Nuts and bolts of RAS-CI methods with general excitation operators

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Abstract

In this talk I will introduce the details describing the restricted active space configuration interaction (RAS-CI) method with the hole and particle truncation of the excitation operator. I will give the motivation for the development of this approach, I will discuss in detail the main expressions defining the RAS-CI wave function with the use of different excitation operators, and the algorithms employed to compute molecular electronic states and their energies. Finally, I will discuss the second order perturbative correction to the RAS-CI energy, i.e. RAS-CI(2), as a path to recover dynamical correlation effects.

During my presentation, I will illustrate the qualities and limitations of these electronic structure models in the computation of ground and excited states in a variety of molecular systems.