

## CHE 481 Applied Bio-Molecular Modeling Fall 2009

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**Lecture Room:** Rm 401 ESB

**Course Format:** 2 Hour lecture, 1 Hour lab

**Prerequisites:** CHE 381, MATH 261, CHEM 231 or 233

**Recommended Texts:**

Andrew R. Leach, *Molecular Modeling: Principles and Applications, Second Edition*, Prentice Hall, 2001.

Daan Frenkel and Berend Smit, *Understanding Molecular Simulations: From Algorithms to Applications, 2<sup>nd</sup> Edition*, Academic Press, 2002.

[http://molsim.chem.uva.nl/frenkel\\_smit/index.html](http://molsim.chem.uva.nl/frenkel_smit/index.html) for additional resources

**Course Objective:** This course will provide an introduction to modern molecular-level computational methods for calculating properties of reaction systems and thermodynamic, transport, and structural properties of materials with a particular focus on biological applications.

**Course Goals:**

1. Students will understand some of the major computational problems in molecular and cellular modeling
2. Deepen students' understanding of principles of macromolecular structure, and of macromolecular structure – function relationships
3. Give students practical experience in building and evaluating molecular models
4. Give students a thorough understanding of the basic principles behind molecular mechanics force fields and algorithms
5. Students will understand the functional construction of force fields, variability, and evaluation of the various force field models
6. Give students practical experience in using standard molecular mechanics algorithms (energy minimization and molecular dynamics)
7. Students will be familiar with a variety of modeling approaches – quantum and molecular mechanics, molecular dynamics, and Monte Carlo
8. Provide students with a survey of a variety of other modeling algorithms
9. Students will have familiarity with computational biology applications such as protein folding, computer assisted drug design, and the prediction of protein-protein and gene regulatory networks
10. Students will understand basic concepts of high performance and grid computing as they help to solve challenging problems in computational biology (e.g., MPI, Condor)

|                  |                              |             |
|------------------|------------------------------|-------------|
| <b>Grading :</b> | 2 Exams (@ 15 % each)        | 30 %        |
|                  | Homework Problem Sets        | 10 %        |
|                  | Term Project (Total 40%)     |             |
|                  | Quality of Work              | 20 %        |
|                  | Quality of Oral Presentation | 20 %        |
|                  | Final Exam                   | <u>20 %</u> |
|                  |                              | 100 %       |

|                          |      |   |
|--------------------------|------|---|
| <b>Grade Assignment:</b> | ≥90% | A |
|                          | ≥80% | B |
|                          | ≥70% | C |
|                          | ≥60% | D |
|                          | <60% | F |

- Grading Policy:**
1. No make-up exams except by prior arrangement with instructor
  2. All problem sets are due at the beginning of class or at the stated time.
  3. A late assignment = no assignment.
  4. Exam grading appeals must be submitted in writing on the day the exam is returned. If you miss that class, you lose the opportunity for regrading.

**HW Assignments:** Homework assignments will be given approximately every week and each assignment will be worth approximately the same credit (Typically there will be between 10 and 12 homeworks each worth the same amount with the total worth 10% of the final grade).

You may (and are encouraged to) work in groups on problem sets. However, what you submit must be your own work except for assignments that are designated as group assignments. Assignments that are obviously copied will receive no credit.

**Attendance Policy:** Consistent with WVU guidelines, students absent from regularly scheduled examinations because of authorized University activities will have the opportunity to take them at an alternate time. Make-up exams for absences due to any other reason will be at the discretion of the instructor.

**Social Justice Statement:**

“West Virginia University is committed to social justice. I concur with that commitment and expect to maintain a positive learning environment based upon open communication, mutual respect, and nondiscrimination. Our University does not discriminate on the basis of race, sex, age, disability, veteran status, religion, sexual orientation, color or national origin. Any suggestions as to how to further such a positive and open environment in this class will be appreciated and given serious consideration. If you are a person with a disability and anticipate needing any type of accommodation in order to participate in this class. Please advise me and make appropriate arrangement with Disability Services (293-6700).”

**Course Schedule:**

| Week | Starting | Topic  |
|------|----------|--|
| 1    | 8/24/09  | Introduction to computational biology: Molecular, cellular, and organism levels, basic concepts – Cartesian and internal coordinates; Boltzmann factors, potential energy surfaces |
| 2    | 8/31/09  | Molecular mechanics force fields – origin, variations, and parameterization, bonds, angles, torsions, and van der Waals interactions   |
| 3    | 9/07/09  | Nonbonded energy computations – molecular mechanics, pair potentials, improper torsions, electrostatics  |
| 4    | 9/14/09  | Molecular mechanics continued – water, united atoms, transferability, periodic boundary conditions, and the Ewald summation  |
| 5    | 9/21/09  | Molecular dynamics – energy minimization, average statistical properties, thermodynamic integration  |
| 6    | 9/28/09  | EXAM 1<br>Monte Carlo methods – Metropolis Method, kinetic MC, phase equilibria, MC vs MD  |
| 7    | 10/05/09 | No Class – GRC Meeting   |
| 8    | 10/12/09 | Protein structure: amino acid repertoire, primary to quaternary structure, protein structure classification. Conformational sampling and protein folding                           |
| 9    | 10/19/09 | Free energy calculations, solvation, free energy partitioning  |
| 10   | 10/26/09 | Problems in biomolecular modeling: Docking and drug design   |
| 11   | 11/02/09 | Problems in biomolecular modeling: Fast methods for the N-body problem   |
| 12   | 11/09/09 | EXAM 2 (AIChE)<br>Term Projects  |
| 13   | 11/16/09 | Problems in biological networks: Predicting protein-protein interactions, Term Projects  |
| 14   | 11/23/09 | Thanksgiving Break   |
| 15   | 11/30/09 | Written and Oral Presentations   |
| 16   | 12/07/09 | Project and Course Review  |
| 17   | 12/14/09 | FINAL  |