Multireference Methods for Extended Systems

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I will describe our latest progress in combining density matrix renormalization group (DMRG) with pair-density functional theory (PDFT) as a new way to calculate correlation energy. Calculations that require active spaces larger than the feasibility limit of the conventional complete active-space self-consistent field (CASSCF) method will be presented. I will also report our advancements in using density matrix embedding theory (DMET) in combination with localized active space self-consistent field (LASSCF) [1] as a solver and its application to realistic models of strongly-correlated systems.

References

1. M. Hermes and L. Gagliardi, *J. Chem. Theory Comput*. **15** (2019) 972.