

PAY ATTENTION to which are P and which are Q problems:

Text Problems

Q12.1 – familiarize yourself with real values to justify the BO approximation

Q12.3 – consider the shapes of the bonding and antibonding orbitals

P12.1 – working with LCAO wave functions / finding normalization constant in terms of S

P12.2 – evaluating H_2^+ MO energies

P12.3 – varying the size of the orbital with a variational parameter

Q13.1-electrons in antibonding orbitals

Q13.3-AO coefficients in MOs for heteronuclear diatomics

Q13.5-g and u labels for heteronuclear diatomics

P13.5-dissociation energies of NO, CF⁻, CF⁺

P13.6-electron configurations for O₂ ions

P13.11-use MO theory to rank vibrational energies

Additional Problems:

1) Write out and compare the MO and VB wave functions for the ground state of H₂

a) What terms are similar? What terms are different?

b) Ascribe a physical interpretation to these terms (ionic terms etc.) and describe the differences and deficiencies between the two wavefunctions.