

Shapes of Common Frontier Molecular Orbitals

Remember:

- (1) If 2 atoms are different, the coefficients will not be the same.
 (a) In HOMO, larger coefficient on more electronegative atom.
 (b) In LUMO, larger coefficient on less electronegative atom.
 (2) Substituent effects
 (3) Use Huckel MO when considering conjugated systems.