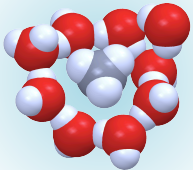


## CHEM 268 – Special Topics in Physical Chemistry

### *Introduction to Molecular Modeling of Chemistry/Biochemistry*



**STRUCTURE?**

**ENERGY?**

**INTERACTION?**

**Time:** 9:40-10:30 AM MWF

**Room:** Lafayette Hall L202

**Lecturer:** Jianing Li ([jianing.li@uvm.edu](mailto:jianing.li@uvm.edu), Cook A223)

**Office Hour:** 4:30-5:30 PM MWF

#### Summary

CHEM 268 explores the techniques and applications of molecular modeling and computational chemistry/biochemistry. This course highlights how to model different molecules (organic, inorganic, and biological) in computers and how to calculate their properties and reactions with modern computational technology. Computational and informatics approaches are introduced from a practical aspect, in conjunction with special topics such as computer-aided drug design and big data. This course is targeted at advanced graduate/undergraduate levels, with the goals to (i) strengthen the understanding of the molecular sciences and (ii) introduce useful modeling skills for solving research problems.

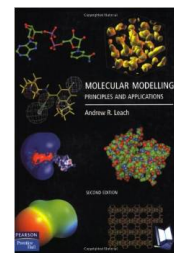
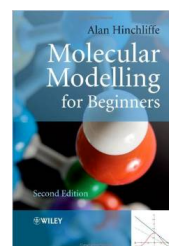
#### Prerequisites

- PHYS 012, 042, or 152.
- MATH 121 or 124.

#### Textbooks

##### Recommended:

- Molecular Modelling: Principle and Applications, 2<sup>nd</sup> Edition, by Andrew R. Leach



##### Other Sources:

- Molecular Modelling for Beginners, 2<sup>nd</sup> Edition, by Alan Hinchliffe
- Big Data for Dummies, by Judith Hurwitz.
- Clusters for Dummies, by Ed Tittel.

#### Topics

Lecture	Topic	Lecture	Topic
<b>1-4</b>	<i>How to build molecular models in a computer?</i>	<b>21-28</b>	<i>Molecular dynamics (MD) simulations &amp; protein folding challenge</i>
<b>5-10</b>	<i>Classical &amp; quantum descriptions of chemical interactions</i>	<b>29-33</b>	<i>Basic quantum chemistry (QC) calculations &amp; molecular property predictions</i>
<b>11-15</b>	<i>From cheminformatics to big (chemistry) data</i>	<b>34-40</b>	<i>Density Functional Theory (DFT) methods &amp; reaction pathways calculations</i>
<b>16-20</b>	<i>Molecular docking &amp; computer-aided drug design (CADD)</i>		

Note: Lecture numbers are very approximate.

#### Grading

- 5-7 homework assignments (60%)
- Final exam or mini project (20%)
- 2 midterm exams (20%, multiple choice)

**Student Learning Accommodations:** In keeping with University policy, any student with a documented disability interested in utilizing accommodations should contact ACCESS, the office of Disability Services on campus. ACCESS works with students and faculty in an interactive process to explore reasonable and appropriate accommodations via an accommodation letter to faculty with recommended accommodations as early as possible each semester.

Contact ACCESS: A170 Living/Learning Center; 802-656-7753; [access@uvm.edu](mailto:access@uvm.edu); [www.uvm.edu/access](http://www.uvm.edu/access)

UVM's policy on disability certification and student support:  
[www.uvm.edu/~uvmppg/ppg/student/disability.pdf](http://www.uvm.edu/~uvmppg/ppg/student/disability.pdf)

**Religious Holidays:** Students have the right to practice the religion of their choice. If you need to miss class to observe a religious holiday, please submit the dates of your absence to me in writing by the end of the second full week of classes. You will be permitted to make up work within a mutually agreed-upon time.

**Academic Integrity:** The policy addresses plagiarism, fabrication, collusion, and cheating.  
<http://www.uvm.edu/~uvmppg/ppg/student/acadintegrity.pdf>

**Grade Appeals:** If you would like to contest a grade, please follow the procedures outlined in this policy:  
<http://www.uvm.edu/~uvmppg/ppg/student/gradeappeals.pdf>

**Grading:** For information on grading and GPA calculation, go to [www.uvm.edu/academics/catalogue](http://www.uvm.edu/academics/catalogue) and click on Policies for an A-Z listing.

**Code of Student Rights and Responsibilities:** [www.uvm.edu/~uvmppg/ppg/student/studentcode.pdf](http://www.uvm.edu/~uvmppg/ppg/student/studentcode.pdf)

**FERPA Rights Disclosure:** The purpose of this policy is to communicate the rights of students regarding access to, and privacy of their student educational records as provided for in the Family Educational Rights and Privacy Act (FERPA) of 1974. <http://www.uvm.edu/~uvmppg/ppg/student/ferpa.pdf>

**Promoting Health & Safety:**

The University of Vermont's number one priority is to support a healthy and safe community:

**Center for Health and Wellbeing** <http://www.uvm.edu/~chwb/>

**Counseling & Psychiatry Services (CAPS)** Phone: (802) 656-3340

**C.A.R.E.** If you are concerned about a UVM community member or are concerned about a specific event, we encourage you to contact the Dean of Students Office (802-656-3380). If you would like to remain anonymous, you can report your concerns online by visiting the Dean of Students website at <http://www.uvm.edu/~dos/>

**Final exam policy:** The University final exam policy outlines expectations during final exams and explains timing and process of examination period. <http://www.uvm.edu/academics/catalogue2013-14/?Page=allpolicies.php&SM=policymenu.html&policy=Exams>