Instructor:
Prof. Pengyu Ren (pren@utexas.edu)
Office: BME 5.202M
Phone: 512-232-1832

Office hour:
Tuesday 1-2 PM, Friday 9:30-10:30 AM, or appointment by email

Class meeting time and location
Tuesday and Thursday, 8-9:30 AM in GDC 4.302

Course Objectives:
Introduction to computational structural biology and molecular modeling, including the fundamentals of biomolecular structure and molecular thermodynamics. The principles and applications of biomolecular modeling used to explore the critical relationship between structure, function, and thermodynamic driving forces in biological molecules.

Knowledge, Abilities, and Skills Students Should Have Entering this Course
Graduate standing (BME383J), upper division undergraduate status (BME346), or permission of the instructor

Required Textbooks and Other Materials
Personal laptop (Windows OS) is required to install and use computer software, online resource and tools. Regular access to the course website (http://canvas.utexas.edu), where the lecture notes and assignments will be posted, is mandatory. If you are unsure about how to use any aspect of Canvas, please contact the ITS Help Desk by calling +1.512.475.9400 or by submitting a help request at https://www.utexas.edu/its/helpdesk/

Recommended Textbook(s):
Molecular Modelling: Principles and Applications (2nd Edition), Andrew Leach, 2001

Other Required Material:
None

Course Objectives:
- Knowledge of the relationship among genetic sequence, protein structure and biological function
- Knowledge of organization of protein and nucleic acid molecular structure
- Knowledge of principles of molecular thermodynamics and biophysical chemistry
- Ability to investigate and interpret the structure, dynamics and interactions of macromolecules using molecular modeling
- Ability to select, design and engineering molecules to interact with and mimic biomolecules using molecular modeling
- Skills in molecular modeling tools and software
- Assessed via homework, lab assignments, and projects

Topics Covered (# of classes per topic):
See Tentative schedule at the end of syllabus for details
1. Introduction (1)
2. Proteins and nucleic acids chemistry and structures (3)
3. Biological databases and visualization (2)
4. Biomolecular thermodynamics and physical chemistry (3)
5. Biophysical chemistry and intermolecular forces (2)
6. Quantum mechanics and Molecular mechanics (4)
7. Molecular dynamics (3)
8. Computer-aided drug discovery and molecular engineering (2)
9. Advanced free energy simulation (1)
10. Research Project (4)

**Class/Laboratory Schedule (Type, number and duration of sessions each week):**
- Class sessions: 2 per week; 90 minutes each
- Lab session: 1 every ~2 weeks in class

**Overview of Major Course Requirements and Assignments:**
- Midterm Exam
- Final project: presentations, critiques, and reports

**Grading Policy:**
- Plus & minus grades will be used
  - Class participation 5% (attendance and in-class project/peer review)
  - Homework & lab assignments 25%
  - Midterm exam 35%
  - Final project 35% (preproposal 5%, half-draft presentation & report 10%, final presentation & report 20%)

Assignments require **electronic** submission to Canvas class website. Late submission of assignments will result in grade reduction (see Attendance policy).

Students taking the course on a credit / no-credit basis must fully participate in all in-class activities and associated preparatory work outside of class but are not required to take the exam or submit the half-draft or the final proposal.

**Class Website:**
[http://canvas.utexas.edu/](http://canvas.utexas.edu/)

**Attendance, Participation, & Late Work Policy**
Participation is required at all class session and failure to participate in class will impact your grade as described above in the Grading & Evaluation section. Absences will be excused and late work accepted only in the cases of a documented emergency (e.g., you or a dependent are ill), observance of a religious holy day, or education-related travel (e.g., presentation at a conference). By UT Austin policy, you must notify the instructors of your pending absence at least fourteen days prior to the date of observance of a religious holy day. If you must miss a class, an examination, a work assignment, or a project in order to observe a religious holy day, you will be given an opportunity to complete the missed work within a reasonable time after the absence. Similar prior notice is expected for non-emergency excused absences.

Peer review is used as a pedagogical strategy extensively in this course. Late submission of assignments disrupts the peer review process. Thus, late submission of assignments will receive severe automatic reductions (see list below) of the max grade possible **unless prior arrangements have been made** with the instructors and extensions have been granted. No late work is accepted after the final class day of the semester.
- Up to 5 minutes late, 20% reduction
- Up to 1 hour late, 40% reduction
- Up to 24 hours late, 60% reduction
- No credit if more than 24 hours late

**Re-grade Policy**
Requests for re-grades will be made using the “assignment comment” feature of Canvas. For assignments graded before the last week of class, re-grade requests must be made within one week. For all other
assignments, re-grade requests must be made within 24 hours. Note that regrading may increase or lower your grade.

**Academic Integrity**
The core values of the University of Texas at Austin are learning, discovery, freedom, leadership, individual opportunity, and responsibility. Each member of the University is expected to uphold these values through integrity, honesty, trust, fairness, and respect toward peers and community.

Students who violate University rules on scholastic dishonesty are subject to disciplinary penalties, including the possibility of failure in the course and/or dismissal from the University. Since such dishonesty harms the individual, all students, and the integrity of the University, policies on scholastic dishonesty will be strictly enforced. For further information please visit the Student Judicial Services Web site: [http://deanofstudents.utexas.edu/sjs/](http://deanofstudents.utexas.edu/sjs/)

Academic integrity topics specific to this course:
- Sample materials will be provided by the instructors to assist students in preparing for assignments, projects, and exams. Any attempt to access copies of assignments, projects, or exams from any source other than the instructors is considered academic dishonesty.
- The instructors will use software designed to detect plagiarism in student work in this course, which may include assignments, projects, and exams. Any concerns raised by such software will be submitted to Student Judicial Services.
- Students are permitted to speak with anyone, including other students in the course, as they work on assignments or projects and prepare for exams. However, all written materials such as computer programs, presentation slides, and papers must be prepared by the individual student.
- Additional guidance on avoiding academic dishonesty or the appearance thereof will be provided on the cover page of each exam.

**Services for Students with Disabilities**
The University of Texas at Austin provides, upon request, appropriate academic adjustments for qualified students with disabilities. For more information, please contact the Division of Diversity and Community Engagement, Services for Students with Disabilities, +1.512.471.6259, [http://www.utexas.edu/diversity/ddce/ssl/](http://www.utexas.edu/diversity/ddce/ssl/)

**Other Campus Resources**
There are many resources and facilities at The University of Texas at Austin. Some key aggregators of helpful information are
- Division of Diversity of Community Engagement ([http://www.utexas.edu/diversity/](http://www.utexas.edu/diversity/)),
- Graduate School ([http://www.utexas.edu/academics/graduate-school](http://www.utexas.edu/academics/graduate-school)),
- Libraries ([http://www.lib.utexas.edu](http://www.lib.utexas.edu)),
- Information Technology Services ([https://www.utexas.edu/its/helpdesk/](https://www.utexas.edu/its/helpdesk/)).

For example, there is a campus map of all-gender restrooms on the Gender and Sexuality Center’s website ([http://ddce.utexas.edu/genderandsexuality/](http://ddce.utexas.edu/genderandsexuality/)).

**Safety Information**
Please review the following recommendations regarding emergency evacuation from the Office of Campus Safety and Security, +1.512.471.5767, [http://www.utexas.edu/safety/](http://www.utexas.edu/safety/):
- Occupants of buildings on The University of Texas at Austin campus are required to evacuate buildings when a fire alarm is activated. Alarm activation or announcement requires exiting and assembling outside.
- Familiarize yourself with all exit doors of each classroom and building you may occupy. Remember that the nearest exit door may not be the one you used when entering the building.
- Students requiring assistance in evacuation shall inform their instructor in writing during the first week of class.
- In the event of an evacuation, follow the instruction of faculty or class instructors.
- Do not re-enter a building unless given instructions by the following: Austin Fire Department, The
University of Texas at Austin Police Department, or Fire Prevention Services office.

- Behavior Concerns Advice Line (BCAL): +1.512.232.5050
- More information regarding emergency evacuation routes and emergency procedures can be found at: www.utexas.edu/emergency

**Tentative schedule (subject to changes)**

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<td>Molecular Simulation &amp; Molecular Dynamics <em>(preproposal review due)</em></td>
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