Exercises

1. Write down a picture of particles of H_2^+ molecular system with their coordinates and describe Schrödinger equation in atomic unit within the Born-Oppenheimer approximation.

picture

Schrödinger equation

2. Solve the H_2^+ molecular system using a linear combination of two 1s orbital of nuclear A and B. Obtain two normalized wave functions and corresponding energy levels.
You can use the following notations for integrals.

$$H_{AB} = H_{BA} = \left\langle \phi_{1s_A} \middle| \hat{H} \middle| \phi_{1s_B} \right\rangle = \left\langle \phi_{1s_B} \middle| \hat{H} \middle| \phi_{1s_A} \right\rangle \quad H_{AA} = H_{BB} = \left\langle \phi_{1s_A} \middle| \hat{H} \middle| \phi_{1s_A} \right\rangle = \left\langle \phi_{1s_B} \middle| \hat{H} \middle| \phi_{1s_B} \right\rangle$$

$$S_{AB} = S_{BA} = \left\langle \phi_{1s_A} \middle| \phi_{1s_B} \right\rangle = \left\langle \phi_{1s_B} \middle| \phi_{1s_A} \right\rangle = S \qquad S_{AA} = S_{BB} = \left\langle \phi_{1s_A} \middle| \phi_{1s_A} \right\rangle = \left\langle \phi_{1s_B} \middle| \phi_{1s_B} \right\rangle = 1$$

3. Write down a picture of bounding and anti-bounding orbitals of H_2^+ system and its' energy diagram.

4. Write down a picture of molecular orbitals and with an energy diagram of 2p group elements such as N_2 molecule.

5. Which is the molecule with the strongest bond among B_2, C_2, N_2, O_2, and F_2? Discuss it from the bond-order concept.