Lecture 9, Jan 30, 2023

Formation of Molecular Bonds

- When two atoms come together, the sign of the electron wavefunctions determine the phase of the electron movements
- When the wavefunctions have the same sign, the wavefunctions interfere constructively and electron density builds up between the two nuclei; this gives the bonding orbital
  - This represent the two electrons being in phase and so they are always staying far away from each other
- When the wavefunctions have different signs, the wavefunctions interfere destructively so electron density in the middle of the nuclei cancels; this gives the antibonding orbital
  - The electrons are out of phase so they feel stronger repulsion
- For every bonding orbital there is an equivalent antibonding orbital
- A *nonbonding* orbital has the constructive and destructive interference parts perfectly cancel out
- The *orbital overlap* $\langle\psi_1|\psi_2\rangle = S_{ab} = S_{ba}$ is the extent to which the two orbitals overlap in space
  - If the two orbitals are orthogonal, they have zero overlap
- When two atoms are brought together, these bonding/antibonding/nonbonding orbitals are created
  - These are shown as states that are lower/higher energy than the original orbitals
  - A nonbonding orbital would be a lone pair
  - Antibonding orbitals are denoted by a star
  - Molecular orbitals are often symmetric; they are denoted g (gerade, even) if they are identical under inversion, or u (odd) if they change sign
- The bond order is defined as the number of electrons in bonding orbitals minus the electrons in antibonding orbitals, divided by 2
  - A bond order of 0 or less cannot exist, e.g. He_2 does not exist because it would have a bond order of $\frac{2-2}{2} = 0$
- In the period 2 elements, the additional states create more molecular orbitals
  - In period 2 there are 8 orbitals (4 pairings of atomic orbitals, times 2 for bonding/antibonding)