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Attenuated second order Mller-Plesset perturbation theory: correcting finite basis set errors and infinite basis set inaccuracies[1]
MATTHEW GOLDEY, Institute for Molecular Engineering, the University of Chicago, MARTIN HEAD-GORDON, Department of Chemistry, University of California, Berkeley — Second order Møller-Plesset perturbation theory (MP2) in finite basis sets describes several classes of noncovalent interactions poorly due to basis set superposition error (BSSE) and underlying inaccurate physics for dispersion interactions. Attenuation of the Coulomb operator provides a direct path toward improving MP2 for noncovalent interactions. In limited basis sets, we demonstrate improvements in accuracy for intermolecular interactions with a three to five-fold reduction in RMS errors. For a range of inter- and intermolecular test cases, attenuated MP2 even outperforms complete basis set estimates of MP2. Finite basis attenuated MP2 is useful for inter- and intramolecular interactions where higher cost approaches are intractable. Extending this approach, recent research pairs attenuated MP2 with long-range correction to describe potential energy landscapes, and further results for large systems with noncovalent interactions are shown.

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