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Equlibrium Configuration of LiH and Li2

The present work describes the equilibrium configuration of the lithium hydride (LiH) and lithium dimer (Li2) calculated using the Hartree-Fock procedure implemented by the Gaussian 03 set of programs. We have also calculated the ground state energy of the lithium atom and ions using the single-center expansion method with the Gaussian shell orbitals. The ground state energies for the lithium atom and ions calculated using the single-center expansion method and the HF procedure agree to each other within 3%. The ground state energy for the lithium atom has been estimated to be -7.432 a.u. and that for Li+ and Li++ ions to be -7.236 a.u. and -4.494 a.u., respectively. With these HF values of energy for the lithium atom and ions, we have estimated the first and second ionization potentials for the lithium atom to be 5.34 eV and 79.95 eV, respectively, which are in close agreement to the previously reported experimental values within 1%. We have also performed calculations using configurations interaction (CI) method and the density functional theory (DFT) to study the equilibrium configurations of LiH and Li2. The ground state energies for LiH and Li2 obtained using the DFT calculation are lower than that obtained with the CI method, which, in turn, are lower than that obtained with the HF approximation. With the DFT calculation we have estimated the binding energy of LiH to be 242.81 kJ/mol, which is in close agreement with the previously reported experimental value of 238.049 kJ/mol within 2%. However, in case of Li2 the DFT value of binding energy is less than the corresponding CI value by around 9%. The binding energy of Li2 using the CI calculation has been estimated to be 94.99 kJ/mol, which is close to the previously reported experimental value of 98.98 kJ/mol within 4%. We have also studied the variation of energy with distance between the constituent atoms of LiH and Li2. From the energy versus distance curves we have estimated the bond lengths for Li-H and Li-Li to be 1.59 Å and 2.70Å, respectively, which are in close agreement with the previously reported experimental values within 1%.

Key words: HF approximation, CI, DFT, binding energy, bond length

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