**20.110 Thermodynamics of Biomolecular Systems, Fall 2013**

**Department of Biological Engineering**

The power of thermodynamics is in its ability to predict chemical and biological events. Will a metabolic reaction occur? Will a drug bind to its protein target and at what concentration will it be active? Will an antibody bind to an antigen? Into what structure will viral coat proteins self-assemble? Will a protein fold? This course is an introduction to the foundations of thermodynamics and its application to biomolecular systems. The first third focuses on the terms that go into the calculation of free energy (G=H-TS), which predicts whether or not a process will occur. This represents the culmination of the zeroth (T), first (H), and second/third (S) laws of thermodynamics. The second third moves to the details of molecular interactions through an introduction to statistical mechanics. Finally, the last third is focused on the application of these tools to biomolecular problem.

Each week there will be three lectures and one recitation devoted to discussion of the assigned problems and lecture material. The TAs and faculty will have office hours in their sections. The detailed lecture schedule is included with the reading assignments. It is important (and useful) that students do the reading before the lecture.

**Prerequisites**: 18.02, 5.111 or 5.112 or 3.091.

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| **Lectures:** | Monday, Wednesday, Friday 10:00 - 10:55 AM, Room 54-100.  Two hours of recitation for each section will be held each week. One hour will be a formal recitation of prepared material by the TA. The other hour will be held as an open-ended office hours. | |
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| **Instructors:** | *Professor Christopher Voigt (20.110)*  Office Hours: 12-1pm on Fridays (Room 47-277)  Office: 617-324-4851  Cell: 617-678-6441  [cavoigt@gmail.com](mailto:cavoigt@gmail.com)  *Professor Linda Griffith (20.110)*  Room 16-429  [griff@mit.edu](mailto:griff@mit.edu)  *Professor Moungi Bawendi (5.60)* | |
|  | Room 6-221  [mgb@mit.edu](mailto:mgb@mit.edu) | |
| **Teaching assistants:** | 20.110 TAs  Raven Reddy ravenr@mit.edu  Jonathan Chien jchien@mit.edu  Vibhuti Agrawal vagrawal@mit.edu  Devin Quinlan dquinlan@mit.edu  Teaching assistant conference hours and contact information will be posted on the course website (Stellar). | |
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| **Administration:** | Catherine Greene Department of Biological Engineering, Room 16-429, x3-0805 or x3-2400 | |
| **Textbooks:** | REQUIRED: Physical Chemistry, 4th ed. R.J. Silbey, R.A. Alberty and M.G. Bawendi, Wiley (2005)  REQUIRED: Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience, 2nd Ed. K. A. Dill and S. Bromberg, Garland (2010)  Other books that may prove useful:  Elements of Chemical Thermodynamics, L. K. Nash, Dover (2005)  Physical Chemistry, P. Atkins and J. de Paula, 8th Edition, Oxford (2006)  Physical Chemistry: Thermodynamics, H. Metiu, Taylor & Francis (2006)  Engines, Energy, and Entropy, J. B. Fenn, W. H. Freeman (1982) Physical Chemistry, Raymond Chang, University Science (2000)  Chemical Kinetics and Reaction Dynamics, P. L. Houston, Dover (2006)  Physical Chemistry for the Biosciences, R. Chang, University Science (2005).  Molecular Thermodynamics, McQuarrie and Simon, University Science (1999) | |
| **Web site:** | https://stellar.mit.edu/S/course/20/fa13/20.110J/#224909 |

**Examinations:** There will be three one-hour examinations during the term and a regularly scheduled final examination. **All mid-term exams will be in the evening**, on dates designated on the syllabus. Exam locations are noted on the syllabus. Class is therefore cancelled during a regular lecture hour, as indicated on the syllabus. Two exam sessions are offered for each exam: 5:45 – 7:15 pm and 7:30 – 9:00 pm. You may attend either exam session (but not both). You will be allowed to use a set of summary equations and notes, no longer than **one** double-sided 8.5" x 11" page per hour exam. In all other respects, the exams will be closed-notes and closed-book. You should also bring a “simple” calculator (a device that only serves as a calculator and cannot take pictures or communicate). Requests for **conflict exams** must be made to the Professor *more than* *two weeks prior* to the scheduled exam date. **Exam excuses for unforeseen circumstances** (sickness, other) require: 1. a note/request from Student Services (S^3) and 2. that you contact Linda Griffith to make arrangements. Requests for **exam re-grades** must be made to your TA *no later than one week after* the exam date.

**Homework**: Homework can (and should) be discussed with your classmates. You are encouraged to work in study groups, but must turn in only your own work. Problems will be assigned roughly every week (10 problem sets), as indicated on the syllabus, and will be due by 3:00 PM on the day specified in the drop boxes next to building 16-220 (next to the elevator). Late problem sets are not accepted. Excuses will not be accepted for late homework; however, the lowest two homework scores will be dropped. Solutions to the problem sets will be posted on the course web site. Homework will be returned in recitation.

**Grades** for the subject will be based on a total of 540 points as follows:

Hour exams 300 points (100 each)

Homework 40 points (5 each – 2 will be dropped)

Final Exam 200 points

**Tutorial reviews** will be held prior to each exam.

**Academic Honesty**

It is expected that students in 20.110 will maintain the highest standards of academic honesty.

With respect to homework assignments, it is expected that no student will turn in work that is not his or her own by copying the work of another student or by using the work or solutions from this subject given in previous years. Discussion of approaches to solving the homework problems, after tempting to work the problems independently, however, is permitted and *encouraged*.

It is expected that during a test or examination, a student will not (1) accept or use information of any kind from other students; (2) represent the work of another student as his or her own; (3) use aids to memory other than those expressly permitted by the examiner. Following a test or examination, a student will not try to deceive teachers or graders by misrepresenting or altering his or her previous work. In advance of a test or exam, a student will not knowingly obtain access to the exam questions.

Departures from the above standards are contrary to fundamental principles of MIT and of the larger scientific community. Such departures are considered serious offenses for which disciplinary penalties, including suspension and expulsion, can be imposed.

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| **20.110 lecture schedule and topics** | | | | | | | |
| Instructors: CV: Chris Voigt, LG: Linda Griffith, JB: Jenn Brophy | | | | | | | |
| **Lec** | **Date** |  | **Topic** | **Readings** | **PS Due** | **PS/Exam Contact** | **Lecturer** |
| 1 | 9/4 | W | Free Energy Overview, Thermodynamic Definitions, 0th Law: Temperature, 1st Law: Conservation, System Boundaries | Ch. 1.1-1.3, 2.1-2.6 |  |  | CV |
| 2 | 9/6 | F | State Functions I: Internal Energy, Heat and Work, Path Dependence | 2.7-2.9, 2.13 |  |  | CV |
| 3 | 9/9 | M | Enthalpy, Calorimetry, Heat Capacity | 2.11-2.12 |  |  | CV |
| 4 | 9/11 | W | Thermochemistry, Hess’ Law, Kirchoff’s Law |  |  |  | CV |
| 5 | 9/13 | F | State Functions II: Equations of State, Ideal Gas Law, Kinetic Theory of Gasses, Real Gases | 1.5-1.11 | #1 | CV | CV |
| 6 | 9/16 | M | Thermodynamic cycles, Reversible and Irreversible Transitions, Isothermal Expansion/Compression, Adiabatic Expansion | 2.10 |  |  | CV |
| 7 | 9/18 | W | 2nd Law: Spontaneous Processes, Entropy, Statistical versus Thermodynamic Interpretations, Isothermal Expansion | 3.1-3.2, 3.6-3.8, 16.1 |  |  | CV |
|  | 9/20 | F | Student Holiday |  |  |  |  |
| 8 | 9/23 | M | Entropy Change of Mixing, Phase Transitions, Heating, and Reactions, 3rd Law | 3.3-3.4, 3.9 | #2 | CV | CV |
| 9 | 9/25 | W | Heat Engines, Carnot Cycle | 3.5, 3.8 |  |  | CV |
| 10 | 9/27 | F | Thermodynamic Efficiency, Standard State Entropies, Criterion for Spontaneity | 4.1 | #3 | CV | CV |
| 11 | 9/30 | M | Gibbs and Helmholtz Free Energy, Free Energy of Reaction | 5.1 |  |  | CV |
|  | 10/2 | W | **EXAM 1** (Through Lec10/PS3) EVENING EXAM location TBA | (no class) |  | CV |  |
| 12 | 10/4 | F | Chemical Work and Fundamental Relationships, Free Energy in Living Systems, Maxwell’s Relations | 1.10; 4.6 |  |  | CV |
| 13 | 10/7 | M | Temperature Dependence of Free Energy, Gibbs-Helmholtz Equation, Pressure Dependence of Free Energy, Chemical Potential | 5.2-5.7 |  |  | CV |
| 14 | 10/9 | W | Phase Diagrams | 5.2-5.7 |  |  | CV |
| 15 | 10/11 | F | Chemical Equilibrium, Temperature Dependence of the Equilibrium Constant, Thermodynamics in Drug Design |  | #4 | CV | CV |
|  | 10/14 | M | Student Holiday |  |  |  |  |
| 16 | 10/16 | W | Powering our World: Energy Sources |  |  |  | MB |
| 17 | 10/18 | F | Pharmaceutical Applications |  | #5 | MB | JB |
| 18 | 10/21 | M | Introduction to Statistical Mechanics. | Dill 1 |  |  | CV |
| 19 | 10/23 | W | Probability & Ensembles | Dill 6 |  |  | CV |
| 20 | 10/25 | F | Microcanonical Ensemble and q; Boltzmann Distribution | Dill 7 | #6 | CV | CV |
| 21 | 10/28 | M | Canonical Ensemble and Q | Dill 10 |  |  | LG |
|  | 10/30 | W | **EXAM #2** (Through Lec20/PS6) EVENING EXAM, Walker Gym | NO CLASS |  |  |  |
| 22 | 11/1 | F | Lattice model, Phase Equilibria, surface & interfacial tension | Dill 15 |  |  | LG |
| 23 | 11/4 | M | Regular solutions, Mixing energy, mean fields | Dill 16 |  |  | LG |
| 24 | 11/6 | W | Colligative Properties: Osmotic Pressure, freezing pt depression | Dill 16 | #7 | LG | LG |
| 25 | 11/8 | F | Phase Partitioning & non ideal solutions | Dill 16 |  |  | LG |
|  | 11/11 | M | Student Holiday |  |  |  |  |
|  |  |  | ***-------------------5.60 AND 20.110 SPLIT-----------------*** |  |  |  |  |
| 26 | 11/13 | W | Binding Polynomials |  | #8 | LG | CV |
| 27 | 11/15 | F | Osmotic pressure and Phase Partioning | Dill 16 |  |  | LG |
| 28 | 11/18 | M | Surface tension | Dill 15 |  |  | LG |
|  | 11/20 | W | **EXAM 3** (Through Lec 28) EVENING EXAM, WALKER GYM | No class |  |  |  |
| 29 | 11/22 | F | Electrolytes I | Dill 22-23 |  |  | LG |
| 30 | 11/25 | M | Electrolytes at Interfaces; Debye length | Dill 22-23 | #9 | MB | LG |
| 31 | 11/27 | W | Polymers 1: Freely jointed chain | Dill 32 |  |  | LG |
|  | 11/29 | F | Student Holiday |  |  |  |  |
| 32 | 12/2 | M | Polymers 2: Chain Conformation | Dill 32 |  |  | LG |
|  | 12/5 | W | Polymers 3: Chain Stretching | Dill 33 | #10 | MB | LG |
| 33 | 12/7 | F | Self-Assembly and complex solutions |  |  |  | LG |
| 34 | 12/9 | M | TBD |  |  |  | LG |
| 35 | 12/11 | W | TBD |  |  |  | LG |