1. Course Details

Instructor: Professor Caroline Taylor  
email: cmtaylor@mtu.edu  
Phone: 7-1645  
Office: ChemSci 701C  
Office Hours: Tuesday 4:00pm – 5:00pm, or by appointment

Lecture*: ChemSci 215  
Wednesday 1:05pm – 1:55pm

Lab*: ChemSci 719 (Chemistry Computer Lab)  
Wednesday 3:05pm – 4:55pm

Primary Text: Molecular Modelling: Principles and Applications 2nd Ed.,  
Andrew R. Leach  
Prentice Hall

D. Frenkel, B. Smit, Understanding to Molecular Dynamics  
M. P. Allen, D. J. Tildesley, Computer Simulation of Liquids  
(Supplemental texts are primarily intended for CH5560)

Webpage: http://www.chemistry.mtu.edu/pages/courses/class.php?class=CH4560&section=0A&sem=20071

Prerequisites: Physical Chemistry, Multivariate Calculus.

Computational Details: Most of the computational work will be carried out in the UNIX environment. You are encouraged to familiarize yourself with Linux/Unix in anticipation of this. A brief review/introduction will be held during the first lab session.

2. Assignments & Grading

Exercises: There will be weekly math and theory exercises, consisting of one problem in each area. These will involve primarily “paper-and-pencil” work, with some plotting or numerical solution.

Problem Sets: During the course of the semester there will be graded problem sets (computational “experiments” and write-ups) due approximately every two weeks. These will be distributed in class and posted on the web site, and the calculations will be performed outside of class. These will be graded on the execution of the computational section, the mathematical analysis, and the write-up, and will count toward the overall course grade.

Critical Analyses: A relevant journal article will be assigned approximately every two weeks, to be read, analyzed, and discussed at the end of lecture on Wednesdays. A one-page written critical analysis of the assigned article will be due at the beginning of lecture the day of discussion. These assignments will be graded both on the written and the discussion portions, and will count toward the overall course grade.

Exams: There are no formal exams for this course.

Final Project: There will be no final examination in the course. In place of a final examination, there will be a final project. A proposal (1-2 pages) for the project will be due Monday, November 26. A final project report, a paper of about 10 pages (in 12pt) including data and figures will be required, to be handed in the Monday of finals week. Details for this assignment will be provided at a later date.

Grade: The course grade will be determined from the math and theory exercises, critical analyses, cumulative problem set scores, the final computational project (including the proposal), and participation in lecture. The anticipated (tentative) breakdown is:

5% participation  
15% exercises  
15% critical analyses  
35% problem sets  
30% final project

Late work will not be accepted.
3. Academic Integrity
Collaboration is both expected and encouraged. However, every student must submit their own work. This extends to the final research project and paper, where scholarly standards must be met. Please review the University’s policy on Academic Integrity, available at http://www.studentaffairs.mtu.edu/dean/judicial/policies/academic_integrity.html. Any violations will be subject to the full range of penalties, from a zero score on the assignment or exam to failure of the course and an indication on the permanent record. If you are at all uncertain, please speak to me.

4. Tentative Schedule

<table>
<thead>
<tr>
<th>Week</th>
<th>General Topics (abridged)</th>
<th>Chapters</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Introduction and quantum review</td>
<td>L1, 2.1-4, 2.7; SZ 1, 2.1, 2.3</td>
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<tr>
<td>2</td>
<td>ES: Basis Sets and Orbitals</td>
<td>L 2.6, 2.8; SZ 2.2</td>
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<tr>
<td>3</td>
<td>ES: Hartree-Fock and SCF</td>
<td>L 2; SZ 3</td>
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<tr>
<td>4</td>
<td>ES: Correlation, <em>ab initio</em> methods</td>
<td>L 3.1-3.4; SZ 4, 6.1, 6.3, 6.5</td>
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<tr>
<td>5</td>
<td>ES: Semi-emperical methods and DFT</td>
<td>L 2.8-11, 3.7-3.9, SZ 2.</td>
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<tr>
<td>6</td>
<td>ES/MS: Conformational Analysis &amp; Forcefields</td>
<td>L 4</td>
</tr>
<tr>
<td>7</td>
<td>MS: Molecular Dynamics</td>
<td>L 6, FS 2, 4</td>
</tr>
<tr>
<td>8</td>
<td>MS: Molecular Dynamics</td>
<td>L 7, FS 6, 12</td>
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<tr>
<td>9</td>
<td>MS: Monte Carlo Simulations</td>
<td>L 8, FS 3</td>
</tr>
<tr>
<td>10</td>
<td>MS: Monte Carlo Simulations</td>
<td>FS 5, 13, 14</td>
</tr>
<tr>
<td>11</td>
<td>MS: MD/MC</td>
<td>L9, FS 15</td>
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<td></td>
<td>BREAK</td>
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<tr>
<td>12</td>
<td>Mixed Methods</td>
<td>L 11, FS 16</td>
</tr>
<tr>
<td>13</td>
<td>Mixed Methods</td>
<td>L 10</td>
</tr>
<tr>
<td>14</td>
<td>Mixed Methods</td>
<td></td>
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<tr>
<td></td>
<td>Finals Week</td>
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Abbreviations:
ES=electronic structure
MS=molecular simulation
L=Leach text
SZ=Szabo and Ostlund text
FS=Frenkel and Smit text

*To be discussed.*