Chemistry 600—Molecular Modeling Spring 2017
Tu,Th 12:30PM-1:45PM
La Tourette Hall 201

Instructor: Professor Linh Nguyen — Office: La Tourette 324
Contact Info: 753-6011; bnguyen2@niu.edu — Office Hours: Friday 10 – 11:50am or by appointment

Objectives: Learn the capabilities and limitations of three major types of computer modeling techniques used in chemistry today—molecular orbital, molecular mechanics, and molecular dynamics methods. By gaining hands-on experience with each method, learn the required input data and how to analyze and interpret results.

Textbook: Recommended (not required) Andrew R. Leach "Molecular Modeling Principles and Applications", 2nd Ed.; Prentice-Hall: New York; 2001. Frank Jensen "Introduction to computational chemistry" 2nd Ed.; Wiley: England; 2007. A reading list of required literature will be provided each week throughout the course.

Grading: Final grades will be assigned based on total points accumulated. Maximum possible score is 1000 points.

850-1000:	A	550-699:	C
700-849:	B	400-549:	D

Each assignment counts toward the final point total in the following amounts:

Molecular orbital calculation	100 points
Molecular mechanics calculation	100 points
Molecular dynamics calculation	100 points
Individual Project	500 points
Quizzes	200 points

Each student is expected to behave according to standards of proper conduct and each student is responsible for knowing Northern Illinois University Academic Misconduct Code. The full text of the Academic Misconduct Code is available in writing and on the NIU Web page at http://www.niu.edu/conduct/academic-misconduct/index.shtml. Any student who chooses to engage in academic misconduct (including cheating, plagiarism, and any other action that may improperly affect evaluation) will be subject to sanctions in accordance with the Academic Misconduct Code. Dr. Nguyen routinely recommends an "F" for the course and expulsion from the University for all such violations.

Laboratories: Computer laboratory assignments are to be completed and a typed, 3 page report submitted on or before the due date. The Center for Research Computing and Data (CRCD - crcd.niu.edu) resources are freely available to everyone at NIU and their collaborators. You will need to request an account on Gaea by sending them this information:
Project: CHEM600S2017
PI: Bao Linh Nguyen a1814870
Student: First name Last name, z#
Gaea is available anytime via the network, unless there is a scheduled maintenance.

Quizzes: Comprehensive quizzes will be given periodically to gauge your ongoing understanding of the material. They may be unannounced.

Projects: Students should select an individual project involving any ONE of the different small molecule passages across any ONE of the integral membrane aquaporin family, using simulation methods emphasized in the course. Your results maybe contributed to one or more publications for the ongoing research in Dr. Nguyen group. A typed 1-2 page outline of the proposed project with 2-3

specific aims should be submitted in writing and I MUST pre-approve the project before work is begun. A typed 1-2 page preliminary results report with figures to show your system is equilibrated, and the path to the output files should be submitted in writing. A typed, 5-10 page ACS publication format report, plus figures and references, is due before the end of the semester.

Plagiarism: Any attempt to represent the work or ideas of others as your own without proper attribution is plagiarism, a form of academic misconduct, and may be dealt with by the procedure described in the Student Code of Responsibility and Conduct. Copies of the Student Code are available on the website. Each student is responsible for knowing and adhering to the Student Code.

Special Situations: If you miss a quiz without a verifiable illness or emergency, a grade of zero will be assigned for that quiz. You have one week after your illness or emergency to document your special circumstances before a grade of zero is assigned.

Accessibility Statement: Northern Illinois University is committed to providing an accessible educational environment in collaboration with the Disability Resource Center (DRC). Any student requiring an academic accommodation due to a disability should let his or her faculty member know as soon as possible. Students who need academic accommodations based on the impact of a disability will be encouraged to contact the DRC if they have not done so already. The DRC is located on the 4th floor of the Health Services Building, and can be reached at 815-753-1303 (V) or drc@niu.edu

Preferred Gender Pronoun Statement: This course affirms people of all gender expressions and gender identities. If you prefer to be called a different name than what is on the class roster, please let me know. Please also inform me and feel free to correct me and your classmates on your preferred gender pronouns. If you have any questions or concerns, please do not hesitate to speak with me in person, or email me. The Gender and Sexuality Resource Center also has a webpage designed to help support people of all genders as they navigate NIU's system: http://niu.edu/gsrc/audience/trans.shtml

Multilingual Student Statement: I am committed to making course content accessible to all students. If English is not your first language and this causes you concern about the course, please speak with me.

Student Sexual Misconduct Policy: Title IX prohibits sex discrimination to include sexual misconduct: harassment, domestic and dating violence, sexual assault, and stalking. If you or someone you know has been harassed or assaulted, you can receive confidential support and advocacy at the Counseling & Consultation Service's Advocacy Services, which can be contacted on at 815-753-1206, or in Campus Life Building-room 200. Alleged violations can be reported non-confidentially to the Affirmative Action & Equity Compliance Office in Lowden Hall-room 101, at 815-753-1118, or online at http://www.niu.edu/sexualmisconduct/help/form.shtml. Reports to law enforcement can be made to NIU Police & Public Safety at 815-753-1212. For an emergency, call 911. For more information about Sexual Misconduct Prevention & Resources, visit http://niu.edu/sexualmisconduct/index.shtml

Note: As an instructor, one of my responsibilities is to help create a safe learning environment on our campus. I also have a mandatory reporting responsibility related to my role as an instructor and a faculty advisor to a student organization. I am required to share information regarding sexual misconduct or information about a crime that may have occurred on NIU's campus with the University. Students may speak to someone confidentially by contacting Counseling & Consultation Service's Advocacy Services at 815-753-1206, or in Campus Life Building-room 200.

Reserve Materials: Lecture notes and answer keys for quizzes, as well as a selection of literature readings, will be placed on Reserve in the university libraries. You are free to make one copy of the notes and answer keys for your own private use.

Tentative Lecture Schedule

Introduction/Quantum Chemical Methods

January	17	Syllabus/Introduction Molecular Modeling
		Laboratory—Introduction to Computers and Operating Systems
	24	Molecular Orbital (MO) Methods
		Laboratory—Using the UNIX Operating System
	31	Self-Consistent-Field (SCF) Molecular Orbital Methods
		Analyzing MO Calculations/Strengths and Limitations
February	7	Density Functional Theory
		Laboratory—Molecular Orbital Calculations
	14	**Laboratory report due (100 points)**

Molecular Mechanics Methods

	14.	Molecular Mechanics Methods
		Laboratory—Molecular Graphics
	21.	Molecular Mechanics Force Fields
		Laboratory—Molecular Mechanics Calculation
	28.	Inventing Force Fields for Molecular Mechanics
		Laboratory report due (100 points)

Molecular Dynamics Methods/Individual Projects

March	**7**	Molecular Dynamics Methods/MD Force Fields
		Laboratory—Molecular Dynamics Simulations
		Project outline due (50 points)
	12-19	Spring Recess
	21	Statistical Analysis of Molecular Dynamics Simulations
		Laboratory —Molecular Dynamics Simulations/Individual projects
	28	Multiple copy MD simulations to find ligand migration pathways
		Preliminary result due (50 points) - Individual projects (energy minimization, and equilibration)
April	4	Analyzing Molecular Dynamics Simulations
		Laboratory—Molecular Dynamics Simulations/Individual projects
	11	Modern Uses of Molecular Dynamics
		Laboratory—Molecular Dynamics Simulations/Individual projects
	18	Miscellaneous Molecular Modeling Methods
		Laboratory—Individual Projects
	25	Laboratory—Individual Projects
		Laboratory—Individual Projects
May	2	Laboratory—Individual projects
		Laboratory—Individual Projects
	5	**Individual projects report due (500 points)**

Disclaimer: The instructor reserves the right to change by addition and/or subtraction any and/or all materials contained in this syllabus. This includes, but is not limited to course content, assignments, due dates, and portion(s) of the grade assigned to individual items within the course.