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Tuning the correlation energy in second-order Møller-Plesset perturbation theory with an effective electron-electron interaction potential TIM KOWALCZYK, TROY VAN VOORHIS, Massachusetts Institute of Technology — For practical electronic structure calculations on large molecules, wave function theories (WFT) remain less popular than density functional theory (DFT) despite the systematic improvability of WFT. The greater computational cost of WFT is largely to blame and is two-fold in nature: WFT generally presents unfavorable scaling with system size relative to DFT, *and* WFT results converge more slowly than those of DFT with respect to basis set size. We propose that each of these issues can be partially mitigated by the introduction of an effective electron-electron interaction potential, in lieu of the true $1/r$ potential, for evaluating the correlation energy in WFT. We discuss the design and optimization of such an effective interaction, in the context of second-order Møller-Plesset perturbation theory (MP2), for two distinct purposes: to accelerate basis set convergence of MP2 correlation energies, and to re-scale the MP2 correlation to improve agreement with experiment and/or higher-level methods.

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