Seminar of the Department. 26
Thin Layers and nanostructures

Fyzikální ústav AVČR, Cukrovarnická 10, Praha 6

Date : 28. 05. 2019 , Tuesday
Time : 10:00 am
Place : Library,Building A, 1st floor

Topic

Density matrix renormalization group method in quantum chemistry

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In the first part of the talk, I will review basic concepts of quantum chemical density matrix renormalization group (QC-DMRG), the method of choice for calculations of strongly correlated molecular systems, which is especially suitable for treatment of one-dimensional and quasi one-dimensional problems. I will also present our recent developments on local orbital optimization matching the two-site DMRG scheme [1] and introduce MOLMPS, the massively parallel QC-DMRG implementation which is currently under development [2].

In the second part, I will introduce the recently developed method for accurate “post-DMRG” treatment of dynamic correlation based on the tailored coupled cluster (CC) theory [3] in which QC-DMRG is responsible for the proper description of non-dynamic correlation, whereas dynamic correlation is incorporated by CC [4].

[1] Ch. Krumnow and L. Veis, et al., Phys. Rev. Lett 117 (2016) 21040.

[2] L. Veis and J. Brabec, et al., in preparation.

[3] T. Kinoshita and O. Hino, et al., J. Chem. Phys. 123 (2005) 074106.

[4] L. Veis and A. Antalik, et al., J. Phys. Chem. Lett. 7 (2016) 4072.

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