

Title: Multi-reference wavefunctions made single-reference on diradical systems

Abstract:

Multi-reference wavefunctions can be made single-reference using electron attachment methodologies. By judiciously removing a certain number of particles in the reference wavefunction, and then adding them back in during an EOM-CCSD calculation, we may circumvent all the difficulties associated with multi-reference wavefunctions. We demonstrate the accuracy of the method on notable multi-reference problems: methylene, para-benzyne, and TMM, using basis set extrapolation methods and CCSD for dynamic correlation on a single-reference problem.