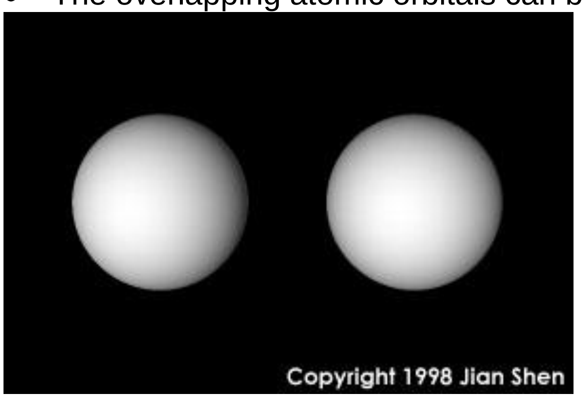
BONDING THEORY

Stable Octet

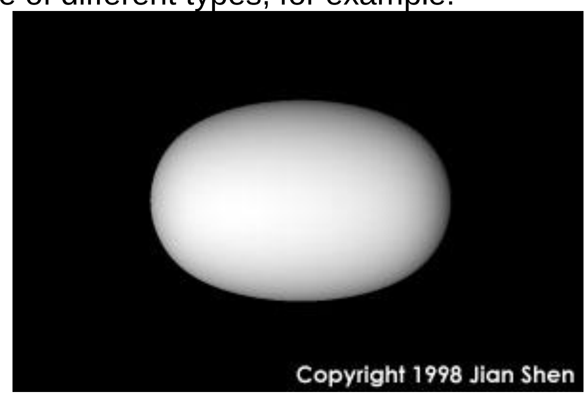
- Taught to you in grade 11
- An atom with a full outer shell had the lowest potential energy and that is why we tried to bond atoms in such a way as to attain a full outer shell (usually 8 valence electrons)
- Electrons were shared (covalent bonds) or transferred (ionic bonds) to give each atom a full outer shell

Valence Bond Theory

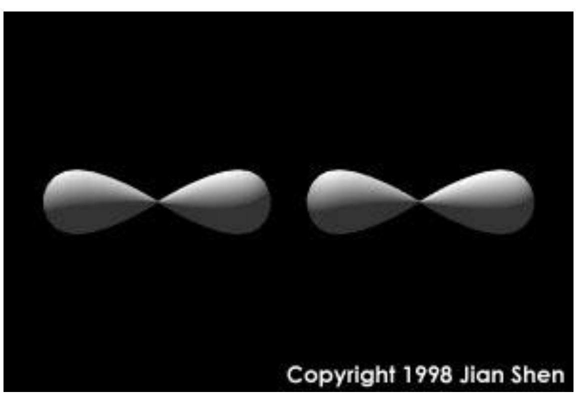
- This approach considers the overlap of the atomic orbitals of the participating atoms to form a chemical bond
- Due to the overlapping, the electrons are localized in the bond region
- The resulting bond is a single bond and is called a sigma (σ) bond
- The overlapping atomic orbitals can be of different types, for example:



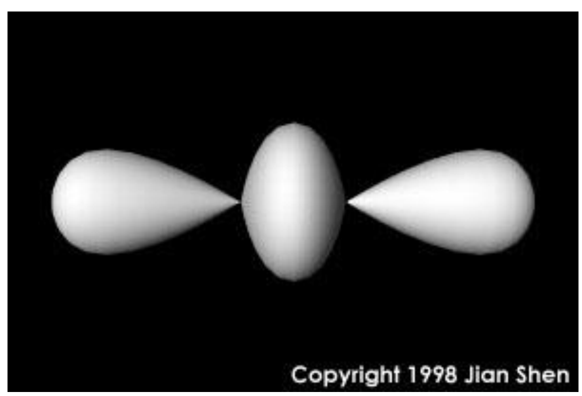
2 unbonded “s” orbitals



s & s sigma bond



2 unbonded “p” orbitals



p & p sigma bond

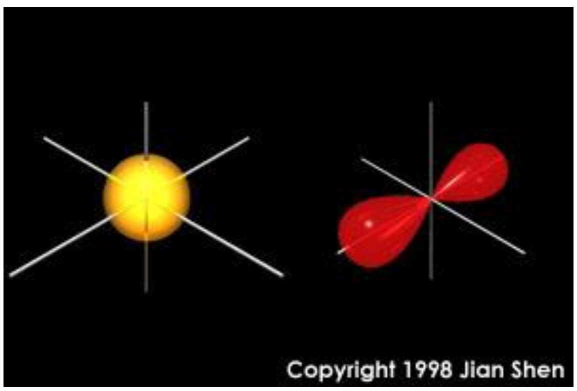
- Not all bonding results in a simple overlap of the “pure” atomic orbitals
- Remember that atomic orbitals can only hold a maximum of 2 electrons so overlapping can only occur when 2 half filled orbitals overlap

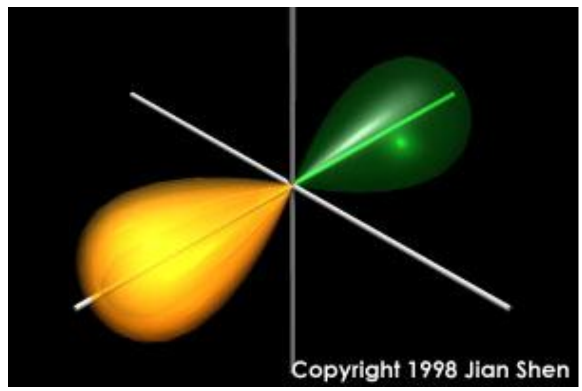
- H_2 1s1 + 1s1 (each hydrogen atom has a half filled orbital that can overlap with the other, forming a FULL overlapped orbital
- In the compound BeF_2,
  F = 1s2 2s2 2px2 2py2 **2pz1** (it has a half-filled orbital to overlap)
  Be = 1s2 2s2 (no half filled orbital therefore it cannot overlap and should not be able to form a bond with fluorine)

<u>Hybridization</u>

- Orbitals in the same atom which lie close to one another in energy have an unusual ability to combine with one another in an additive way
- This phenomenon is called HYBRIDIZATION
- The resulting hybrid orbitals contain properties of their parental atomic orbitals
- Each hybrid orbital is oriented as far apart from one another as possible resulting in the largest possible break angle

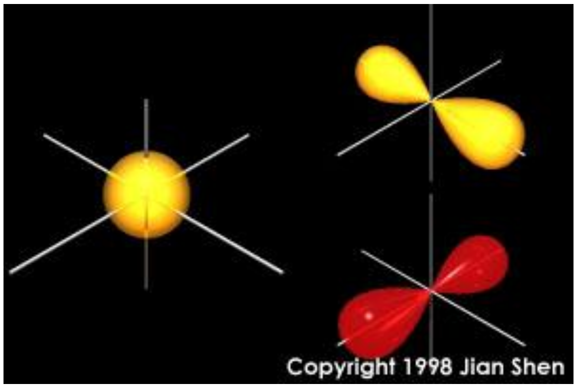
<u>sp Hybridization</u>

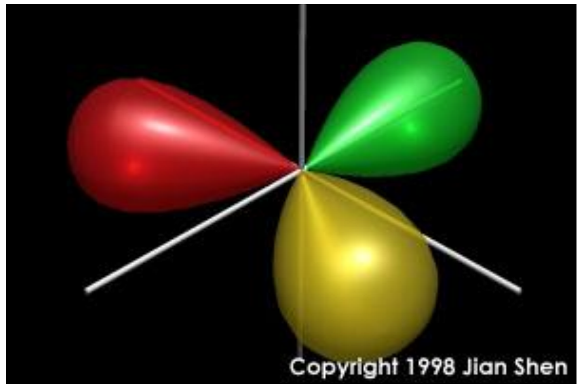




- One s and one p orbital combine to form a new set of 2 sp hybrid orbitals
- Each of the 2 sp hybrid orbitals are equivalent but oriented in opposite directions in space
- Together, the 2 hybrid orbitals form the combined sp hybrid orbital which is capable of 2 bonds
- The shape of this hybrid orbital is linear and thus has a break angle of 180°
  - $BeCl_2$, C_2H_2, HCN and CO_2 all have sp hybrid orbitals

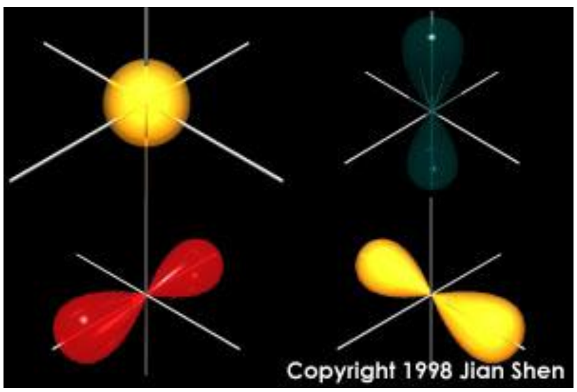
sp2 Hybridization

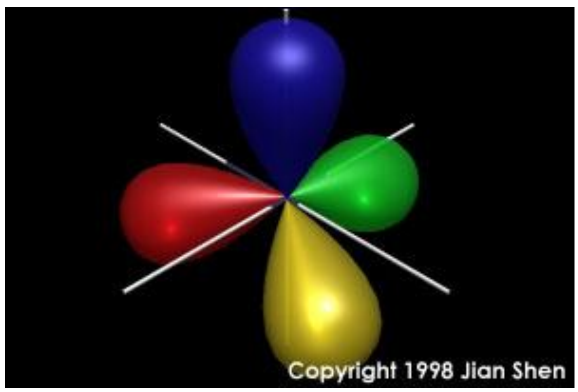




- One s and 2 p orbitals combine to form a new set of 3 sp2 hybrid orbitals
- Each of the 3 sp2 hybrid orbitals are equivalent but oriented as far apart from each other in space
- Together, the 3 sp2 orbitals are capable of 3 bonds
- The shape of this hybrid orbital is trigonal planar and thus has a break angle of 120°
    - BF_3, CO_3^{-2}, NO_3^{-1}, NO_2, SO_2, benzene all have sp2 hybrid orbitals
- *Not all three sp2 hybridized orbitals have to be used in bonding*
- *One of the orbitals may be occupied by a pair or single electron; this will yield one of the derivative shapes of the trigonal planar*

sp3 Hybridization





- One s and 3 p orbitals combine to form a new set of 4 sp3 hybrid orbitals
- Each of the 4 sp3 hybrid orbitals are equivalent but oriented as far apart from each other in space
- Together, the four sp3 hybrid orbitals are capable of 4 bonds
- The shape of the hybrid orbital is tetrahedral and thus has a break angle of 109.5°
    - CH_4, NH_3, H_2O, SO_4^{-2}, CH_3Cl, NH_4^{+1}, PF_3, all have sp3 hybrid orbitals

- *One or two of the sp3 hybrid orbitals may be occupied by non-bonding electrons which will form one of the tetrahedral derivative shapes* sp3d Hybridization

- One s orbital, 3 p orbitals and one d orbital combine to form a new set of 5 sp3d hybrid orbitals
- Not all 5 of these hybrid orbitals are equivalent; the 2 axial orbitals are equivalent (90° from the equatorial orbitals; 180° apart from each other) and the 3 equatorial orbitals are equivalent (120° apart from one another)
- Together, the 5 hybrid orbitals form the combined sp3d hybrid orbital and is capable of 5 bonds
- The shape of this hybrid orbital is trigonal bipyramidal
    - PCl5, PClF4, TeCl4, BrF3, SF_4, IF_3, XeF_2, I_3^{-1} all have sp3d hybrid orbitals
- *Some of the sp3d hybrid orbital can contain pairs of unbonded electrons which will form one of the trigonal bipyramidal derivative shapes*

sp3d2 Hybridization

- One s orbital, 3 p orbitals and 2 d orbitals combine to form a new set of 6 sp3d2 hybrid orbitals
- Not all 6 of these hybrid orbitals are equivalent; the 2 axial orbitals are equivalent (180° apart from one another) and the 4 equatorial orbitals are equivalent (90° for each other)
- Together the 6 hybrid orbitals form the combined sp3d2 hybrid orbital and is capable of 6 bonds
- The shape of this hybrid orbital is octahedral
    - SF_6, IF_5, IOF_5, XeF_4, BrF_5, SiF_6^{-2}, PF_6^{-1} all have sp3d2 hybrid orbitals
- *Some of the sp3d2 hybrid orbitals can contain pairs of unbonded electrons which will form one of the derivative shapes of the octahedral*