Course goals: The central idea of this course is the free energy, the quantitative way we understand driving forces, i.e., the equilibria and rates in chemistry, physics and biology. We describe the underpinning components, the entropy and energy. We explore the microscopic interactions -- including hydrogen bonding, van der Waals, electrostatics and hydrophobic forces -- that explain physical and chemical mechanisms in biology and are the workhorse tools in computational drug discovery. We show how these basic ideas are applied: binding affinities are the basis for drug discovery; coupled binding is the basis for how biological machines convert energy and transduce signals; and polymer free energies are the basis for the folding of protein and RNA molecules.

1/30) Probabilities. Counting states as a basis of entropy (MDF 1, 2).
2/1) Entropy and Energy as driving forces (MDF 3).

2/4) Partial derivatives (MDF4) (a).
2/6) Max Ent and the Boltzmann distribution law (MDF 5) (a).
2/8) Energies and enthalpies. Thermodynamic states (MDF 6).

2/11) Free energies, chemical potentials (MDF 8, 9).
2/13) Microscopic modeling and the Boltzmann law (MDF 10).

2/18) Liquids & phase equilibria (MDF 14).
2/20) Solvation. Free energies of transfer (MDF 16).


3/6) Electrochemical equilibria (MDF 22).

3/11) Intermolecular forces: van der Waals, dipolar, hydrogen bonds (MDF 24).
3/13) Properties of water. Hydrophobic solvation (MDF 30, 31)


4/1) Polymer entropies, constraints and folding (MDF 33, 34) (d).
4/3) Protein structures (PP1) (c).
4/5) Protein function and mechanisms (PP2) (c).

4/8) Protein stability (PP3).
4/10) Protein cooperativity: helix-coil transitions (PP4).
4/12) Protein folding & aggregation (PP4).

4/17) Protein evolution and sequence space (PP6).
4/19) Bioinformatics, sequence comparisons (PP7) (d).

4/26) Role of physical & computational modeling in biopharma (c or f).

4/29 –) Student project presentations.

(a) Jin Wang (3)?
(b) Helmut Strey (2) – OK for 3/29 and 4/3, not 4/1.
(c) Markus Seeliger (2-4)?
(d) ??
(e) Rob Rizzo group (2).
(f) Wendy Cornell (1)?