Beyond the LPNO-TCC: Introduction of DLPNO-TCCSD

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Coupled cluster (CC) methods tailored by matrix product state (TCC)[1] are highly accurate post-DMRG methods, which provide an accurate treatment of non-dynamic correlation with DMRG and dynamic correlation with CC framework. While being tremendously successful, canonical TCC method cannot handle large systems. Recently developed local variant of TCC (LPNO-TCC) is able to describe these systems and provide excellent results[2]. Unfortunately, due to the lack of proper linear scaling, calculations of very large systems is prohibitive even for LPNO-TCC. Therefore, one has to go beyond the LPNO-TCC.

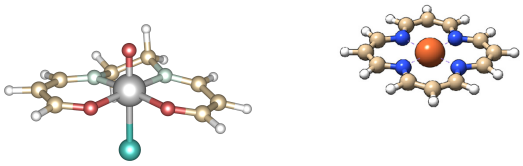

Figure 1: Studied systems.

In this poster, we present a benchmark of a novel domain-based local tailored coupled cluster singles and doubles method (DLPNO-TCCSD). We tested the performance of DLPNO-TCCSD on the rotational barrier of tetramethyleneethane, energetics of oxo-Mn(salen). iron porphyrin and model of NiFe hydrogenase with several different CAS spaces. These tests shows that DLPNO-TCCSD provides about 99.9% of the canonical correlation energy, which is a large improvement wrt. LPNO-TCCSD results, while being several times faster.

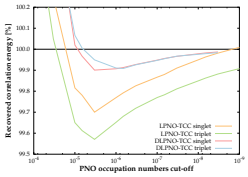

Figure 2: Comparison of DLPNO-TCCSD and LPNO-TCCSD.

References

1. Veis, L., Antalík, A., Brabec, J., Neese, F., Legeza, Ö., and Pittner, J., *The Journal of Physical Chemistry Letters* **7** (2016), 4072.
2. Antalík, A., Veis, L., Brabec, J., Legeza, Ö., Pittner, J. 2019. Towards the Efficient Local Tailored Coupled Cluster Approximation and the Peculiar Case of Oxo-Mn(Salen). *JCP* submitted