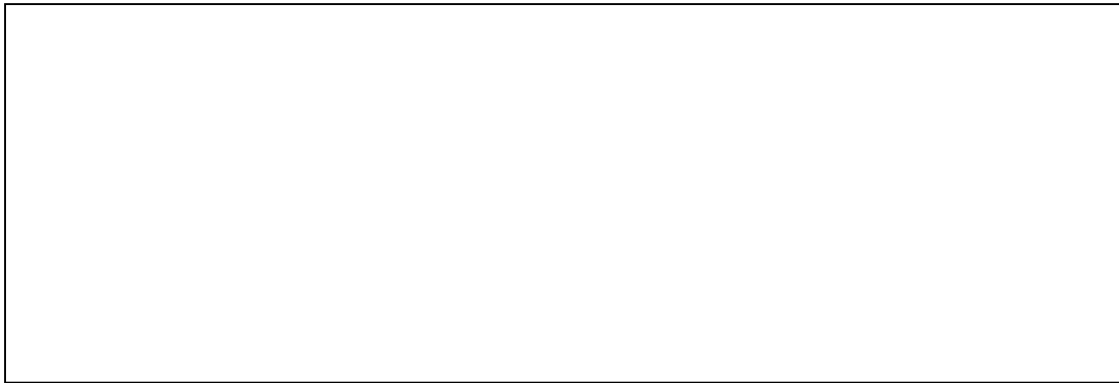


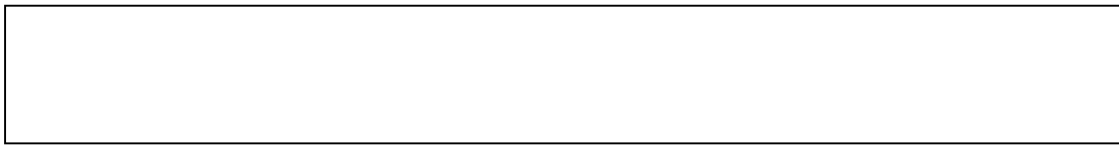
Exercises

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.

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

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.