On a quest for fast and reliable black-box methods

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The coupled cluster theory, although very reliable for the dynamical correlation (starting from CCSD(T) method), is much less suitable for the static correlation. The multi-reference methods on the other hand are far from being black-box methods. Additionally, these methods have steep scaling in computational time and resources with the molecular size, and therefore in the canonical form are applicable only to small molecules.

In the first part of my talk the distinguishable cluster approach [1,2] will be presented, which is able to accurately describe strongly correlated states. In a combination with explicitly correlated treatment it allows to achieve nearly chemical accuracy for single-reference test cases [3].

In the second part I will present new techniques to speed up linear-scaling local correlation methods [4].

1. D. Kats and F. R. Manby, *J. Chem. Phys.*, **139**, 021102 (2013)
2. D. Kats, *J. Chem. Phys.*, **141**, 061101 (2014)
3. D. Kats, D. Kreplin, H.-J. Werner, and F. R. Manby, *submitted*
4. D. Kats, *J. Chem. Phys.*, **141**, 244101 (2014)