Low-Order Scaling Electronic Structure Methods for Non-Covalent Interactions in Psi4

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Many methods in electronic structure theory (EST) are limited in application by their high asymptotic scaling. This is particularly unfortunate for investigations of non-covalent interactions, which are often long-range in nature and therefore require computations on large chemical systems. We developed and implemented several approximate, reduced-cost EST methods in the Psi4 software package which exhibit better scaling properties than their conventional counterparts. These low-order scaling methods extend the range of chemical systems that can be studied with EST.