Electronic structure of the MoLi, MoBe, and RuB molecules: Ground and Low-Lying States

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Transition metal compounds play significant role in many research fields such as Organometallic Chemistry, Catalysis, Surface Science and Astrophysics.[2] The accurate theoretical description of these molecules is a demanding task, because of their computational complexity due to their high density of states and the high space-spin angular momentum of the transition metal atom. As a result, the understanding of the chemical bond between a transition metal element and a main group element is not an easy task.[2]

In the present work, the electronic structure of three diatomic molecules, i.e., MoLi, MoBe, and RuB have been studied employing accurate ab initio methodologies. The complete active space self-consistent field (CASSCF) and the multireference configuration interaction plus single and double excitations (MRCISD) methodologies in conjunction with the aug-cc-pV5Z(-PP) basis sets have been used. The dissociation energies, bond lengths, dipole moments and usual spectroscopic data have been calculated for all studied states. Their potential energy curves of all low-lying electronic states have been plotted. Finally, their bonding has been analyzed. MoBe presents specific interest due to the type of bonds that form the Be atom, while the ground state of the RuB presents a quadruple bond.

References:
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