I. COURSE ABSTRACT

From the Course Catalogue:

CHEM 6481. Statistical Mechanics
3-0-3. Prerequisite: CHEM 6471 or consent of School.

Statistical thermodynamics, lattice statistics, molecular
distribution and correlation functions, the theories of liquids
and solutions, phase transitions, cluster theory, and
measurement.

The course should be accessible to graduate students in chemistry, physics, chemical engineering,
and related fields. (Talented undergraduates may also be capable of mastering the material.)
What makes this a Chemistry Course is that modern chemical dynamics will be the underlying
theme. Which is to say that time-dependent and spectroscopically-measurable quantities will be
emphasized. In practice, the course prerequisite is a good understanding of the undergraduate
physical chemistry sequence. (Thermodynamics will be reviewed briefly in the first two weeks.)

II. GENERAL INFORMATION

Classroom: Boggs 3-39S

Texts: DC: “Introduction to Modern Statistical Mechanics,” David Chandler (Ox-

- A terse, but modern treatment.

RZ: “Nonequilibrium Statistical Mechanics,” Robert Zwanzig (Oxford Press,

- A relatively new book by one of the founders of the field.

“Statistical Mechanics,” Donald McQuarrie (HarperCollins, New York,
1976). Approximate cost: $95.00, Recommended.

- Expensive and wordy, but may be a useful reference to those who find
Chandler lacking in detail.

Office Hours: Fridays, from 10:00 to 11:00 AM in Boggs 3-15. (A limited number can be
scheduled by appointment.)

E-Mail: edu@theor.chemistry.gatech.edu. Do not use my chem-mail address!
You are strongly encouraged to use e-mail as a way to extend my office
hours beyond the scheduled period.
### Course Schedule

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### Grading:

- 5% Problem Sets
- 30% In-Class Exam with your Higher Score
- 20% In-Class Exam with your Lower Score
- 45% 3-Page Study of JCP paper + proposal

Problem sets will be handed out one week before they are due. The expected due dates are boxed on the syllabus. Late problem sets will not be accepted.

Collaboration on problem sets is permitted, but you must hand in your own hand-written solutions.

Problems sets will be graded on a scale from 0 to 3 with:

- **1** = anything with your name handed in
- **2** = some attempt was made to complete the problems
- **3** = a reasonable attempt was made to complete all the problems, with most being correct.

### Reading Assignments:

Mandatory, as per the syllabus.

### Attendance:

Strongly recommended. You will be responsible for any material covered in class even if it is nowhere to be found in the assigned textbooks. Because of the cancellation of 4 lectures due to the APS and ACS meetings, the exams have been rescheduled outside of lecture, and up to 2 additional lectures may be scheduled.

### Absences:

In the event that you miss an exam with a valid excuse, you will be given an oral exam at a mutually agreed date and time.

All in-class exams will be closed book, closed notes, but with a single cheat sheet. The exams are underlined above and are scheduled for Feb. 3 and Apr. 7 between 9:30AM and 11:00AM. Note that those dates fall at an unscheduled class time. It will be rescheduled if a conflict appears in the first week of classes. **There will be no final exam.**
Paper: A 3-page paper will be due on April 28. You will choose a paper from the Journal of Chemical Physics published in 2005 or 2006 which is in some way relevant to this course. (You can not have studied this same paper in a previous or current class nor can it have been published by your research group.) You will discuss the important findings in the paper, and provide and justify a proposal extending the work in some way.

Exam #1: You should expect to have a question on Exam #1 asking you to provide the literature citation of your chosen JCP paper, and a justification of your choice in terms of the criteria above.

Exam #2: You should expect to have a question on Exam #2 asking you to provide the literature citation of your chosen JCP paper, and a justification of your choice if it has changed. In addition, you will be asked to provide a thesis for your proposal and a brief abstract justifying the feasibility of your approach.