Linear scaling multireference coupled cluster methods

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The coupled cluster ansatz can be used combined with the multireference perturbation theory to develop rigorously size-extensive multireference methods. Similarly to single-reference coupled-cluster based methods the polynomial scaling in computational time and memory can be reduced using local correlation approaches.[1] In my talk I will present progress on implementation of linear scaling multirefrence coupled cluster methods. The methods are implemented using local integrated tensor framework [2] which allows fast implementation of linear scaling methods. An extension to computation of excitation energies in a Hermitian linear response formalism [3,4] will be discussed.

- 1. F. Menezes, D. Kats and H. J. Werner, J. Chem. Phys., 145, 124115 (2016)
- 2. D. Kats and F. R. Manby, J. Chem. Phys., 138, 144101 (2013)
- 3. D. Kats, D. Usvyat and M. Schütz, *Phys. Rev. A*, **83**, 062503 (2011)
- 4. G. Wälz, D. Kats, D. Usvyat, T. Korona and M. Schütz, Phys. Rev. A, 86, 052519 (2012)