Frozen-pair Coupled Cluster methods for strong and weak correlation

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The major part of the strong correlation can be provided by the pair Coupled Cluster Doubles (pCCD) model combined with a (variational) orbital optimization protocol [1,2]. The orbital-optimized pCCD method is size-consistent and computationally inexpensive in comparison to various multi-reference approaches. However, it does not account for all electron correlation effects. [3] One way to include the missing (dynamic) electron correlation effects is to use a (linearized) Coupled Cluster correction on top of the pCCD wave function. [4,5] The frozen-pair Coupled Cluster Singles Doubles (fpCCSD) method is one efficient way to improve the wave function with the cost of CCSD. [4] In fpCCSD or its linearized variant, the singles and non-pair doubles amplitudes are optimized, while the pair doubles amplitudes are kept frozen. Such an optimization routine provides a balanced description of strongly-correlated systems, where traditional CCSD usually fails. In this work, we will scrutinize the performance of various Coupled Cluster corrections on top of pCCD.

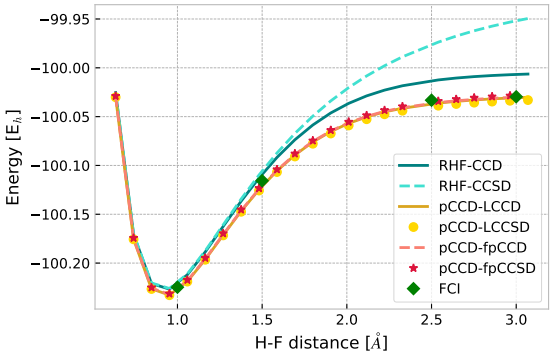

Figure 1: Potential energy curves of fluorine molecule (cc-pVDZ basis set).

References

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