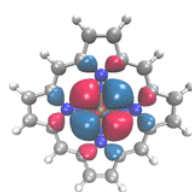
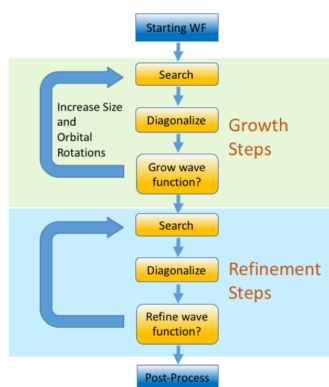
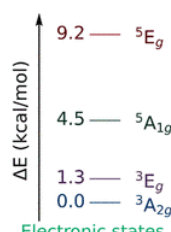


Adaptive Sampling Configuration Interaction (ASCI) Method

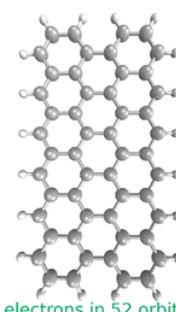


40 electrons in 42 orbitals

CASSCF quality results at greatly reduced cost!

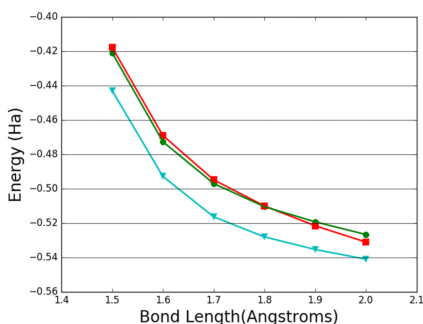


Electronic states of Fe-Porphyrin

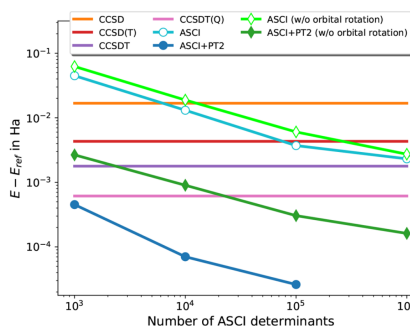


52 electrons in 52 orbitals

- ASCI is a compact approximation to the unattainable full CI ansatz. In ASCI, a trial CI wave function is iteratively improved by the inclusion of new determinants for which the estimated CI coefficients are significant.
- The ASCI energy can be further improved through second-order Epstein-Nesbet perturbation theory (PT2).
- The ASCI scheme can be applied in CASSCF calculations (ASCI-SCF), affording much larger active spaces than conventional CASSCF calculations and extending CASSCF calculations to medium-sized molecules.



(a) Cr_2 binding curves. Green, ASCI+PT2 energies; red, DRMG energies for (24e,30o); blue, ASCI energies without the frozen core (48e,42o)



(b) Convergence rate of ASCI and ASCI+PT2 energies for the CN radical in the cc-pVDZ basis, with increasing size of ASCI wave functions

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