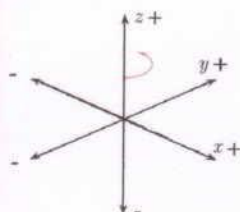
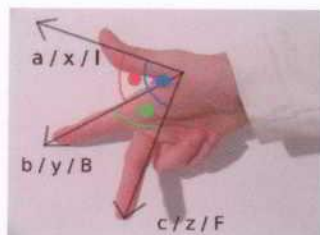


Lab. 2 Linear Combination of Atomic Orbitals (LCAO): VB & MO Theories Atomic Orbitals

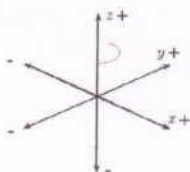
Right handed Cartesian coordinate system



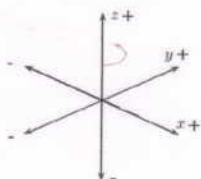
A. Atomic Orbitals

Draw the Angular portion of the wave function of the following atomic orbitals on a right handed Cartesian coordinate system

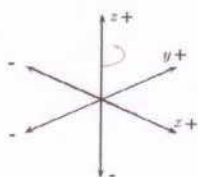
i) s orbital



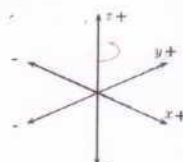
ii) p_x orbital



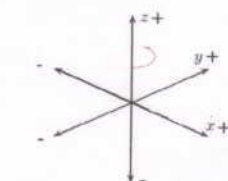
p_y orbital



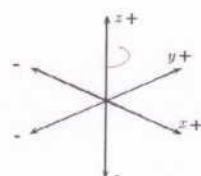
p_z orbital



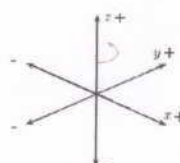
iii) dz^2 orbital



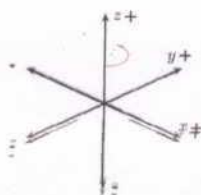
dx^2-y^2 orbital



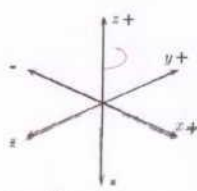
dxy orbital



dxz orbital



dyz orbital



v) Draw hybrid orbitals resulting from sp^3d hybridization

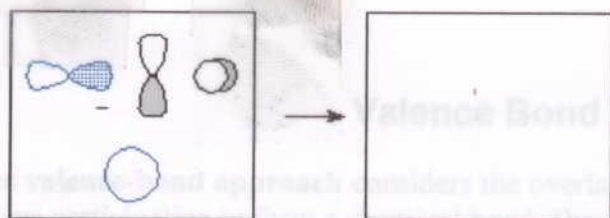
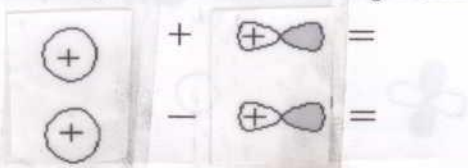
Hybridization of Atomic Orbitals

It is the **Linear Combination of Atomic Orbitals (LCAO)** in the valance of **an atom**: Individual wave functions (orbitals) combine to form hybrid atomic orbitals (sp , sp^2 , sp^3 , sp^3d , sp^3d^2) Quantum mechanical approaches by combining the wave functions to give new wavefunctions are called **hybridization** of atomic orbitals. Hybridization has a sound mathematical fundation, but it is a little too complicated to show the details here. Leaving out the jargons, we can say that an imaginary mixing process converts a set of atomic orbitals to a new set of **hybrid atomic orbitals** or **hybrid orbitals**.

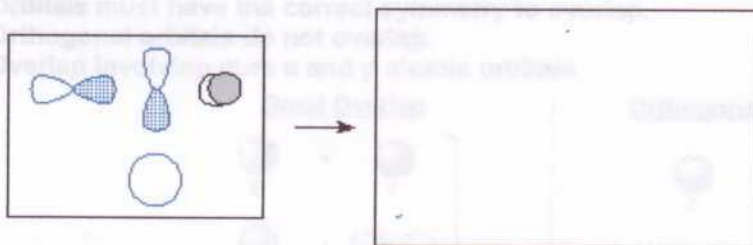
Hybrid Atomic Orbital: Combination of atomic orbitals from the **same atom**

At this level, we consider the following hybrid orbitals:

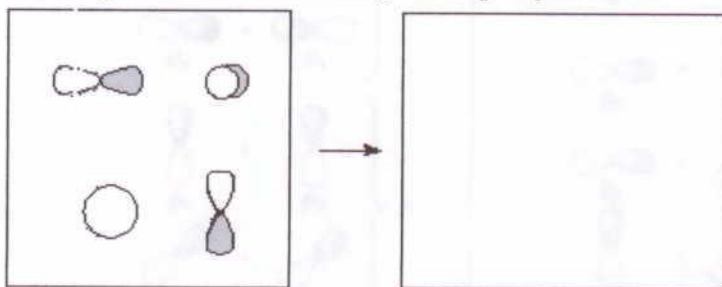
i) Draw hybrid orbitals resulting from sp hybridization



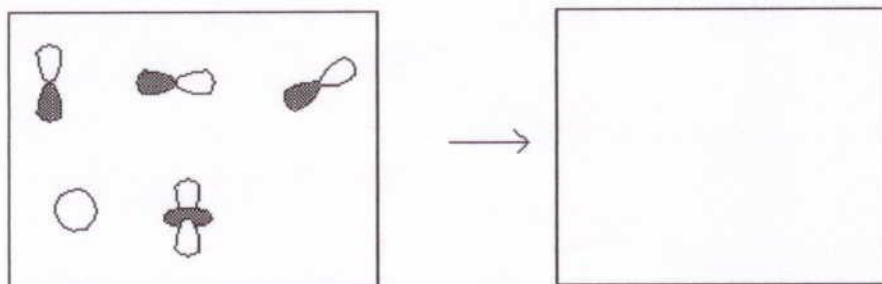
ii) Draw hybrid orbitals resulting from sp^2 hybridization



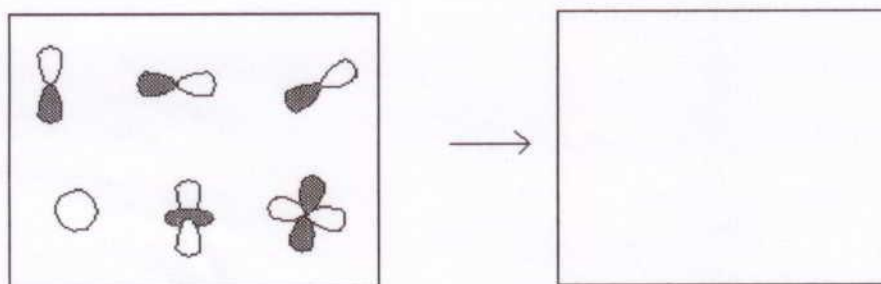
iv) Draw hybrid orbitals resulting from sp^3 hybridization



- v) Draw hybrid orbitals resulting from sp^3d hybridization



- vi) Draw hybrid orbitals resulting from sp^3d hybridization



Valence Bond Theory

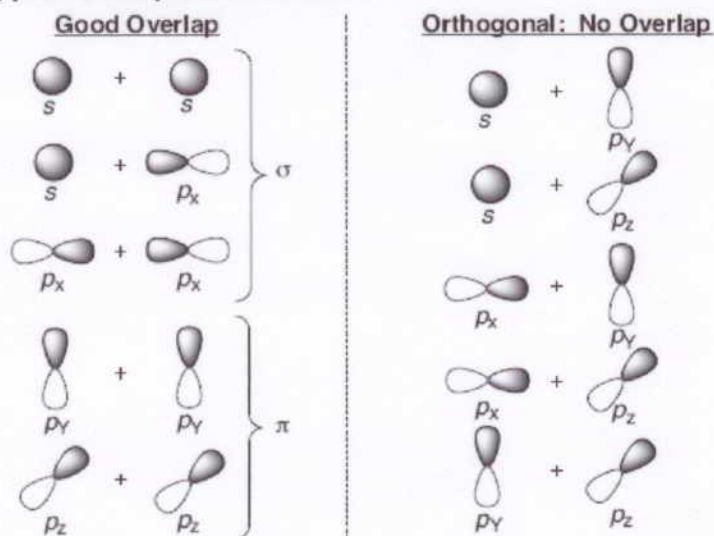
The **valence-bond approach** considers the overlap of the atomic orbitals (AO) of the two atoms participating to form a chemical bond. Due to the overlapping, electrons are localized in the bond region.

Orbital Overlap

Orbitals must have the correct symmetry to overlap.

Orthogonal orbitals do not overlap.

Overlap involving pure s and p atomic orbitals



What is a delta (δ) bond? Draw an example.

Show overlap between following atomic orbitals to form covalent bond

Pure atomic orbitals

i) s-s overlap

bond type:

ii) p_x - p_x overlap

bond type:

iii) p_x - d_{xz} orbital overlap

bond type:

iv) d_{xz} - d_{xz} orbital overlap

bond type:

Pure atomic orbitals

i) sp - sp overlap

bond type:

Draw example

ii) sp^2 - sp^2 overlap

bond type:

Draw example

iii) sp^3 - sp^3 overlap

bond type:

Draw example

iv) sp^3d - p overlap

bond type:

Draw example

v) sp^3d^2 - sp^2 orbital overlap

bond type:

Draw example

bond type:

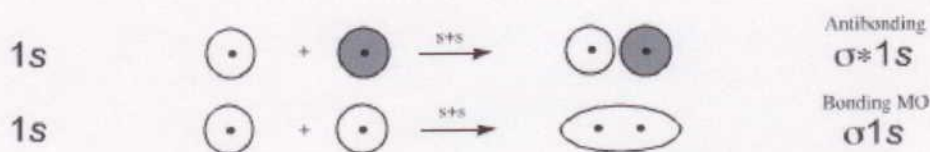
Molecular Orbital Theory

In Molecular Orbital Theory, the orbitals undergo the **Linear Combination of Atomic Orbitals (LCAO)** in a molecule to form molecular orbitals from the overlap of atomic orbitals of the atoms that satisfy two criteria:

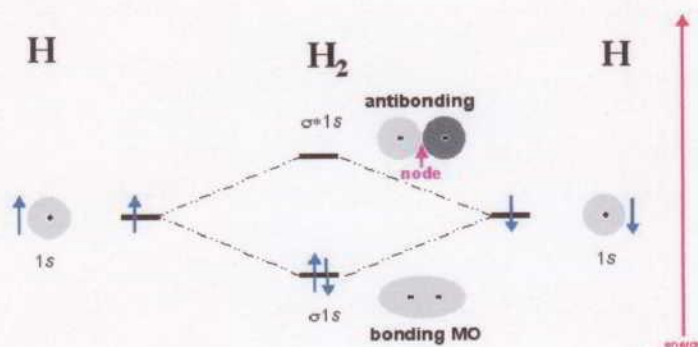
- The orbitals have compatible symmetry
- The orbitals are similar in energy

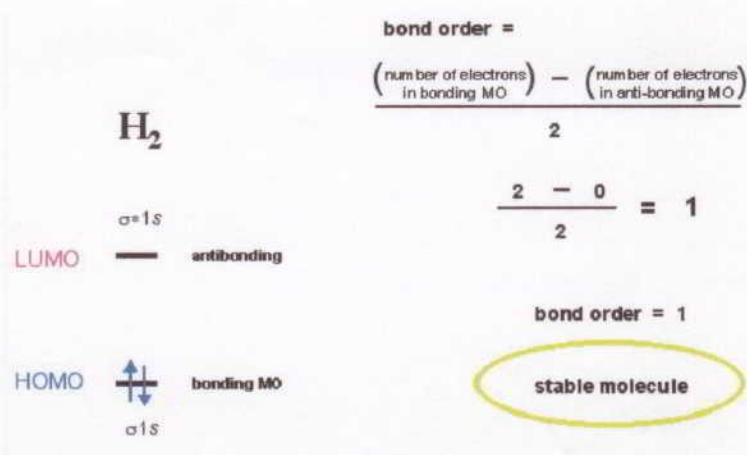
The interactions of the atomic orbitals to form molecular orbitals is represented by an energy diagram called a molecular orbital diagram. The diagram displays the orbitals arranged vertically from lowest to highest energy. The atomic orbitals for the various atoms are listed in columns at the left and right sides of the diagram. The molecular orbitals are listed in a column down the center of the diagram.

The atomic orbitals are given the usual s , p_x , *etc.* designation. The molecular orbitals, which are often identified by their symmetry properties, may be identified by their bonding properties: σ , σ^* , π , π^* , or n (nonbonding).

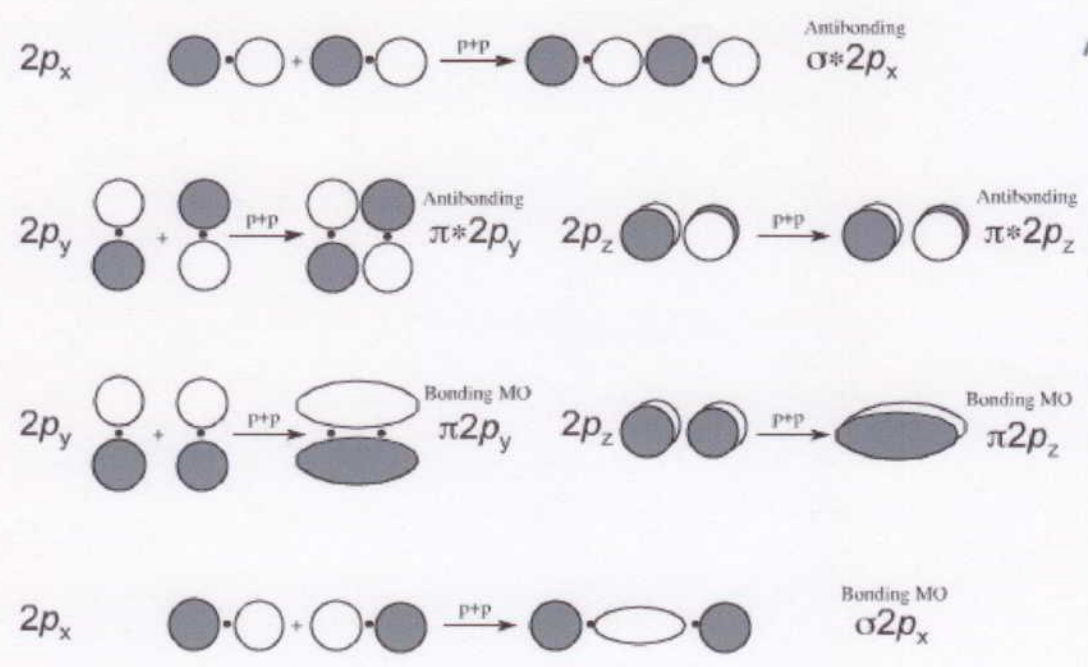


Example H_2 molecule



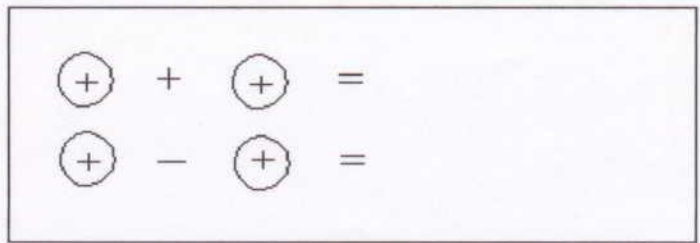


P orbitals linear combinations

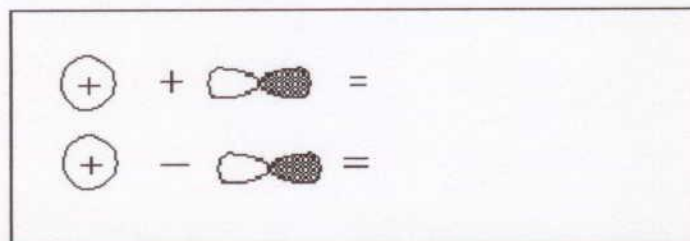


A. At this level, we consider the following hybrid orbitals:

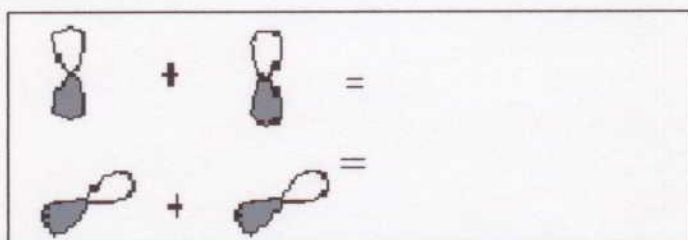
i) Draw sigma molecular orbitals resulting from s and s linear combination of atomic orbitals



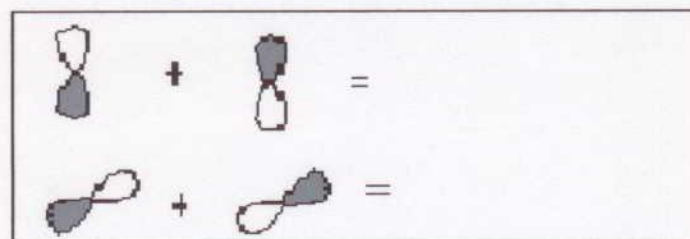
ii) Draw sigmamolecular orbitals resulting from s and p linear combination of atomic orbitals



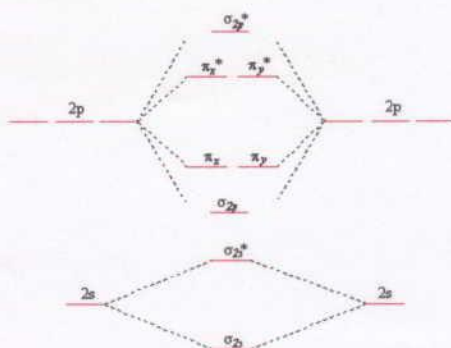
iii) Draw bonding pi molecular orbitals resulting from p and p linear combination of atomic orbitals



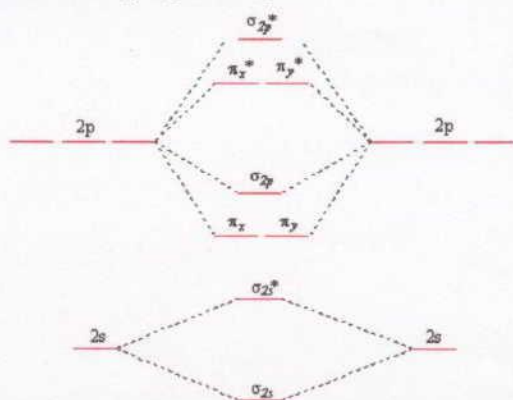
iv) Draw anti-bonding pi molecular orbitals resulting from p and p linear combination of atomic orbitals



B. Draw molecular orbitals for homonuclear diatomic molecules of the 2nd period elements O_2 , F_2 and Ne_2



C. Draw molecular orbitals for homonuclear diatomic molecules of the 2nd period elements B₂, C₂ and N₂



D. Using the molecular orbital diagram for the homonuclear diatomic molecules of the 2nd period elements calculate the following:

Energy ↑	Li ₂	Be ₂	B ₂	C ₂	N ₂	O ₂	F ₂	Ne ₂
	σ_{2p}^*	σ_{2p}^*	σ_{2p}^*	σ_{2p}^*	σ_{2p}^*	σ_{2p}^*	σ_{2p}^*	σ_{2p}^*
	π_{2p}^* π_{2p}^*	π_{2p}^* π_{2p}^*	π_{2p}^* π_{2p}^*	π_{2p}^* π_{2p}^*	π_{2p}^* π_{2p}^*	π_{2p}^* π_{2p}^*	π_{2p}^* π_{2p}^*	π_{2p}^* π_{2p}^*
	σ_{2p}	σ_{2p}	σ_{2p}	σ_{2p}	σ_{2p}	π_{2p} π_{2p}	π_{2p} π_{2p}	π_{2p} π_{2p}
	π_{2p} π_{2p}	π_{2p} π_{2p}	π_{2p} π_{2p}	π_{2p} π_{2p}	π_{2p} π_{2p}	σ_{2p}	σ_{2p}	σ_{2p}
	σ_{2s}^*	σ_{2s}^*	σ_{2s}^*	σ_{2s}^*	σ_{2s}^*	σ_{2s}^*	σ_{2s}^*	σ_{2s}^*
	σ_{2s}	σ_{2s}	σ_{2s}	σ_{2s}	σ_{2s}	σ_{2s}	σ_{2s}	σ_{2s}

i) Number of valence electrons in each molecule:

$$\text{Li}_2 = \quad \text{B}_2 = \quad \text{C}_2 = \quad \text{N}_2 = \quad \text{O}_2 = \quad \text{F}_2 = \quad \text{Ne}_2 =$$

ii) Bond order of each molecule:

$$\text{Li}_2 = \quad \text{B}_2 = \quad \text{C}_2 = \quad \text{N}_2 = \quad \text{O}_2 = \quad \text{F}_2 = \quad \text{Ne}_2 =$$

iii) Unpaired electrons in each molecule:

$$\text{Li}_2 = \quad \text{B}_2 = \quad \text{C}_2 = \quad \text{N}_2 = \quad \text{O}_2 = \quad \text{F}_2 = \quad \text{Ne}_2 =$$