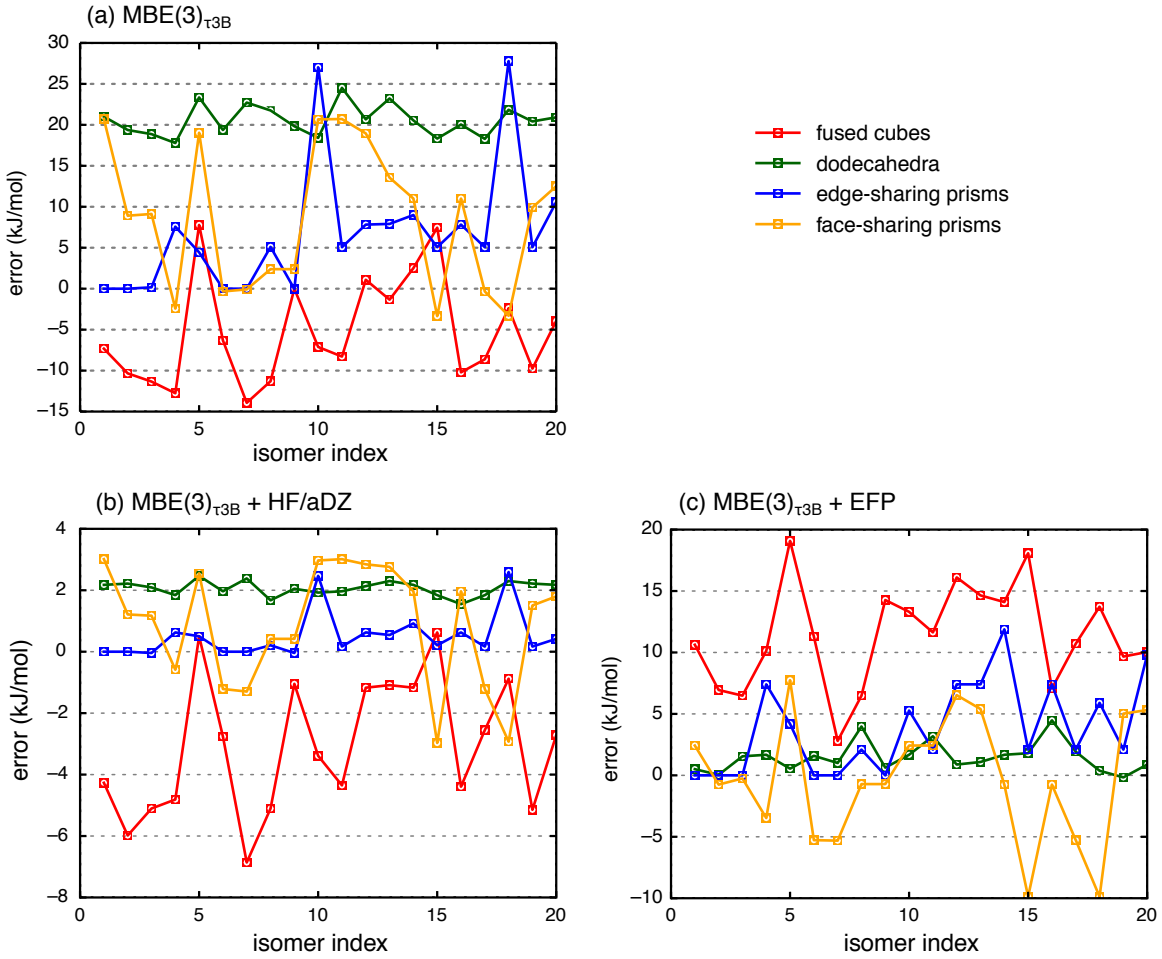

FIG. S3: Signed errors (relative to a supersystem calculation) for relative energies of $(H_2O)_{20}$ isomers computed at the ωB97X-V/aTZ level of theory, using (a) MBE(3)$_{\tau 3B}$, (b) MBE(3)$_{\tau 3B}$ + HF/aDZ, and (c) MBE(3)$_{\tau 3B}$ + EFP. All fragment approximations used an energy threshold $\tau_{3B} = 0.25$ kJ/mol. Note that the energy scale is different in each panel. The isomers and color scheme are the same as in Figs. 7 and 8.

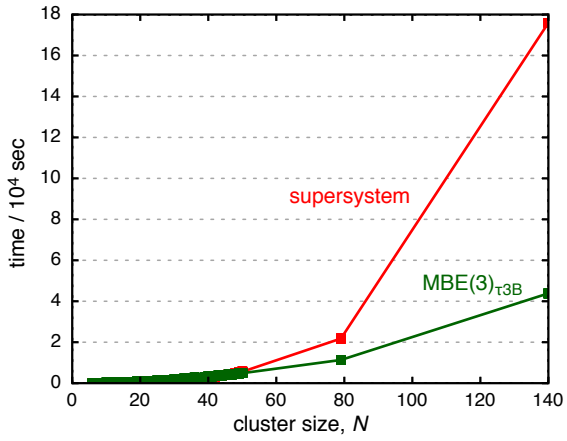

FIG. S4: Wall time for B3LYP/aDZ calculations on clusters $(H_2O)_N$ for N = 6–50, 79, and 140. All calculations were performed on a single 40-core compute node, including all of the subsystem calculations for MBE(3)$_{\tau 3B}$. The latter method uses $\tau_{3B} = 0.25$ kJ/mol as the energy threshold.