NJIT New Jersey Institute of Technology

THE COLLEGE OF SCIENCE AND LIBERAL ARTS

THE DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE

Chemistry:
Spring 2025 Course Syllabus

NJIT Academic Integrity Code: All Students should be aware that the Department of Chemistry & Environmental Science (CES) takes the University Code on Academic Integrity at NJIT very seriously and enforces it strictly. This means that there must not be any forms of plagiarism, i.e., copying of homework, class projects, or lab assignments, or any form of cheating in quizzes and exams. Under the University Code on Academic Integrity, students are obligated to report any such activities to the Instructor.

COURSE INFORMATION

Course Description: Principles and applications of quantum chemistry; Static electronic structure calculations, Solving Schrodinger equation via Hartree-Fock method, Density Functional Theory; Molecular dynamics simulations, building force-fields, concept of ensembles; Ab-initio molecular dynamics. Introduction to software Gaussian and CP2K as well as visualizing packages Avogadro, Gaussview and VMD.

Number of Credits: 3

Course-Section and Instructors

Course-Section	Instructor
CHEM 737-102, M 6pm – 8:50 pm	Farnaz A. Shakib (Website)

Course Presentation:

In person: **Guttenberg Info Tech Center 2400**

Course Partitions:

Lectures on theoretical concepts/Hands-on lab sessions January 27 – April 7
Exam on theoretical concepts April 14
Working on Projects and Final Presentations: April 21 – May 5

Office Hours: Arranged by email.

In-person: Tiernan hall Rm 368

There is no textbook for this course. The materials covered are on the frontline of research and online resources are numerous.

University-wide Withdrawal Date: The last day to withdraw with a **W** is Monday, April 7, 2025. It will be strictly enforced.

Learning Outcomes: At the end of the course, the student will be able to

- Construct the Schrödinger equation for simple systems
- Create input configuration of molecules for static electronic structure calculations
- Create input files for molecular dynamics simulations
- Be familiar with bash scripting
- Be able to turn numerical data to visual plots and results
- Be able to run calculations on high performance computing clusters
- Describe the differences between classical and quantum mechanics
- Build force fields for molecular dynamics
- Describe the differences between classical and quantum-mechanical dynamics simulations
- Analyze the molecular dynamics trajectories
- Be able to carry out a computational project all the way from making the input files to analyzing the results

Canvas: There is a course Canvas site that will include significant resources and updates of importance to this course, both for the lecture and laboratory portions. Please check it frequently, and also make sure to check or forward your NJIT email in order to receive important announcements. Furthermore, all the office hours and discussions will be conducted through Canvas.

POLICIES

All CES students must familiarize themselves with, and adhere to, all official university-wide student policies. CES takes these policies very seriously and enforces them strictly.

Grading Policy: The final grade in this course will be determined as follows:

Lab Homework	25
Class Participation Solving problems in class, active role in asking and answering questions, active participation in the lab section	20
Exam on Theoretical Concepts	25
Final Presentation	30

Your final letter grade in this course will be based on the following tentative curve:

A	88-100	**C**	60-64.5
B+	78-87.9	**F**	< 60
B	70-77.9		
C+	65-69.9		

Attendance Policy: Attendance at all classes is not mandatory but extremely encouraged due to the nature of the topic which cannot be simply learnt through "getting the notes."

Homework Policy: Homework is an expectation of the lab section of the course. They are meant to help you honing your basic scripting and computational skills. Homework is due for grading one day before the class (i.e. till 6pm on the Sunday before the class). Graded homework will be returned the next day after the lecture and they will be discussed during the lecture.

Exams: There will be one exam covering the theoretical concepts discussed in the class. The exam is closed book/notebooks but students are allowed to prepare a double sided A4 page of any material related to class and keep it with themselves during the exam.

Makeup Exam Policy: There will normally be **NO MAKE-UP EXAMS** during the semester. In the event that a student has a legitimate reason for missing an exam, the student should contact the Dean of Students office and present written verifiable proof of the reason for missing the exam, e.g., a doctor's note, police report, court notice, etc. clearly stating the date AND time of the mitigating problem. The student must also notify the CES Department Office/Instructor that the exam will be missed so that appropriate steps can be taken to make up the grade.

Cellular Phones: All cellular phones and other electronic devices must be switched off during all class times. Such devices must be stowed in bags during exams or quizzes.

ADDITIONAL RESOURCES

Accommodation of Disabilities: Office of Accessibility Resources and Services (***formerly known as Disability Support Services***) offers long term and temporary accommodations for undergraduate, graduate and visiting students at NJIT.

If you are in need of accommodations due to a disability please contact Chantonette Lyles, Associate Director at the Office of Accessibility Resources and Services at 973-596-5417 or via email at lyles@njit.edu. The office is located in Fenster Hall Room 260. A Letter of Accommodation Eligibility from the Office of Accessibility Resources Services office authorizing your accommodations will be required.

For further information regarding self-identification, the submission of medical documentation and additional support services provided please visit the Accessibility Resources and Services (OARS) website at:

- http://www5.njit.edu/studentsuccess/disability-support-services/

Tentative Course Outline

Lecture	Date	Theoretical Concepts	Hands-on Lab
1	01/27/2025	Introduction to Computational Chemistry	Introduction to Linux/Bash scripting/vi editor/homework
2	02/03/2025	Quantum mechanics (QM), Time-dependent and time-independent Schrödinger equations, Matrix representation of QM	Gnuplot/plotting functions/homework
3	02/10/2025	Electronic structure calculations, Hartree-Fock (HF) method	Creating input files with Avogadro software/simple minimization
4	02/17/2025	density functional theory (DFT)	Electronic structure calculations of benzene in the gas phase/MOs/vibrational analysis/Comparing HF and DFT
5	02/24/2025	Basis sets	Analysis of accuracy and efficiency of different basis sets
6	03/03/2025	Chemical reactions, Thermochemistry	Related calculations
7	03/10/2025	Solvent effect	Electronic structure calculations of organic compounds in solution/Implicit solvent
8	03/17/2025	Spring recess, no class	
9	03/24/2025	Introduction to Ab Initio Molecular Dynamics (AIMD), concept of periodic boundary conditions	Compiling Packmol, Preparing input files with Packmol for AIMD simulation of organic compounds in aqueous solution
10	03/31/2025	Classical molecular dynamics (MD), Equations of motions, concept of force fields	Analysis of AIMD and MD trajectories with VMD package, Convergence of E, T, P/ concept of RDF
11	04/07/2025	Concept of ensembles for MD simulations and thermostats	Related simulations
12	04/14/2025	Exam on theoretical concepts	
13	04/21/2025	Discussing the topics for the final project, assigning projects to groups (2 groups of 2 and 1 group of 3)	Working on projects
14	04/28/2025	Working on projects	
15	05/05/2025	Final presentations	