The low-lying excited states of LiYb+

Marta Gałyńska

Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Torun, Poland

Various quantum chemical methods can predict fundamental properties asso- ciated with the ground and lowest-lying excited states of atoms and molecules at absolute zero temperature. Only recently, experimental investigations on compounds in their electronic ground state have been rendered possible by the discovery of laser cooling. During the last two decades, many sophisticated experimental methods such as helium buffer gas cooling, photoassociation, and magnetic Feshbach resonances were extensively applied to explore the chemistry and physics of so-called cold and ultracold atoms and molecules, which are typically studied in the range of 1.0 mK and 1.0 K. These experiments facilitate measurements of atoms or molecules with remarkable precision by controlling their specific quantum state. Thus, cold and ultracold chemistry can join theory and experiment in discovering fundamental properties of matter in the quantum realm.

The ytterbium atom is a highly-valuable element because of its closed f-shell and the $4f^{14}6s^2$ ground-state electronic configuration, which makes its electronic structure similar to the group II-atoms. However, ytterbium has 70 electrons and is classified as a heavy element, which is an extraordinary challenge for state-of-the-art quantum chemistry because of nonnegligible spin-orbit coupling (SOC) effects and the large number of electrons that need to be correlated. How- ever, the spin-orbit coupling effects are often omitted during quantum chemistry investigations of ytterbium compounds because of the higher cost of the calcu- lations. During the current project, we investigate the influence of relativistic effects on the low-lying excited states of $LiYb^+$ using the Equation of Motion CCSD and Fock Space CCSD methods. All presented calculations were done with relativistic four-component Hamiltonian implemented in the DIRAC quan- tum chemistry software.