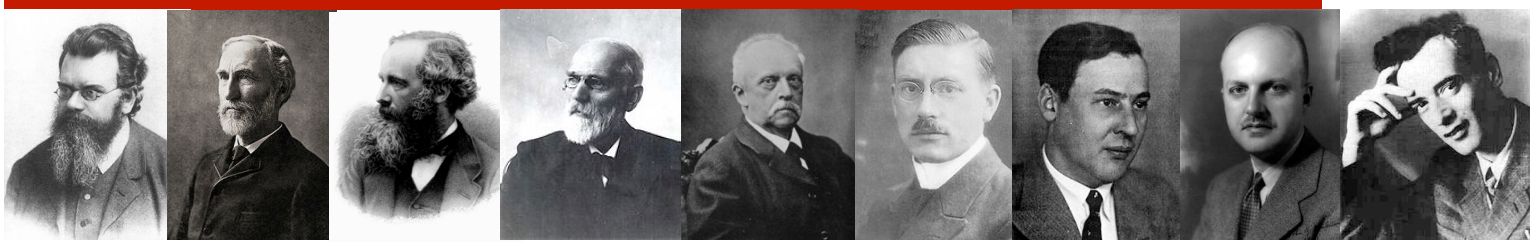
Fall 2017

# Chem. 661 Introduction to Statistical Mechanics



## Class Synopsis

Fundamental ideas of thermodynamics and statistical mechanics will be discussed. These include a brief review of thermodynamics, introduction of various ensembles, methods for computing thermodynamic observables of molecular systems using microscopic models, basic theories of phase transitions, imperfect gases, liquids and polyelectrolytes. If time permits, topics related to interface and polymer dynamics will also be covered.

Homework problems are largely of the pencil & paper type. There will be two mid-term exams and one cumulative final exam.

**Instructor**: Qiang Cui, Theoretical Chemistry Institute, Chem 8305i
Email: cui@chem.wisc.edu
**Lectures:** Chem 8335 MWF 11:00AM-11:50AM

## Textbook and References

- *Introduction to Modern Statistical Mechanics*, David Chandler, Oxford University Press, 1987 [An elegant basic introduction]
- *Statistical Mechanics*, Donald A. McQuarrie, University Science Books, 2000 [A classic text]
- *An Introduction to Statistical Thermodynamics*, T. L. Hill, Dover, 1986 [A classic text that includes clear explanations on key topics]
- *Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology,* Ken Dill and Sarina Bromberg, Garland Science, 2010 [A wonderfully clear introduction with many chemical and biological applications]
- *Basic concepts for simple and complex liquids*, Jean-Louise Barrat and Jean-Pierre Hansen, Cambridge University Press, 2003 [A collection of somewhat advanced topics related to simple and complex liquids]

| | Lec | Discussion Topic | Reference |
|---|---|---|---|
| Sept. 4 | L1 | **Goal; Rev. Thermo (1st Law)** | **Chandler, Ch1** |
| Sept. 6 | L2 | **2nd Law and equilibrium condition** | **Chandler, Ch1** |
| Sept. 9 | L3 | **Legendre transform; Maxwell relation** | **Chandler, Ch1** |
| Sept. 11 | L4 | **Euler Theorem; Extensive variables; Gibbs-Duhrem** | **Chandler, Ch1; Dill, Ch 9** |
| Sept. 13 | L5 | **Equilibrium Statistical Thermodynamics; probabilities I** | **Chandler, Ch1** |
| Sept. 16 | L6 | **Probabilities II** | **Dill, Ch1; Kardar Ch 2** |
| Sept. 18 | L7 | **Probabilities III** | **Dill, Ch1; Kardar Ch 2** |
| Sept. 20 | L8 | **Ensembles I: microcanonical** | **Chandler, Ch3** |
| Sept. 23 | L9 | **Ensembles II: canonical I** | **Chandler, Ch3** |
| Sept. 25 | L10 | **Ensembles III: canonical II** | **Chandler, Ch3** |
| Sept. 27 | L11 | **Ensembles IV: Generalized ensembles** | **Chandler, Ch3** |
| Sept. 30 | L12 | **Grand-canonical ensemble; Ideal gas law from uncorrelated fluctuati** | **Chandler, Ch3** |
| Oct. 2 | | **Ideal System I: Photon gas, Bose-Einstein/Fermi-Dirac distributions** | |
| Oct. 4 | L13 | **Ideal System II: Classical limit, monoatomic gas; Gibbs paradox** | **Chandler, Ch4** |
| Oct. 7 | L15 | **Diatomics II; Equipartition; Classical expression** | **Pathria** |
| Oct. 9 | L16 | **-------** | **McQuarrie, Ch6,7** |
| Oct. 11 | L17 | **Chemical equilibrium** | **Chandler, Ch4** |
| Oct. 14 | L18 | **Lattice vibration I - NMA** | |
| Oct. 14 ev | L19 | **Lattice vibration II - Einstein vs. Debye** | **McQuarrie, Ch11** |
| Oct. 18 | | **Mid-term Exam 1 (thermo; probabilities and ensembles)** | |
| Oct. 21 | | **Review of the first mid-term** | |
| Oct. 23 | L20 | **Phase Transition I - the Ising model, transfer matrix** | **Chandler, Ch5; Yeomans, Ch1** |
| Oct. 25 | L21 | **Phase Transition II - 1D vs. 2D and Tc [<M>]** | **Chandler, Ch5** |
| Oct. 28 | L22 | **Phase Transition III - Symmetry breaking, Correlation & susceptibili** | **Chandler, Ch5** |
| Oct. 30 | L23 | **Phase Transition IV - Mean Field theory** | **Chandler, Ch5** |
| Nov. 1 | L24 | **Phase Transition V: Variational & perturbation theory** | **Chandler, Ch5** |
| Nov. 4 | L25 | **Co-operativity: Helix-coil transition** | **Dill; Ch26** |
| Nov. 6 | L26 | | |
| Nov. 8 | | **----------** | |
| Nov. 11 | L27 | **Gibbs phase rule; Clausius-Clapeyron; interface; Gibbs adsorption isc** | **Chandler, Ch2** |
| Nov. 13 | L28 | **Lattice model for liquids and solution mixtures** | **Chandler, Ch2** |
| Nov. 15 | L29 | **Lattice model for transfer between phases; another look at chemical** | **Dill, Ch14-15** |
| Nov. 15 ev | L30 | **Convention of chemical potential & Dimerization in solution** | |
| Nov. 18 | L31 | **Virial coefficients 1 - derivations** | **Dill, Ch15-16** |
| Nov. 20 | | **Virial coefficients 2 - examples; Liquid State 1 - Basic Intro of g(r)** | |
| Nov. 22 | L32 | **Mid-term Exam 2 (Chemical equilibrium; Lattice Vibration; Phase tra** | **Chandler, Ch6** |
| Nov. 25 | L33 | **Review of the second exam** | **Chandler, Ch6** |
| Nov. 27 | L34 | **Liquid State 2 - Thermodynamics and g(r)** | **McQuarrie, Ch12** |
| Nov. 28-Nov. 30 | | **Thanksgiving** | |
| Dec. 2 | L35 | **Liquid State 3 - Chemical Potential; thermodynamic integration** | **Chandler, Ch7; McQuarrie, Ch13** |
| Dec. 4 | L36 | **Liquid State 4 - Perturbation theory; vdW theory** | **Chandler, Ch7; McQuarrie, Ch13** |
| Dec. 6 | L37 | **Liquid State 5 - Debye-Huckel 1** | **Hill/McQuarrie** |
| Dec. 9 | L38 | **Liquid State 6 - Debye-Huckel 2** | **Hill/McQuarrie** |
| Dec. 11 | L39 | **Polymers - a few relations** | **Dill** |
| Dec. 13 | L40 | **Final review** | |
| Dec. 20 | | **Final Exam (Cumulative)** | |
| **Other possible top** | | **Monte Carlo I: Metropolis scheme** | |
| | | **Monte Carlo II (umbrella sampling); imperfect gas** | |