# Vibrational levels of selected excited electronic states of $Li_2$ molecule by multireference coupled cluster method

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The intermediate Hamiltonian Fock space coupled cluster scheme in (2,0) sector is used for the accurate description of electronic states of $Li_2$ molecule. The method has a useful feature that the description of the electronic states of the neutral molecule is obtained for the doubly ionized reference. This approach is particularly advantageous in the studies of the potential energy curves (PECs) for the alkali metal diatomics which after removal of two electrons dissociate into closed shell fragments.

In the current work we study the potential energy curves of low lying electronic states of lithium dimer. Contrary to the previous studies the current approach is based on the first principle calculations with all correlated electrons. In all cases we were able to compute the smooth PECs for the whole range of interatomic distances from equilibrium to the dissociation limit. The theoretical PECs stay very close to the experimental curves and the computed scpectroscopic parameters reproduce the experiment with very good accuracy. The other advantage of the approach is its rigorous size-extensivity allowing to reproduce the atomic excitation energies at the infinite interatomic distance. Moreover, we observe a perfect agreement between theoretical and experimental vibrational energy levels.