Multireference Fock space coupled cluster method based on the RHF reference for the description of the potential energy curves

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The Fock space (FS) coupled cluster (CC) method reported recently [1] is introduced to study double electron attached states. The method has a useful feature that when applied to the doubly ionized atoms or molecules it provides the full characteristics of the neutral system since the description of the neutral system is accomplished via attaching two electrons to the corresponding doubly ionized system. This way is particularly advantageous when a closed shell molecule dissociates into open shell fragments while its doubly positive cation generates the closed shell units.

A critical point of the succesful application of the FS-CC theory in molecular applications is the intermediate Hamiltonian technique. Using it we were able to compute the potential energy curves (PECs) for the series of alkali metal dimers. Moreover, the size-extensivity property of the Fock space formalism ensures the proper dissociation limit for all studied species. In all cases PECs are smooth for the entire range of interatomic distances (from the equilibrium point to the dissociation limit). Based on the calculated potential energy curves we are able to compute spectroscopic parameters of the systems studied.

[1] Musiał, M. *J. Chem. Phys.*, 136:134111-1–14, 2012.