Frozen density embedding of CASSCF wavefunctions in CP2K

L. Schreder[1], S. Luber[1]*

[1]University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

Most chemical processes happen at a local scale where only a subset of the molecular orbitals (MOs) is excited, and only a subset of covalent bonds may be rearranged. To capture such excited states or reactions, the efficient Density Functional Theory (DFT) is often inadequate, and the use of correlated wavefunction (CW) methods is required for accurate results. Due to their unfavorable computational scaling compared to DFT, this usually limits their use to small systems. Thus, studying a local excitation or chemical reaction in an extensive, relatively static environment is a balancing act between the accuracy of CW methods and the system size DFT can afford. A mixed-resolution approach backed by embedding theory is therefore preferable. Based on the self-consistent frozen density embedding algorithm, we developed a method of embedding complete active space self-consistent field (CASSCF) simulations run in the OpenMolcas code in a DFT environment calculated in CP2K.