Lecture 2 Notes

* **Review**
  + Weak interactions are significant
  + Functional groups determine behavior of molecules and are interchangeable (change group = change behavior)
  + Changing functional group = chemical reaction
  + Hydrolysis of ATP
    - ATP + H2O 🡪 ADP + Pi + Free Energy
    - Major source of energy for cell
    - The bonds are high energy because the phosphate groups are negative and naturally repel each other
* **Thermodynamics**
  + Energy is conserved (1st law of thermo)
    - Energy is neither created/destroyed but can be transformed from one form to another but it is always conserved
    - Can exchange energy with the universe in many ways (potential, mechanical, kinetic, heat, …)
  + Entropy increases (2nd law of thermo)
    - Not necessarily disorder/randomness
    - More accurately, entropy is the amount of possible microstates something can form
  + Living organisms transform energy through bonds (breaking, forming, shifting electrons)
    - This allows us to process macromolecules and derive energy from them
* **ΔG describes a reaction’s spontaneity**
  + When positive, not spontaneous
  + When negative, spontaneous
  + Most biological processes are not spontaneous
    - They can become spontaneous by adding reactions together
* **How can we get a reaction to become spontaneous?**
  + They can become spontaneous by adding reactions together
  + ΔG is additive
    - Coupled by a common intermediate (most often phosphate group)
    - Coupled half reactions through enzyme active site (squishing 2 reactions together)
    - Coupled to ion transport
* **ATP is the energy currency of the cell**
  + Bonds do not store energy (breaking bonds requires energy input)
  + Energy is released from products having lower energy
  + ATP hydrolysis is highly exergonic
  + Transfer of phosphate groups between biological compounds is like a transfer of free energy
    - Kinases- enzymes that add phosphate groups
    - Phosphatase- enzymes that cleave phosphate groups off
* **Why is ATP hydrolysis reaction so exergonic**
  + Decreasing electrostatic repulsion
  + Increasing resonance structures/stabilization
    - Electrons can wiggle from state to state giving multiple confirmations
  + Increasing ionization
  + Increasing solvation
    - Ionization and solvation go hand in hand; creating more ions allows it to become hydrated with a water shell and become more soluble
  + Most exergonic reactions have one or more of these above characteristics
  + Endergonic reactions will have the opposite characteristics
* **Equilibrium**
  + Keq shows which direction a reaction will head to
    - Keq >> 1, ΔG is large and negative
    - Keq << 1, ΔG is large and positive
    - Keq = 1, ΔG is 0
* **Spontaneity does not equal rate**
  + ΔG tells us nothing about the reaction rate
* **Activation energy is a barrier to reaction**
  + The transition state of any reaction is at the highest energy state that is possible
  + Activation energy barrier requires input energy (heat, …)
    - Our bodies can’t really use heat input
* **What physical factors contribute to EA**
  + Stability of the transition state
    - Weak interactions between reactants (H bonds)
  + pH
    - Deals with ionization (alters polarity and charge between functional groups)
  + Temperature
    - As temperature goes up, the likelihood of molecules rearranging themselves into the transition state goes up
  + Enzymes
    - Lower activation energy directly
* **Enzymes are proteins that catalyze reactions**
  + They do so by stabilizing the transition state
  + Active site- place on enzyme shaped to receive particular substrate
  + Enzymes are left unchanged after a reaction
  + E + S, ES, EP, E + P
  + Enzymes are highly specific
  + Nomenclature almost always ends in “-ase”
  + Enzymes are fully complementary (shaped correctly) with a substrate in the transition state
  + Covalent interactions lower activation energy by providing an alternate pathway (breaking covalent bonds)
  + Noncovalent interactions stabilize the transition state and release free energy (holding substrate through weak interactions until reaction occurs)
* **Enzymes lower a reaction’s activation energy by stabilizing the transition state**
  + This is done through weak interactions
    - This includes hydrophobic interactions (separates substrates from water)
* **Transition state is not a reaction intermediate**
  + Transition state is the highest energy state of the reaction
  + Transition states are highly unfavorable and highly unlikely to occur without an input of energy
* **Entropy reduction**
  + As entropy of the reactants decreases (they are more ordered and resemble the products more), the likelihood of the reaction occurring and the rate at which it will occur is much larger
* **Desolvation**
  + Compounds are often surrounded by a hydration shell
    - An enzyme, through hydrophobic interactions, can separate it from water and allow the substrates to interact alone
    - Enzyme does so by forming its own H bonds with substrate
* **Compensation for substrate distortion**
  + If a substrate can reach its transition state through an enzyme, an enzyme will hold it there to make the reaction more likely to go to completion
* **Catalytic alignment**
  + Induced fit/conformational change
    - The substrate binds first to enzyme, and then enzyme moves to conform substrate into a different conformation