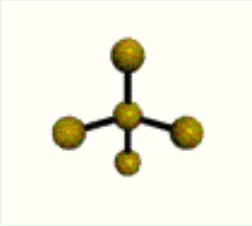
Valence-Shell Electron-Pair Repulsion(VSEPR) Theory:

Theory which predicts the geometric arrangement of atoms in a molecule. The valence electron pairs occupy positions as far as possible from one another. All electron pairs are considered.

In VSEPR theory double and triple bonds are treated as single bonds.

Number of Electron Pairs	Number of Lone Pairs	Geometry	Example
4	0	Tetrahedral	
4	1	Trigonal pyramidal	
4	2	Bent	

Valence-Shell Electron-Pair Repulsion(VSEPR) Theory:

In VSEPR Theory double and triple bonds are treated the same as single bonds.

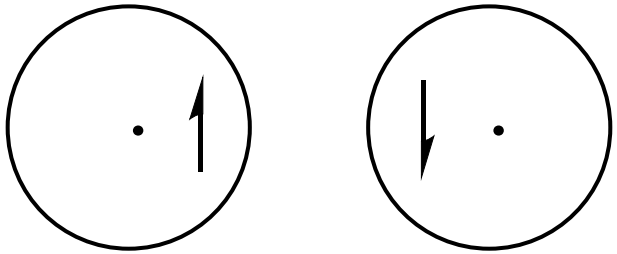
Lone-pair Lone-pair repulsion	**>**	**Lone-pair Bonding-pair repulsion**	**>**	**Bonding-pair Bonding-pair repulsion**

Valence Bond Theory:

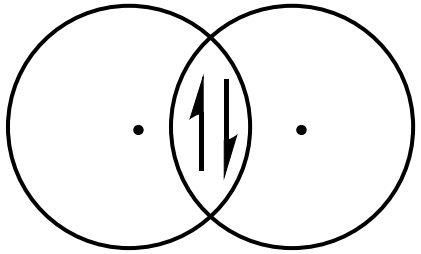
A covalent bond results when a singly occupied valence orbital of one atom overlaps a singly occupied valence orbital of another atom.

Consider H_2 molecule.

H: $1s^1$



$1s^1$:H

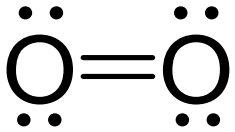


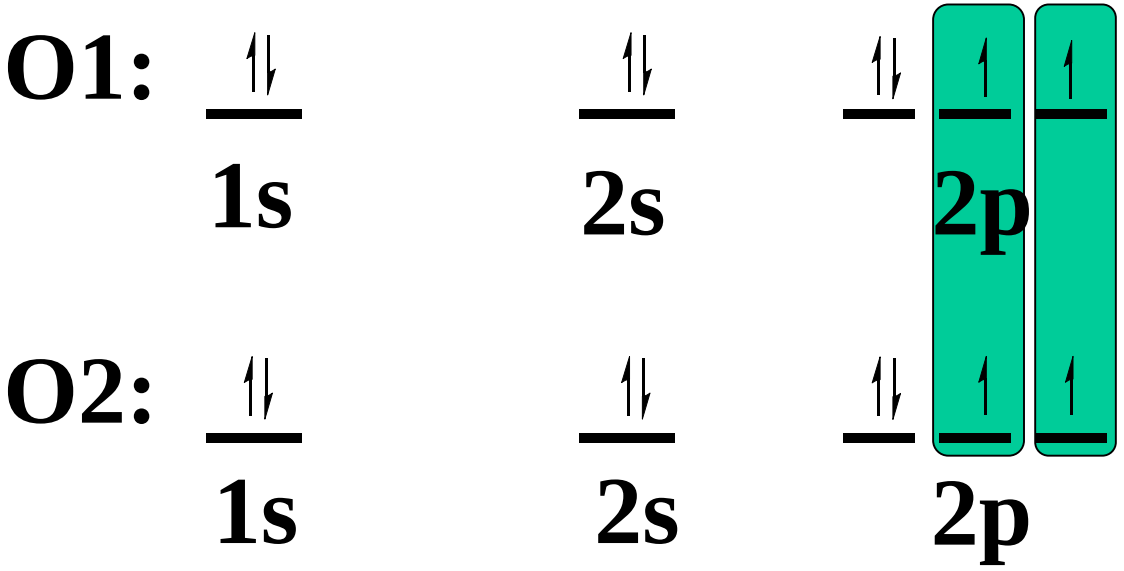
H—H

Hybridization:

Consider H_2. According to valence bond theory each atom contains a single unpaired electron. Each atom can form a single bond.

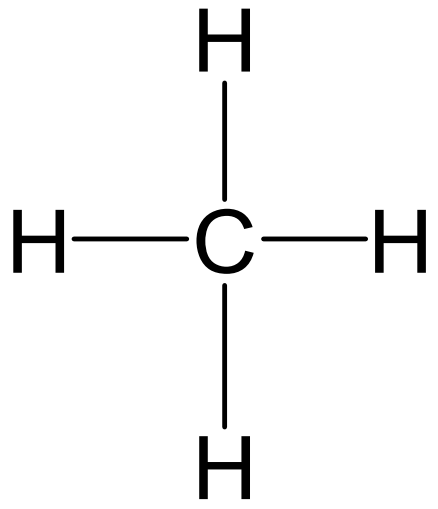
Consider oxygen(O_2). Each O atom should be able to form two bonds.





Hybridization:

Consider CH_4.



4H: $\frac{\uparrow}{1s}$

C: $\frac{\uparrow\downarrow}{1s}$ $\frac{\uparrow\downarrow}{2s}$ $\frac{\uparrow}{}\ \frac{\uparrow}{}\ \frac{}{2p}$

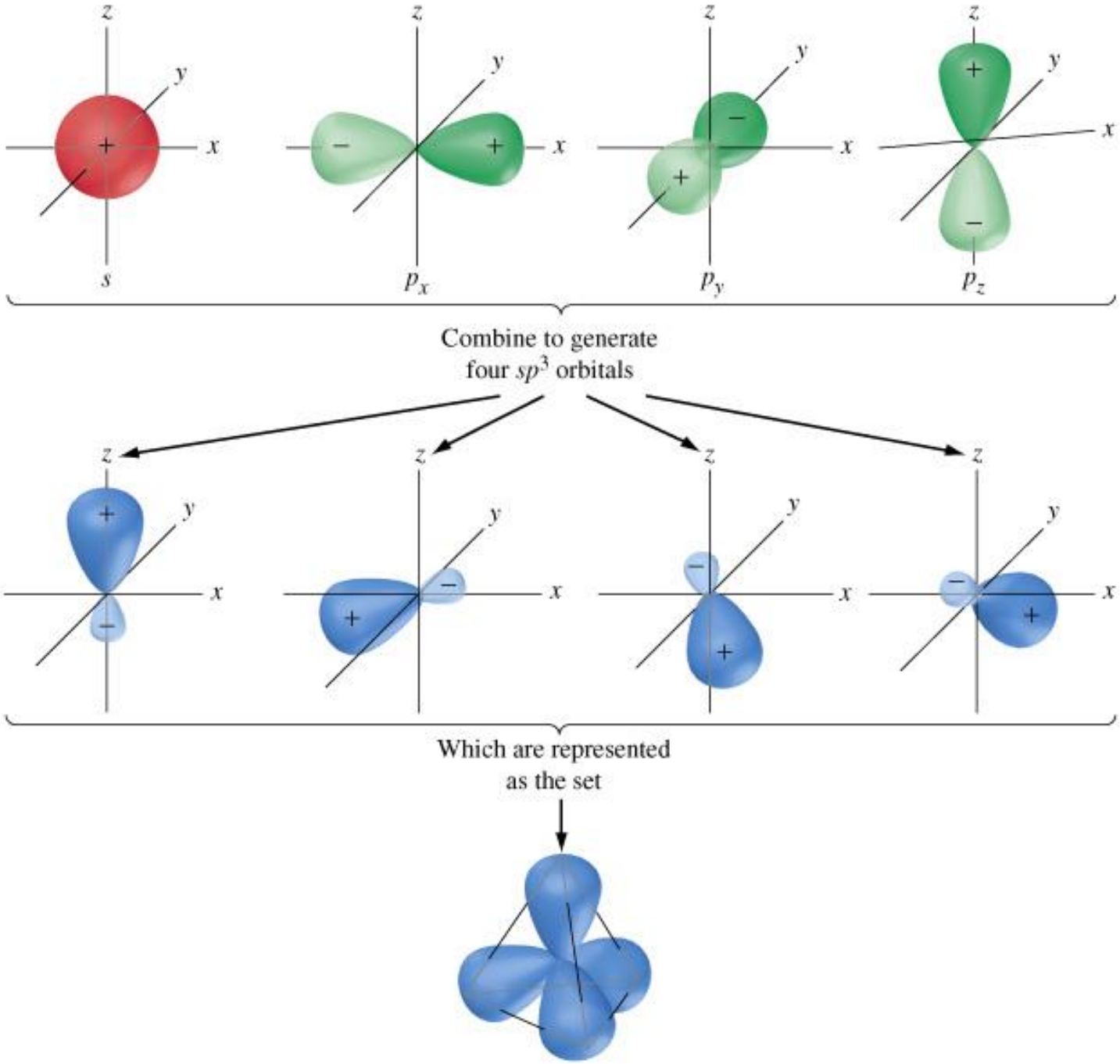
According to Valence Bond theory, C should only form 2 bonds. We know it form 4 bonds. Why??

Hybridization:

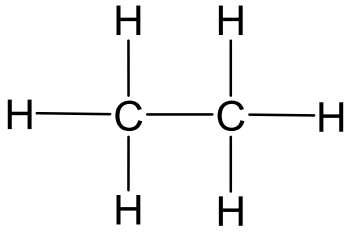
Hybridization is the mixing of atomic orbitals.

sp^3 ¼ s character

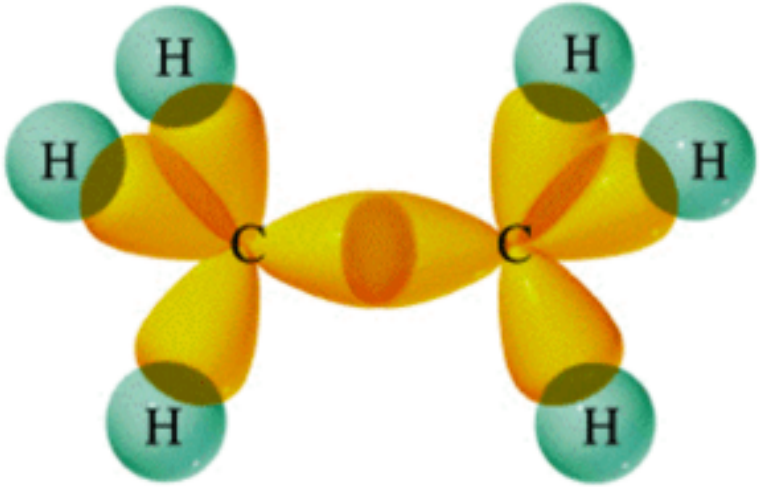
¾ p character



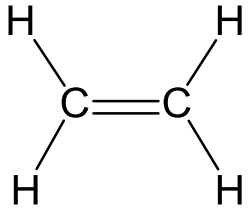
Reference: http://davidjohnewart.com/Chemistry/chemtheft/12.html



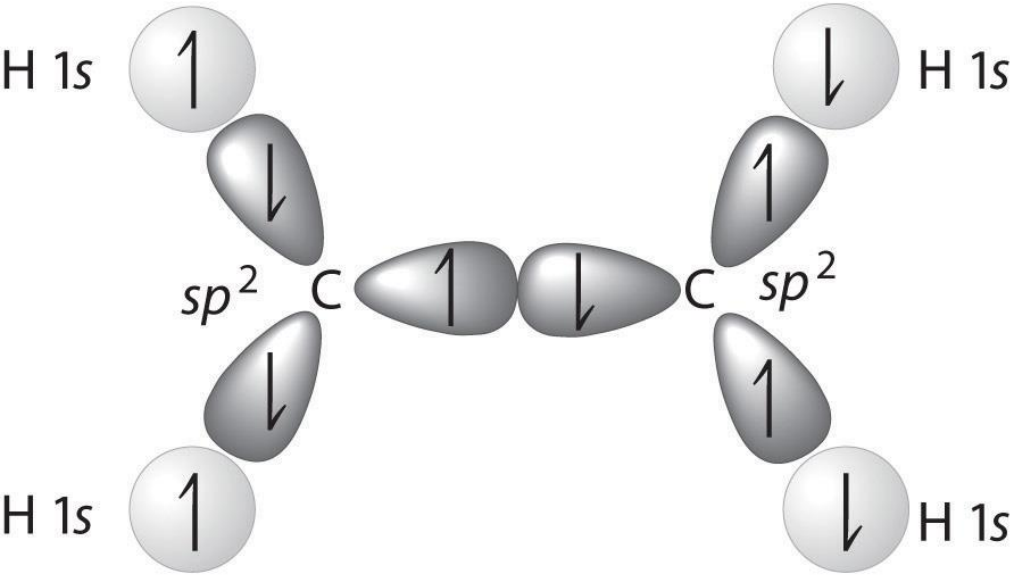
ethane



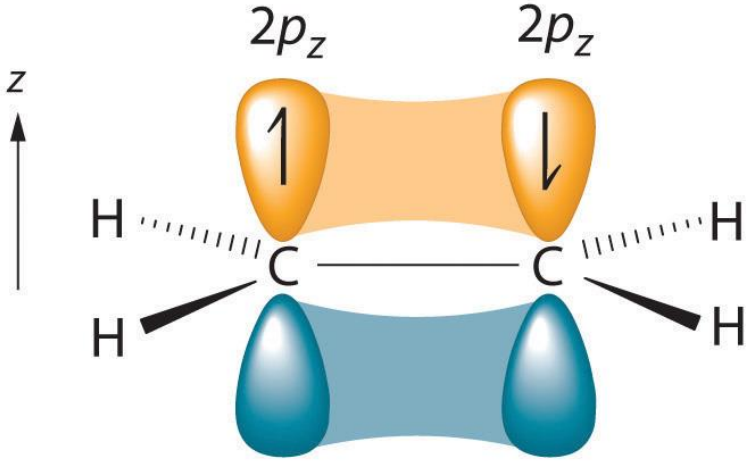
Reference: http://classnotes.org.in/class11/chemistry/chemical-bonding-molecular-structure/hybridisation/



ethene



(a) C_2H_4 σ-bonded framework



(b) C_2H_4 π bonding

Dipole Moment:

If two equal and opposite charges are separated by a known distance, the dipole moment is defined as follows.

$$\text{Dipole Moment}(\mu) = Q \times r$$

Q: charge **r: distance between charges**

Ex: δ^+ δ^-

H–F **polar molecule**

Expressed in Debye Units(D).

1 D = 3.33×10^{-30} C·m

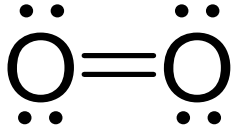
Polar vs. Non-polar Molecules:

Factors Determining the Polarity of a Molecule:

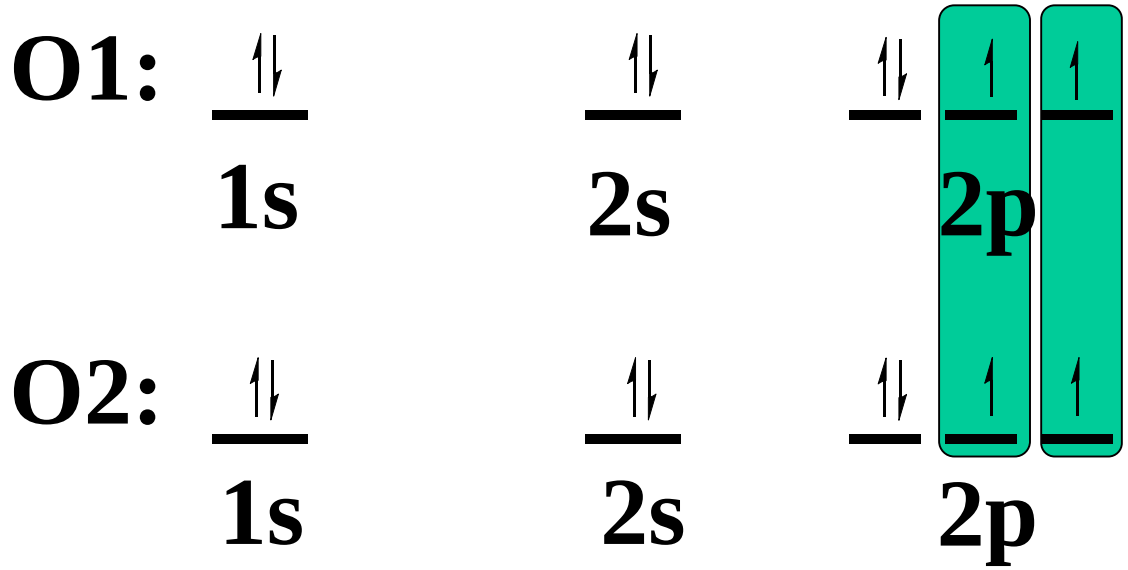
1. **Dipole moment.**
2. **Shape of the molecule.**

MO Theory:

Consider oxygen(O_2).



According to Lewis and Valence Bond Theory, O_2 has all paired electrons. Not so!!!



MO Theory:

When atoms bond, atomic orbitals(AO's) combine to form molecular orbitals(MO's).

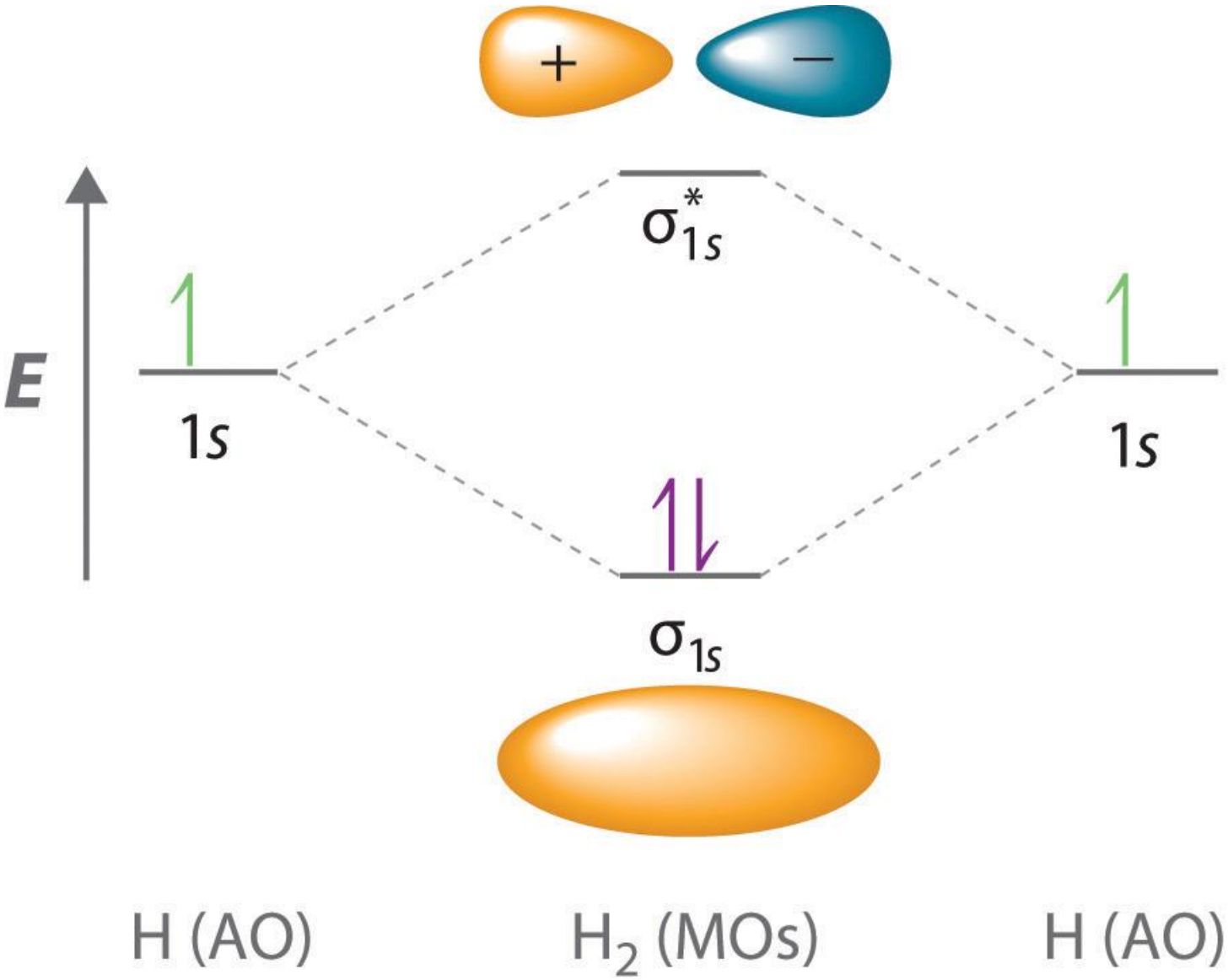
 # AO's = # MO's

Orbital interaction can be additive or subtractive.

Subtractive – Do not promote bonding. Higher energy. Ex: σ^*

Additive – Promote bonding. Lower energy. Ex: σ

Consider MO diagram for H_2.



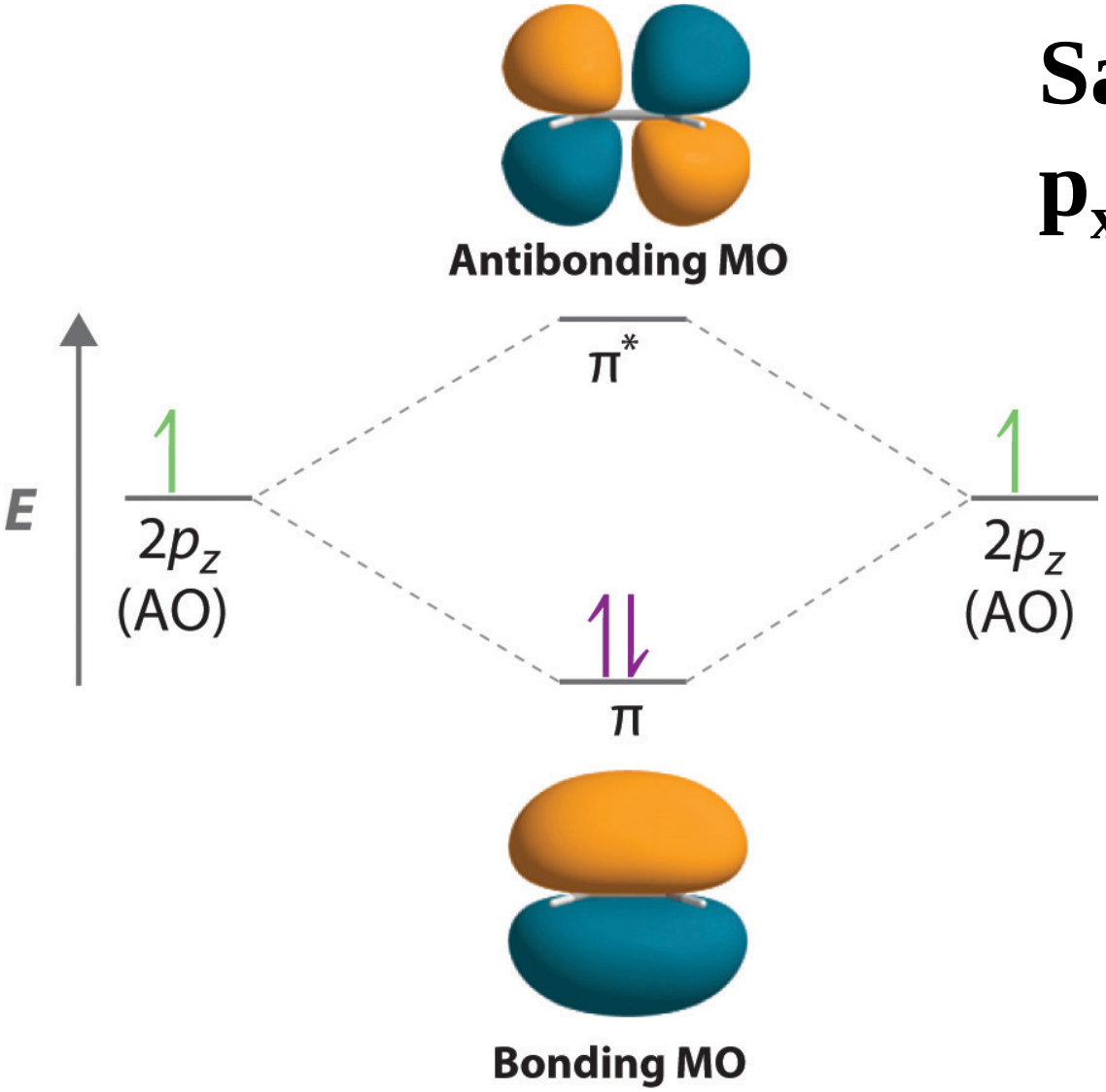
Reference: https://www.pinterest.ca/pin/322851867015938399/

Bond Order:

Bond Order is a measure of the number of electron pairs shared between atoms.

$$\text{Bond Order} = \frac{\#\text{ bonding electrons} - \#\text{ antibonding electrons}}{2}$$

Molecular Orbitals from p orbitals:



Same for p_x and p_y.

Reference: https://chem.libretexts.org/LibreTexts/Mount_Royal_University/Chem_1201/Unit_4%3A_Chemical_Bonding_II_-_Advanced_Bonding_Theories/4.11%3A_Multiple_Bonds_in_MO_Theory

MO Diagram for Oxygen(O_2) :