

How good is pair coupled-cluster doubles (pCCD)?

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As both of our honorees have devoted substantial effort toward further developing pair CCD (pCCD), the amazingly simple, correlated theory of Cullen, it is interesting to investigate a wide range of potential applications compared to the more complex and expensive CCSD and its triple and quadruple excitation corrections. Applications of interest include IP, EA, and excited states, as well as its role in MR applications. Unlike virtually any normal CC method, pCCD is critically sensitive to orbital optimization and for bond breaking, localization. Its features and its performance will be addressed in this talk.