Lecture 7, Jan 23, 2023

Stability and Bonding

- Elements with a high Z_{eff} have higher electron affinity, and tend to form nonmetals (e.g. the halogens)
- When two atoms are brought near each other, the electron density builds up between them and screens the proton charge
  - When the two electrons are moving towards each other, the state has higher energy; this is an *antibonding* state
  - When they are moving away from each other, the state has lower energy; this is a *bonding* state
- We can solve the problem of one electron and two protons, which corresponds to the case of ${H_2}^+$
  - In the antibonding state electron density depletes in the centre due to the destructive interference, so the electrons are concentrated near the outside
    * The higher energy of the antibonding state tends to pull the molecule apart
  - In the bonding state electron density builds up in the centre; the electrons are concentrated near the centre
    * The bonding state has lower energy since the high electron density in the centre is closer to the protons
  - In the bonding state, there is a minimum in the energy as a function of the inter-proton distance, which facilitates bonding
- Both bonding and antibonding states are reflected by a superposition of atomic orbitals to form molecular orbitals (LCAO-MO)
  - The two ways we can superimpose the two hydrogenic wavefunctions are $\Psi^+ = \Psi_1 + \Psi_2$ and $\Psi^- = \Psi_1 - \Psi_2$
  - In the case of Ψ^+, the two wavefunctions are in phase, so in the middle between the two atoms they add constructively; this reflects the buildup in electron density that lowers the energy
  - In the case of Ψ^-, the two wavefunctions are out of phase so interfere destructively between the two atoms; this reflects the depletion in electron density that raises the energy
- When the overlap is spherically symmetric you get a σ bond (s orbitals)