Course Syllabus for CH4590/CH6590 Fall 2016
Molecular Driving Forces
Department of Chemistry

Instructor Information

Instructor: Loredana Valenzano, PhD, Assistant Professor
Office Location: ChemSci 701-A
Telephone: (906) 487-1602
E-mail: lvalenza@mtu.edu
Office Hours: MWF 2:30 PM – 3:30 PM
Or by appointment

Course Identification

Course Number: CH4590-0A / CH6590-0A
Course Name: Molecular Driving Forces
Course Location: ChemSci 215
Class Times: MWF 9:05 AM - 9:55 AM

Course Description/Overview

The course is intended for senior undergraduates and graduate students in chemistry, biochemistry, biology, physics, biophysics, polymer science, materials science, nanoscience, with interests in molecular interactions, molecular self-assembly, crystal growth, etc.

Spanning from classical thermodynamics to kinetics, from statistical thermodynamics to quantum chemistry, it deepens concepts covered in other courses to provide the students with an overall understanding of the forces driving molecular interactions at both microscopic and macroscopic level.

The topics covered in this course will allow students to gain not only a fundamental theoretical knowledge about the description of the physical-chemical properties characterizing the different types of molecular interactions, but it will also provide a direct link to the manifestation and the interpretation of such phenomena in real-world scenarios.

Course Learning Objectives

• To provide students with a deepen understanding of classical thermodynamics, equilibrium, kinetics, statistical thermodynamics, foundations of quantum mechanics, and the inner links between them.
• To provide students with the understanding of the fundamental principles governing the forces ruling the interaction between molecules, and driving molecular and material assembly.
• To provide students with the theoretical aspects linking classical and statistical thermodynamics.
• To guide students in developing quantitative reasoning, problem solving, rigorous thinking but also physical-chemical intuition.

Course Resources

Online Resources
• Canvas: http://courses.mtu.edu
• E-mail List: ch4590-fa16-l@mtu.edu and ch6590-fa16-l@mtu.edu

Required Course Text


Other useful sources are:

• Donald A. McQuarrie and John D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, Sausalito-California, ©1997
## Grading Scheme

### Grading System

<table>
<thead>
<tr>
<th>Points</th>
<th>Letter Grades</th>
</tr>
</thead>
<tbody>
<tr>
<td>93-100</td>
<td>A</td>
</tr>
<tr>
<td>87-92</td>
<td>AB</td>
</tr>
<tr>
<td>82-86</td>
<td>B</td>
</tr>
<tr>
<td>76-81</td>
<td>BC</td>
</tr>
<tr>
<td>70-75</td>
<td>C</td>
</tr>
<tr>
<td>65-69</td>
<td>CD</td>
</tr>
<tr>
<td>60-64</td>
<td>D</td>
</tr>
<tr>
<td>0-59</td>
<td>F</td>
</tr>
</tbody>
</table>

*Note that NO CURVING will be applied*

### Grading Policy

Your grade for this course will be based on the following:

<table>
<thead>
<tr>
<th>Assignment</th>
<th>Max points per type of assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 Homework (25 points each)</td>
<td>150</td>
</tr>
<tr>
<td>3 Term Exams (50 points each)</td>
<td>150</td>
</tr>
<tr>
<td>1 Final Exam (100 points)</td>
<td>100</td>
</tr>
<tr>
<td><strong>Total Points</strong></td>
<td><strong>400</strong>*</td>
</tr>
</tbody>
</table>

*Your total score in the Course will be converted to 100%.

### Late Assignments

No late assignment will be considered.

### Preparation for Class & Class Attendance (please, read this carefully!)

Reading material will be assigned to students before each class. This will not constitute a compulsory assignment students will be graded on, but given the nature of the material covered in this course it is in the interest of the students to come to class prepared, or at least with some pre-acquired knowledge. Students’ proactive attitude in getting familiar with the topics ahead of class will facilitate their learning process which will develop through assigned in-class discussion, homeworks, and exams.
Attendance in class is not compulsory but it is highly recommended to keep track of the topics covered and discussed. Coming to class will provide guidance to develop good reasoning, and mathematical skills which are essential to succeed in this class.

Course Policies

Your grade will be based on:

- 6 homeworks;
- 3 term exams;
- 1 final term exam.

The 6 Homeworks will be assigned roughly every 1.5 weeks, with exceptions due to class recesses, and Thanksgiving break. Homeworks will be due in class the same day one week after (example: homework assigned on Friday, 7th will be due on Friday, 14th). No late homework will be accepted. Students who will not turn in homework without documented and satisfactory explanation will receive a grade of 0.0 (see the last page of this document “Excused Absence”).

The 3 Term Exams and the Final Exam will be assigned in the form of problem solving, and potentially short essay; in both cases, students will be asked to show both the development of their reasoning skills and their capabilities in solving and deriving equations related to the material covered in class, and that they worked on in homeworks. Students who will not show up for Midterm and Final Exams without documented and satisfactory explanation will receive a grade of 0.0 (see the last page of this document “Excused Absence”).

Laptops are allowed in class only, not during exams. The following are not allowed at any time: cell phones, Blackberries, iPods, PDAs, or any other electronic devices. Calculators on other devices are strictly prohibited during the exams. Information exchanges on electronic devices during class and exams are also prohibited and violate the Academic Integrity Code of Michigan Tech.
University Policies

Student work products (exams, essays, projects, etc.) may be used for purposes of university, program, or course assessment. All work used for assessment purposes will not include any individual student identification.

Academic regulations and procedures are governed by University policy. Academic dishonesty cases will be handled in accordance the University's policies.

If you have a disability that could affect your performance in this class or that requires an accommodation under the Americans with Disabilities Act, please see me as soon as possible so that we can make appropriate arrangements. The Affirmative Action Office has asked that you be made aware of the following:

Michigan Tech complies with all federal and state laws and regulations regarding discrimination, including the Americans with Disabilities Act of 1990. If you have a disability and need a reasonable accommodation for equal access to education or services at Michigan Tech, please call the Dean of Students Office, at 487-2212. For other concerns about discrimination, you may contact your advisor, department head or the Affirmative Action Office, at 487-3310

Academic Integrity:
http://www.studentaffairs.mtu.edu/dean/judicial/policies/academic_integrity.html

Affirmative Action:
http://www.admin.mtu.edu/aaq/

Disability Services:
http://www.admin.mtu.edu/urel/studenthandbook/student_services.html#disability

Equal Opportunity Statement:
**Tentative Course Schedule**

<table>
<thead>
<tr>
<th>Main Topics</th>
<th>Chapter</th>
<th>Tentative Week</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multivariable Calculus, Entropy, Thermodynamic Driving Forces</td>
<td>4-5-6</td>
<td>2</td>
</tr>
<tr>
<td>Thermodynamic Paths, Thermodynamic Cycles, Laboratory conditions and Free Energies</td>
<td>7-8</td>
<td>3</td>
</tr>
<tr>
<td>Maxwell’s Relations, Boltzmann Distribution</td>
<td>9-10</td>
<td>4</td>
</tr>
<tr>
<td>Statistical Mechanics, Temperature, Heat Capacities</td>
<td>11-12</td>
<td>5</td>
</tr>
<tr>
<td>Equilibria between Liquids, Solids, and Gases</td>
<td>13-14</td>
<td>6</td>
</tr>
<tr>
<td>Solutions, Mixtures, Solvation</td>
<td>15-16</td>
<td>7</td>
</tr>
<tr>
<td>Diffusion, Permeation, Flow, Microscopic Dynamics</td>
<td>17-18</td>
<td>8</td>
</tr>
<tr>
<td>Chemical Kinetics, Transition States, Electrostatic Forces, Electrostatic Potential</td>
<td>19-20-21</td>
<td>9</td>
</tr>
<tr>
<td>Electrochemical Equilibria, Salt Ions Shielding in Solutions, Intermolecular Interactions</td>
<td>22-23-24</td>
<td>10</td>
</tr>
<tr>
<td>Multi-site and Cooperative Ligand Binding, Bio and Nano Machines</td>
<td>28-29</td>
<td>12</td>
</tr>
<tr>
<td>Water, Water as Solvent, Polymer Solutions</td>
<td>30-31-32</td>
<td>13</td>
</tr>
<tr>
<td>Polymer Elasticity and Collapse, Polymers Confinement and Deformation</td>
<td>33-34</td>
<td>14</td>
</tr>
</tbody>
</table>

Students will be asked to read before hand those sections of the textbook which will be covered in class. This will allow them to approach the class with some prebuilt awareness which will put them in the condition to better grasp the theoretical content of each class.

If needed, and only for topics which will need a more in depth knowledge, I will provide external notes and/or I will record videos that will be available on Canvas. This implies that students are highly encourage to come to class, and take notes which they will then improve through the reading of the textbook. Students able to do so constantly throughout the semester will highly benefit in terms of time and effort required solving problem sets, and succeeding in the term and final exams.

Links to short videos will be also provided as additional help and tips to solve the problems assigned through the homeworks. Full solutions of the problems/exercises assigned in homeworks and exams will be also made available.
Topics listed above and not covered in class or in videos, and not clearly assigned as external additional reading will not be part of any assignment.

**More Information about Homework, Midterm and Final Exams**

Please, note that the adopted textbook contains problems at the end of each chapter that you may consider to solve even though they will be not assigned as homework. Homework and Exams may be partially based on them and/or related to them.

**Homeworks** will be assigned and returned in class according to the following schedule:

<table>
<thead>
<tr>
<th>Assignment</th>
<th>Assigned</th>
<th>Due Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homework #1</td>
<td>Wednesday, September 7th 2016</td>
<td>Friday, September 16th 2016</td>
</tr>
<tr>
<td>Homework #2</td>
<td>Wednesday, September 21st 2016</td>
<td>Friday, September 30th 2016</td>
</tr>
<tr>
<td>Homework #3</td>
<td>Monday, October 3rd 2016</td>
<td>Wednesday, October 12th 2016</td>
</tr>
<tr>
<td>Homework #4</td>
<td>Wednesday, October 26th 2016</td>
<td>Friday, November 4th 2016</td>
</tr>
<tr>
<td>Homework #5</td>
<td>Monday, November 7th 2016</td>
<td>Wednesday, November 16th 2016</td>
</tr>
<tr>
<td>Homework #6</td>
<td>Wednesday, November 30th 2016</td>
<td>Friday, December 9th 2016</td>
</tr>
</tbody>
</table>

Homework can be solved with the support of books, notes, and calculators. Students are allowed to work together.

**Midterm Exams are scheduled for:**

1) **Monday, 26th September 2016, M&M U115, 6:05 PM - 6:55 PM**
2) **Monday, 31st October 2016, DOW 641, 6:05 PM - 6:55 PM**
3) **Wednesday, 16th November 2015, DOW 641, 6:05 PM - 6:55 PM**

Midterm Exams can be solved with the support of calculators only.
No books or notes will be allowed.
The formula sheet will be provided.

**To compensate for evening Exams, the class will not meet the following days:**

1) **Friday, 14th October 2016;**
2) **Friday, 21st October 2016;**
3) **Friday, 18th November 2016.**
**Final Exam** is not scheduled at the time this Syllabus has been completed. The final exam will be scheduled by the Registrar’s office later on in the semester.

The Final Exam can be solved with the support of calculators only. No books or notes will be allowed. I will provide the formula sheet.

The Final Exam will be a comprehensive 2-hour examination.

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**Getting Help in Learning**

*From me, as your Instructor*

Please, know that I am always available to my students! Therefore, do not hesitate in contacting me for any problem or for guidance regarding the material covered in class.

In particular, my office hours are scheduled on **MWF, 2:30 PM – 3:30 PM** in my office in ChemSci 701-A. In order to arrange for assistance by appointment you can contact me by email at lvalenza@mtu.edu or by phone at (906) 487-1602.

On Canvas you will find, prior to the lectures, the slides which will be commented in class, extra notes, text, and solutions of practicing exams. Text and solutions for the 4 homeworks, and the 3 midterms will be published accordingly.

**VIDEOS CONTENT:**

- Before each Midterm (and before the Final), videos will be posted spanning/summarizing the material covered in class.
- Videos containing hints for solving homework, fully commented solutions for homework, midterm exams (after the due dates, of course!), and other learning material will also be posted.
- Additional material will eventually be posted about topics treated in more depth.
Excused Absenses

Events beyond your control may cause you to miss a homework deadline or an exam. Whenever possible, contact me prior to your absence to arrange to make-up missed work. If you are unable to notify me concerning an absence or if you need to notify several instructors on short notice, contact the Office of Student Affairs for assistance. The Dean of Students will then inform all your instructors that you face a situation that requires that you miss class, and you are granted an excused absence. It is then your responsibility to contact each of your instructors after you recover from your illness or return to campus.

An absence is excused under the following conditions:

- If you participate in off-campus University-sponsored activities such as field trips, fine arts performances, intercollegiate athletics, job fairs, etc., you are granted an excused absence if your activity conflicts with an exam. Furthermore, I consider plant trips, job interviews requiring travel, and professional society meetings as excusable. It is imperative that for an absence of this type, for which a conflict with an exam is known well ahead of time, that you arrange with me to take the exam earlier than its normally scheduled time.

- If you encounter circumstances beyond your control such as illness, the funeral of any relative or close friend, or other personal emergency, you are granted an excused absence. You must provide verification of the special circumstances that led to your absence. In the event of a missed exam due to an excused absence, it is not possible to make-up the exam. Instead, an excused absence from an exam will receive the score EX. At the end of the semester, exam EX scores will be replaced by a weighted average of all of your non-EX scores on exams (midterms and final exams). If the final exam is missed as a result of an excused absence, you will be awarded the letter grade of I (incomplete) and must take the CH 3510 final exam at the end of any one of the next semesters that you’re in residence. Two or more exams missed as a result of excused absences will be handled on an individual basis.

If a homework due date is missed as a result of an excused absence, the due date will be extended after you notify me.