

Homework 10, Due April 17

1. Write the expression of all the Coulomb and exchange integrals for the Li atom ground state ($1s^2 2s^1$).
2. Write the electronic Hamiltonian of H_2 molecule in atomic units.
3. For H_2 , the molecular orbitals are expressed in terms of linear combinations of atomic orbitals:

$$|\psi^\pm\rangle = c[|\phi_{sa}\rangle \pm |\phi_{sb}\rangle]$$

Determine the coefficient c by normalization.

4. Draw the molecular orbital energy level diagram for N_2^- and write down its electronic configuration. Compute the spin multiplicity of the molecular ion and the bond order.