Lecture 11, Feb 3, 2022

Correspondence Principle

- Quantum effects are important when de Broglie wavelength is comparable to the spacial scale of the phenomenon
  - The phase of wavefunctions also need to be conserved – if the time scale of action is comparable to quantum decoherence then quantum effects are important
  - Important for quantum computers
- The core of quantum mechanics is the quantization of energy given as ΔE
  - The classical limit is defined as $\Delta E \ll kT$
  - In this limit thermal collisions blur out any resemblance of a wave and the system behaves classically
- The correspondence principle states that there is a continuous bridge from discrete quantized resonance conditions of the quantum world to the continuum variables of classical mechanics
  - e.g. for the infinite potential well $E = \frac{h^2 n^2}{8mL^2}$, if L or m are on the classical scale, then E is extremely small and energy approaches a continuum
- Example: Protein motion
  - Functionally relevant motions of proteins are on the scale of 1 to 10 angstroms
  - de Broglie wavelength calc be calculated using the mass and thermal velocity, and turns out to be 1.8×10^{-13} m
  - This is much smaller than an atom so the system is not quantum

Long Range Intermolecular Forces

- Ionic bonds, covalent bonds, metallic bonds
- Metallic bonds are covalent bonding with different degrees of ionic character
  - Metals typically involve 3d or higher valence orbitals
  - This creates an electronic continuum and facilitates conduction

Short Range Intermolecular Forces

- Ion Coulombic dipole coupling: polar molecule with a permanent dipole moment interact with ions
  - Dipole moments result from large differences in electronegativities between bonded atoms
  - Potential function on the order of $\frac{1}{r^6}$
  - Bonding from 40-600 kJ/mol
  - e.g. dissolving a sodium ion in water perturbs 80 water molecules
- The hydrogen bond
  - Hydrogen bonds to oxygen, nitrogen or fluorine
  - The high specificity of this force imposes directions on biological molecules
  - Hydrogen bonds encode information in DNA, provide protein building sites, nucleation sites, etc
  - Also on the order of $\frac{1}{r^6}$
  - Bond energies of 10-40 kJ/mol
- Dipole-dipole interactions
  - Same physics as hydrogen bonds but 2 to 8 times weaker
  - Bond orders of 5-25 kJ/mol
  - Also on the order of $\frac{1}{r^6}$ for potentials
- Ion induced dipole interactions
  - Ions polarize an otherwise neutral atom, creating a dipole
  - Only occurs when the ion is in close proximity
  - Oxygen transport uses this to bind oxygen to ion in heme proteins
  - 3-15 kJ/mol
  - Potential on the order of $\frac{1}{r^4}$

- Dipole-induced dipole interaction
  - Even weaker, works the same
- Induced dipole-induced dipole: van der Waals force (aka dispersion or London forces)
  - Spontaneous movement of charges create temporary dipoles that induce more dipoles
  - Occurs when all molecules are strictly nonpolar
  - Weakest force, but powerful in numbers