ELECTRONIC EXCITATIONS OF ALKALI-ALKALINE EARTH DIATOMIC MOLECULES - RESULTS FROM AB INITIO CALCULATIONS

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Recently interest in polar diatomic molecules with a magnetic dipole moment has been growing. An example for such molecules is the combination of an alkali metal atom and an alkaline earth metal atom. These systems are quite small, containing only three valence electrons. Nevertheless calculations of excited states are challenging. Ab initio calculations for two sample systems, LiCa[a] and RbSr, will be presented. The potential energy curves and transition dipole moments for the ground state and several excited states were determined, up to 25000 $\mathrm{cm}^{-1}$for LiCa and up to 22000 $\mathrm{cm}^{-1}$for RbSr. Multireference configuration interaction calculations (MRCI) based on complete active space self-consistent field wave functions (CASSCF) were used to determine the properties of the system as implemented in the MOLPRO software package.[b] Effective core potentials (ECPs) and core polarization potentials (CCPs) were applied to reduce the computational effort, while retaining accuracy. The similarities and differences of the two systems will be discussed. In both systems the accurate description of the asymptotic values of the PECs corresponding to atomic D-states proved to be difficult. The results will be compared to recent experiments, showing that a combination of theory and experiment gives a reliable description of the systems.

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[a] G. Krois, J.V. Pototschnig, F. Lackner and W.E. Ernst, J. Phys. Chem. A, 117, 13719-13731 (2013)

[b] H.-J. Werner and P. J. Knowles and G. Knizia and F. R. Manby and M. Schütz et al., MOLPRO, version 2010.1, see http://www.molpro.net/