

5.3: Diatomic MO Diagrams

Learning objectives for this unit are to:

- Derive molecular orbital energy diagrams for homonuclear and heteronuclear diatomic molecules, taking into account atomic orbital overlap and mixing of molecular orbitals
 - Predict the bond orders for homonuclear and heteronuclear diatomic molecules and ions, and correlate bond lengths, strengths, and stabilities of molecules with bond order
 - Predict the magnetic properties of molecules (diamagnetic/paramagnetic) based on the MO diagram
 - Identify the HOMO and LUMO on an MO diagram
 - Explain the origin and consequences of sp mixing
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