CCSD tailored with orbital-optimized pair-CCD and matrix-product-state wave functions.

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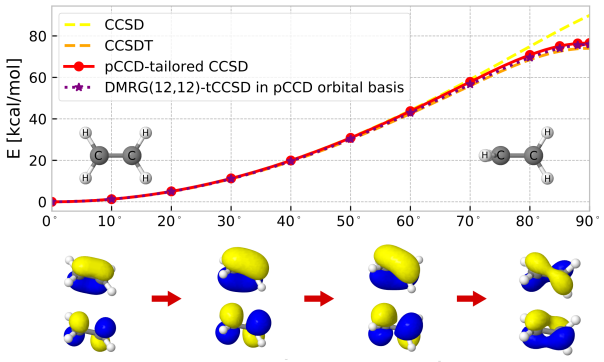

Coupled cluster theory provides a robust and accurate treatment of electron correlation effects. In its standard single-reference formulation, this model is one of the most reliable tools to describe dynamic electron correlation. However, it fails when the quantum system under study has a multireference nature. In such cases, the hierarchy of approximations breaks down, and the cluster operator's truncation provides an incorrect wave function model with unphysical coupling between cluster amplitudes.[1]
One of the treatments dedicated to capturing strong electron correlation effects is the tailored coupled-cluster method. The subset of cluster amplitudes is extracted from the external model that provides the proper description of the multireference nature of the molecular system.[2–4] Our work studies coupled cluster models tailored by orbital-optimized pair coupled cluster doubles (pCCD) and the density matrix renormalization-group algorithm (DMRG). These methods scale polynomially with the system size and provide an efficient way to capture strong electron correlation effects.

References

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