Introduction to Bonding

- Molecule forms if total energy of molecule is lower than the total energy of the separated atoms
- Simplest case: ionic compound, like NaCl
- Could use IE, EA, Coulomb’s Law to find energy

NaCl Energetics

- IE for Na is 495.8 kJ/mol
- EA for Cl is –349.0 kJ/mol
- So forming the ions costs energy: 495.8 – 349.0 = 146.8 kJ/mol
- Coulomb energy for attraction between the ions is –490.8 kJ/mol
- Overall process releases energy
NaCl Crystal Structure

Other Types of Bonding
- Most compounds are not ionic.
- H₂, N₂, etc.
- Bonding based on electron sharing rather than electron donation.
- “Covalent bonding”

Bonding in H₂: Orbital Picture
- Interaction between valence atomic orbitals
- H-atom has 1s¹ electron configuration
- Picture the bond between 2 H-atoms as interaction between the 1s orbitals.
H₂ Molecule

- Bond strength maximized at optimum distance
  - "equilibrium bond length."
- Further apart:
  - weaker electron-nucleus interactions
- Closer together:
  - strong nucleus-nucleus repulsion

H₂ Potential Curve

HF - Lewis Picture

- Try using overlap of valence orbitals, like in H₂
- HF
  - H: 1s¹, F: 2s², 2p⁶
- Lewis structure:
  H⁺ + F⁻ → H⁺F⁻
HF - Orbital Overlap?

- H: 1s¹, F: 2s², 2p⁵
- Bond formed from overlap of 1s orbital on hydrogen and a 2p orbital on F. (say 2p₂)

Types of Bonds

- Ionic Bonding → e⁻ donation
- Covalent bonding → e⁻ sharing
- Most bonds are a combination of the two.
- Polar covalent → uneven e⁻ sharing
Electronegativity

• “... ability of an atom in a molecule to attract the shared electrons in a chemical bond”
• Related to IE and EA
• How would you expect electronegativity to vary in the periodic table?

Electronegativity

• High electronegativity means atom attracts electrons strongly
• Low electronegativity means it is fairly easy to pull electron density away from an atom
Electronegativity

- Large (negative) EA $\rightarrow$ high electronegativity
- Small IE $\rightarrow$ low electronegativity

Electronegativity

- Values approximate, scale arbitrary
- Highest electronegativity: F, $\chi = 4.0$
- Lowest electronegativity: Cs, $\chi = 0.7$
- Generally $\chi$ increases as you move up or to the right in periodic table

Electronegativity Difference

- In a purely covalent bond, the 2 atoms are identical: H$_2$, N$_2$, etc.
- Same electronegativity, so perfectly even sharing
**Electronegativity Difference**

- In an ionic bond, one atom has high electronegativity, one low: NaCl
  \( \chi(\text{Na}) = 0.9, \chi(\text{Cl}) = 3.0 \)
  so \( \Delta\chi = 2.1 \)
- Chlorine pulls an electron away from sodium, forming ions

**Polar Bonds**

- For most bonds, \( \Delta\chi \) is small but not zero
- This gives an intermediate case: electrons shared, but not equally
- CO: \( C: \chi = 2.5, \text{ O: } \chi = 3.5; \Delta\chi = 1.0 \)
- Not ionic, but not purely covalent, either

**Electronegativity difference**

- If \( \Delta\chi \geq \sim 2 \), bond is ionic
- If \( \Delta\chi = 0 \), bond is purely covalent
- If \( 0 < \Delta\chi < \sim 1.8 \), bond is polar
- There’s a bit of a gray area between “very polar” and “ionic.”
- Example:
  - HF has \( \Delta\chi = 1.9 \), but is a gas \( \rightarrow \) polar
  - MgCl\(_2\) has \( \Delta\chi = 1.8 \), but is a high m.p. solid \( \rightarrow \) ionic