Course Syllabus for CH3520 Spring 2016
Physical Chemistry II: Molecular Structure
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 1:00 PM – 2:00 PM
Or by appointment

Course Identification
Course Number: CH3520-0A
Course Name: Physical Chemistry II: Molecular Structure
Course Location: ChemSci 104 B
Class Times: MWF 12:05 PM - 12:55 PM

Course Description/Overview
To introduce concepts useful in explaining and interpreting the nature of physical and chemical properties of matter at electronic structure level. This course will cover the following areas of Physical Chemistry: foundations of quantum chemistry, foundations of electronic structure theory, theoretical methods in determining molecular properties, the theory behind spectroscopic methods, statistical thermodynamics, basic properties of crystalline solids.

Overall, the knowledge acquired in this course will allow students to appreciate the “secrets behind the scenes” about the description of the physico-chemical properties of matter which, naturally, occurs at electronic level.

Course Learning Objectives
• To provide students with foundations in quantum mechanics, and electronic structure theory as applied to chemistry. Such concepts will be used to understand the basic principles governing the formation and the breaking of chemical bonds mostly in molecules, with a glimpse to solids as well.
• To provide students with the theoretical aspects linking classical and statistical thermodynamics.
• To provide students the opportunity to apply advanced mathematical concepts to the solution of complex problems daily occurring in (quantum) chemistry.
• 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](http://courses.mtu.edu)
- E-mail List: ch3520-sp16-l@mtu.edu

**Required Course Text**


**Other useful sources are:**


**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>
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<tr>
<td>70-75</td>
<td>C</td>
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<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>10 Homework (30 points each)</td>
<td>300</td>
</tr>
<tr>
<td>3 Term Exams (40 points each)</td>
<td>120</td>
</tr>
<tr>
<td>1 Final Exam (80 points)</td>
<td>80</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 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:

- 10 homeworks;
- 3 term exams;
- 1 final term exam.
**The 10 Homeworks** will be assigned roughly **every week**, with exceptions due to class recesses, and Spring 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 Absense”).

**The 3 Term Exams and the Final Exam** will be assigned in the form of **problem solving, and potentially short essay**; in both cases, you will be asked both to show the development of your reasoning skills and your capabilities in solving and deriving equations related to the material covered in class, and that you worked on in your 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 Absense”).

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](http://www.studentaffairs.mtu.edu/dean/judicial/policies/academic_integrity.html)
Affirmative Action:
http://www.admin.mtu.edu/aaomt/mtu

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

Equal Opportunity Statement:
**Tentative Course Schedule (see Calendar for detailed tentative schedule!)**

<table>
<thead>
<tr>
<th>Main Topics</th>
<th>Chapter</th>
<th>Tentative Week</th>
</tr>
</thead>
<tbody>
<tr>
<td>From Classical to Quantum Mechanics, Schrödinger Equation, State/Wave Function, Particle in a 1D box, Particle in a 3D box, Degeneracy, Operators, 1D Harmonic Oscillator, Two-Particle Problems, Two-Particle Rigid Rotor, Approximation Methods, Hermitian Operators</td>
<td>17: Quantum Mechanics</td>
<td>Weeks 1, 2, 3</td>
</tr>
<tr>
<td>Canonical Ensemble and Thermodynamical Properties, Canonical Partition Functions, Boltzmann Distribution, Statistical Thermodynamics of Ideal Gases, Entropy and Third Law of Thermodynamics</td>
<td>21: Statistical Mechanics (a taste of...)</td>
<td>Week 12, 13</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. For a detailed list of sections, and topics covered during the 40 times class will meet, students are warmly invited to consult the Calendar for the course which is also posted on Canvas.

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 Online Quizzes, 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>Friday, January 15&lt;sup&gt;th&lt;/sup&gt;</td>
<td>Friday, January 22&lt;sup&gt;nd&lt;/sup&gt;</td>
</tr>
<tr>
<td>Homework #2</td>
<td>Friday, January 22&lt;sup&gt;nd&lt;/sup&gt;</td>
<td>Friday, January 29&lt;sup&gt;th&lt;/sup&gt;</td>
</tr>
<tr>
<td>Homework #3</td>
<td>Monday, February 8&lt;sup&gt;th&lt;/sup&gt;</td>
<td>Monday, February 15&lt;sup&gt;th&lt;/sup&gt;</td>
</tr>
<tr>
<td>Homework #4</td>
<td>Monday, February 15&lt;sup&gt;th&lt;/sup&gt;</td>
<td>Monday, February 22&lt;sup&gt;nd&lt;/sup&gt;</td>
</tr>
<tr>
<td>Homework #5</td>
<td>Monday, February 22&lt;sup&gt;nd&lt;/sup&gt;</td>
<td>Monday, February 29&lt;sup&gt;th&lt;/sup&gt;</td>
</tr>
<tr>
<td>Homework #6</td>
<td>Monday, March 14&lt;sup&gt;th&lt;/sup&gt;</td>
<td>Monday, March 21&lt;sup&gt;st&lt;/sup&gt;</td>
</tr>
<tr>
<td>Homework #7</td>
<td>Monday, March 21&lt;sup&gt;st&lt;/sup&gt;</td>
<td>Monday, March 28&lt;sup&gt;th&lt;/sup&gt;</td>
</tr>
<tr>
<td>Homework #8</td>
<td>Monday, March 28&lt;sup&gt;th&lt;/sup&gt;</td>
<td>Monday, April 4&lt;sup&gt;th&lt;/sup&gt;</td>
</tr>
<tr>
<td>Homework #9</td>
<td>Monday, April 4&lt;sup&gt;th&lt;/sup&gt;</td>
<td>Monday, April 11&lt;sup&gt;th&lt;/sup&gt;</td>
</tr>
<tr>
<td>Homework #10</td>
<td>Friday, April 15&lt;sup&gt;th&lt;/sup&gt;</td>
<td>Friday, April 22&lt;sup&gt;nd&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

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

**Term Exams** are scheduled for:

1) Monday, February 1<sup>st</sup>, ChemSci 104-B, 12:05 PM - 12:55 PM
2) Wednesday, March 2<sup>nd</sup>, ChemSci 104-B, 12:05 PM - 12:55 PM
3) Monday, April 4<sup>th</sup>, ChemSci 104-B, 12:05 PM - 12:55 PM
Term Exams can be solved with the support of calculators only. No books or notes will be allowed. The formula sheet will be provided.

**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.

**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 after each lecture (*MWF, 1:30 PM – 2:30 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, all the slides which will be commented in class, extra notes, text, and solutions of practicing exams. Text and solutions of the 13 online quizzes, 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.