# Chemistry 534 – Chemical Statistical Mechanics (3 cr., Fall 2015)

| Instructor:   | Prof. Kirk Peterson   | Fulmer 104B (335-7867) |  |  |
|---|---|------------------------|--|--|
| Office Hours:   | By appointment  |                        |  |  |
| Email:  | kipeters@wsu.edu  |                        |  |  |
| Class web page:   | http://tyr0.chem.wsu.ed   | lu/~kipeters/Chem534/  |  |  |
| Recommended Texts:  |   |                        |  |  |
| Statistical Mechanics, by Donald A. McQuarrie (Univ. Press) |   |                        |  |  |
| <u>c</u>  | Statistical Mechanics, by Norman Davidson (Dover)                       |                        |  |  |
| Ī   | Introduction to Modern Statistical Mechanics, by David Chandler (Oxford |                        |  |  |
| S   | Statistical Mechanics: A Concise Introduction for Chemists, by Benjamin |                        |  |  |
| I.  | Widom, Cambridge University Press, 2002.                                |                        |  |  |

### Tues/Thurs. (12-1:15) Todd 202

# **Point Distribution:**

| Hour Exams (2 x 250 pts) | 500  |
|--------------------------|------|
| Final Exam (cumulative)  | 300  |
| Homework (9 total)       | 200  |
| TOTAL                    | 1000 |

# Grading:

| 850 –1000 A     |
|-----------------|
| 801 - 849 B+/A- |
| 650 – 800 B     |
| 600 – 649 C+/B- |
| < 600 C         |

#### Topics to be covered

Ensembles, Probabilities, Probability distributions, Boltzmann distribution, partition

functions, intro to stat thermo

Ideal gases: Boltzmann statistics, molecular partition functions

Diatomic and polyatomic partition functions

Chemical Equilibria

Ideal solids and blackbody radiation (harmonic crystals, Rayleigh-Jeans, Debye theory)

Classical statistical mechanics (phase space averages, equipartition theorem), the grand canonical partition function

Non-ideal gases (virial expansion, intermolecular potentials)

Liquids (molecular dynamics, Monte Carlo) Quantum ideal gases (Bose-Einstein and Fermi-Dirac statistics)

# **Learning Outcomes**

| Student Learning  | Course Topics/Dates    | Evaluation of Outcome:  |
|---|------------------------|-------------------------|
| Outcomes  | The following          | This outcome will be    |
| At the end of this course,  | topic(s)/dates(s) will | evaluated primarily by: |
| students should be able to:   | address this outcome:  |                         |
| Define basic terms and<br>concepts in statistical<br>mechanics  | Throughout course      | Homework and Exams      |
| Apply statistical mechanical<br>methods to standard<br>problems in statistical<br>thermodynamics  | Weeks 1–8              | Homework and Exams      |
| Develop a foundation in<br>statistical mechanics that<br>can be applied to practical<br>problems involving more<br>complex liquids and solids | Weeks 9-15             | Homework and Exams      |

# **University boilerplate**

### **Academic Integrity:**

I encourage you to work with classmates on assignments. However, each student must turn in original work. No copying will be accepted (including from textbooks or homework assignments from earlier semesters). Students who violate WSU's Standards of Conduct for Students will receive an F as a final grade in this course, will not have the option to withdraw from the course and will be reported to the Office Student Standards and Accountability. Cheating is defined in the Standards for Student Conduct WAC 504-26-010 (3). It is strongly suggested that you read and understand these definitions.

### **Reasonable Accommodation Statement:**

Students with Disabilities: Reasonable accommodations are available for students with a documented disability. If you have a disability and need accommodations to fully participate in this class, please either visit or call the Access Center (Washington Building 217; 509-335-3417) to schedule an appointment with an Access Advisor. All accommodations MUST be approved through the Access Center. For more information contact a Disability Specialist on your home campus:

# Pullman or WSU Online: 509-335-3417

http://accesscenter.wsu.edu, <u>Access.Center@wsu.edu</u> **Spokane**: <u>http://spokane.wsu.edu/students/current/studentaffairs/disability/</u> **Tri-Cities**: <u>http://www.tricity.wsu.edu/disability/</u> Vancouver: 360-546-9138 <u>http://studentaffairs.vancouver.wsu.edu/student-resource-center/disability-services</u>

# Safety and Emergency Notification:

Washington State University is committed to enhancing the safety of the students, faculty, staff, and visitors. It is highly recommended that you review the Campus Safety Plan (http://safetyplan.wsu.edu/) and visit the Office of Emergency Management web site (http://oem.wsu.edu/) for a comprehensive listing of university policies, procedures, statistics, and information related to campus safety, emergency management, and the health and welfare of the campus community.