Seminar 10

1- Which is the bond order for: $H_2$, $O_2$, $N_2$ and $B_2$?

2- For the homonuclear diatomic molecules and ions write their ground electronic states: $H_2$, $H_2^+$, $Be_2$, $Be_2^-$, $C_2^+$, $C_2$, $C_2^-$.

3- Suppose that two MOs of a molecule are given by the formulas:
   \[
   \phi_1 = (\frac{1}{\sqrt{3}})\chi_1 + (\frac{1}{\sqrt{3}})\chi_2 + (\frac{1}{\sqrt{3}})\chi_3 \\
   \phi_2 = (\frac{1}{\sqrt{3}})\chi_3 + (\frac{1}{\sqrt{3}})\chi_4 + (\frac{1}{\sqrt{3}})\chi_5
   \]
   where the $\chi$’s are AOs which are assumed to be orthonormal. By inspection, what is the overlap between these MOs?

4- Being $|1\rangle$ and $|2\rangle$ the AOs for the hydrogen atoms forming the molecule:
   a) Write the wavefunctions for $H_2$
   b) The energies
   c) Identify the bonding and the antibonding.

5- Considering benzene:
   a) Find the energy levels.
   b) Indicate which energy levels are degenerate.
   c) Make a plot of the energy levels and fill them with the $\pi$ electrons.
   d) Identify the bonding and antibonding orbitals in the plot.

6- Which kind of hybridisation do you find in the following organic compounds: ethane ($C_2H_6$), ethene ($C_2H_4$) and ethine ($C_2H_2$)?