Chemistry 484 covers statistical mechanics and thermodynamics, based on quantum mechanical results. The course follows CEM 483 (Fall semesters), which provides an introduction to quantum chemistry. However, CEM 484 also works as a stand-alone course in thermodynamics, from a molecular point of view.

**Goals for this course**
- Use statistical mechanics to obtain thermodynamic properties and the distribution of molecules among energy levels, based on quantum chemical results
- Develop expertise in thermodynamic calculations
- Strengthen physical intuition about thermodynamics and quantum mechanics
- Solve representative problems in statistical mechanics and molecular thermodynamics
- Apply course concepts to solve problems in new situations

**Instructor**
Professor Katharine Hunt  
17A Chemistry Building  
353–1152  
[huntk@msu.edu](mailto:huntk@msu.edu)  
[klich@chemistry.msu.edu](mailto:klich@chemistry.msu.edu)

Room 17A is located in the basement of the Chemistry building. To reach this office, please enter through the door to Room 19, then turn right and go down the interior corridor. The door along the main hallway in the basement does not go to this office.

**Lectures**
MWF 10:20 am–11:10 am, 101 Biochemistry

**Recitation Sections**

<table>
<thead>
<tr>
<th>Section</th>
<th>Day</th>
<th>Time</th>
<th>Room</th>
</tr>
</thead>
<tbody>
<tr>
<td>001</td>
<td>Thursday</td>
<td>10:20–11:10</td>
<td>110 CEM</td>
</tr>
<tr>
<td>002</td>
<td>Wednesday</td>
<td>9:10–10:00</td>
<td>109 CEM</td>
</tr>
<tr>
<td>003</td>
<td>Friday</td>
<td>11:30–12:20</td>
<td>109 CEM</td>
</tr>
<tr>
<td>004</td>
<td>Friday</td>
<td>9:10–10:00</td>
<td>109 CEM</td>
</tr>
</tbody>
</table>

**Office Hours**

<table>
<thead>
<tr>
<th>Instructor</th>
<th>Time and Day</th>
<th>Room</th>
</tr>
</thead>
<tbody>
<tr>
<td>Katharine Hunt</td>
<td>11:10 am–12:00 noon, MTWTF</td>
<td>17A</td>
</tr>
</tbody>
</table>

**TAs for this course:** Nathan Jansen and Arnab Chakraborty  
TA Office Hours (TBA) will be held in the CEM Basement Help Room.
Textbook

*Thermodynamics, Statistical Thermodynamics, and Kinetics*, by Thomas Engel and Philip Reid. This book is a companion volume to the text used for CEM 483.

Problem Sets

Problem sets will be assigned, normally on a weekly basis after the first week of classes. You are encouraged to collaborate on the problem sets. Due to the size of the class, these sets will not be graded, but the problems will form the basis for quizzes in the recitation sections.

Recitations

Recitation quizzes normally will be held weekly at the end of each of the sessions, during the weeks when there is no midterm. The quizzes will consist of one problem or a part of a problem from the problem set. Each quiz will last roughly ten to fifteen minutes.

Course Project

The course project will involve calculations of thermodynamic quantities for a chemical reaction, starting from quantum mechanical information about the reactants and products. Individual steps in the calculations will be done as the semester progresses. You will have the opportunity to update your answers based on feedback, before the project is completed.

Grading

1. Midterm Exams
   a. Midterm 1, February 12, 2020  17%
   b. Midterm 2, March 11, 2020  17%
   c. Midterm 3, April 8, 2020  17%
2. Recitation Quizzes  12%
3. Class Project  12%
4. Final Exam  25%

Thursday, April 30, 2020
7:45 am-9:45, 101 Biochemistry

*The date and time for the final are fixed by the university.*

Guaranteed Grading Scale

<table>
<thead>
<tr>
<th>Percentage Range</th>
<th>Grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>85.0% and higher</td>
<td>4.0</td>
</tr>
<tr>
<td>77.0-84.9%</td>
<td>3.5</td>
</tr>
<tr>
<td>70.0-76.9%</td>
<td>3.0</td>
</tr>
<tr>
<td>63.0-69.9%</td>
<td>2.5</td>
</tr>
<tr>
<td>55.0-62.9%</td>
<td>2.0</td>
</tr>
<tr>
<td>47.0-54.9%</td>
<td>1.5</td>
</tr>
<tr>
<td>40.0-46.9%</td>
<td>1.0</td>
</tr>
</tbody>
</table>

If your percent score for the semester reaches the corresponding cut-off, you will be guaranteed that grade. It is possible that the cut-off scores may be reduced slightly depending on the difficulty of the exams. We will also compute your percent score after dropping the lowest midterm (using the same relative weights as above), and will use that
score if it results in a higher grade for the semester. Adjustments may also be made for differences in the difficulty of quizzes. Since the lowest midterm score can be dropped, make-up exams will be offered only in unusual circumstances; in that case, please see the instructor.

**i>clickers**

After the first few weeks, i>clickers will be used, so that you can answer questions and provide feedback. There will be an announcement before the i>clicker questions start. The questions should be helpful in adjusting the pace and depth of CEM 484.

Extra credit will be available, based on i>clicker responses. This will be computed as follows: 2 points will be awarded for every correct answer (or other full-credit response) and 1 point for an incorrect answer (0 points for no response). At the end of the semester, if you have gained at least 50% of the total available i>clicker points, 2% will be added to your semester total. If you have gained 75% or more of the total available i>clicker points, 5% will be added to your semester total. Intermediate values of the added percentages are also possible.

Information on registering your i>clicker will be provided in class and on the D2L site.

**Office Hours**

You are encouraged to come to office hours! If you have a time conflict with the scheduled office hours, please contact the course instructor or TA to arrange an appointment at an alternate time.

**Accommodations for Students with Disabilities**

Text from the Course Information for CEM 483 (Prof. John McCracken):

“Michigan State University is committed to providing equal opportunity for participation in all programs, services, and activities. Requests for accommodation by persons with disabilities may be made by contacting the Resource Center for Persons with Disabilities by phone at 517-884-RCPD or through the web at rcpd.msu.edu. Once your eligibility for an accommodation has been determined, you will be issued a verified individual services accommodation (‘VISA’) form.”

Please provide your VISA form to Prof. Hunt at the beginning of the semester or at least two weeks prior to the date when accommodation is required (midterms, final exam, quizzes, etc.). We will also honor requests received closer to the need for accommodation, whenever that is possible.

**Emergency Guidelines**

Each classroom has posted emergency guidelines that tell how to deal with Secure-in-Place situations, Evacuation, Seeking Shelter, Hazardous Material Leaks, or Spills. This is a lecture course, but the room is located in a research building. In the event of an evacuation, you should go to one of the rally points identified on the Classroom Emergency Guideline form posted in the classroom. Staff members of the Emergency Action Team can be identified by yellow vests/hats. If you anticipate any difficulty in evacuating in the event of an emergency, please let the instructor know as soon as possible.
Course Outline

1. The Boltzmann Distribution: How Probable are Various Energies? 13
2. Partition Functions for Individual Molecules and Distributions 14
5. Thermochemistry: ΔU and ΔH for Chemical Reactions 4
7. Third Law of Thermodynamics: Approaching 0 K 5
8. Free Energies and Equilibrium: ΔA and ΔG 6
9. Properties of Real Gases 7
10. Phase Transitions and Solutions 8, 9
11. Kinetic Theory of Gases 16

The chapter references come from the text, *Thermodynamics, Statistical Thermodynamics, and Kinetics*, by Thomas Engel and Philip Reid.

H Option

An H option is available for CEM 484 in two forms:

1) *Short research project*. If you are interested in this form of the H option, please see the course instructor within the first three weeks of class, so that we can identify a course-related project of interest to you.

2) *Problem-solving option*. Starred problems which go beyond the required level of the course will be distributed with some of the problem sets and practice exams. You can complete an H option for this course by providing good solutions for half of these problems.