Lecture 10, Feb 2, 2022

Heteronuclear Diatomic Orbitals

- When two atoms come together with different energies in the orbitals, the electrons in the molecular orbitals will be closer to the one with the lower energy
  - Electron density is greater in the negative ion (lower energy) side
- When the difference in energy is very large, the filled orbital on the negative ion has the same energy as the atomic orbital
- Atomic orbitals most effectively overlap to form molecular orbitals when:
  1. Shapes are conductive to good overlap – symmetry
  2. Their energies are similar in the separated atoms
- Electronegativity difference χ between a pair of atoms in a bond defines the unbalanced electron sharing or formation of a polar bond
  - $|\chi_A - \chi_B| = \sqrt{D_{AB} - (D_{A_2} D_{B_2})^{\frac{1}{2}}}$
  - Normalized so that fluorine is 4
- $\Delta\chi > 1.8$ is ionic; $\Delta\chi < 0.6$ is covalent; in between is polar covalent
- With polar covalent bonds, the bonds have a dipole; the vector sum of the all the bond dipoles is the overall molecular dipole
  - The dipole moment $\mu = qr$ where r is the distance between charges and q is the magnitude of charge separation

Hybridization

- Add together the s orbitals and p orbital wavefunctions to create hybridized orbitals in order to follow VSEPR shapes
- Examples:
  - Tetrahedral: NH_4
    * Nitrogen has valence shell electron configuration $2s^2 2p^3$
    * 1 electron from the s shell gets promoted into the same energy as a p shell, and then the s shell and 3 p shells hybridize to form sp^3 orbitals
    * The sp^3 orbitals have 4 symmetric lobes arranged in a tetrahedral pattern; each lobe will have 1 electron in it, which can σ bond with the s shell in the hydrogen
  - Linear: CO_2
    * The middle carbon forms sp hybrid orbitals, with 2 symmetric lobes arrange linearly
    * The 2 lobes from the sp orbitals σ bond with the p orbitals in the oxygen atoms
    * The remaining 2 p unhybridized orbitals form π bonds with the p orbitals in the hydrogen atoms