New Jersey Institute of Technology
Digital Commons @ NJIT

Chemistry, Environmental and Forensic Science Syllabi

NJIT Syllabi

Spring 2022

CHEM 437-102: Applying Computational Chemistry & Molecular Models

Farnaz Shakib

Follow this and additional works at: https://digitalcommons.njit.edu/chem-syllabi

Recommended Citation

Shakib, Farnaz, "CHEM 437-102: Applying Computational Chemistry & Molecular Models" (2022). *Chemistry, Environmental and Forensic Science Syllabi*. 421.
https://digitalcommons.njit.edu/chem-syllabi/421

This Syllabus is brought to you for free and open access by the NJIT Syllabi at Digital Commons @ NJIT. It has been accepted for inclusion in Chemistry, Environmental and Forensic Science Syllabi by an authorized administrator of Digital Commons @ NJIT. For more information, please contact digitalcommons@njit.edu.

NJIT New Jersey Institute of Technology

THE COLLEGE OF SCIENCE AND LIBERAL ARTS

THE DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE

Chemistry:
Spring 2022 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, force-fields, Path integral formalism of dynamics, ensembles; Ab-initio molecular dynamics, non-adiabatic quantum dynamics.

Number of Credits: 3

Course-Section and Instructors

Course-Section	Instructor
CHEM 437-102, R 6pm – 8:50 pm	Farnaz A. Shakib (Website)
CHEM 737-102, R 6pm – 8:50 pm	Farnaz A. Shakib

Course Presentation: Converged Mode

In person: Guttenberg Info Tech Center 2315C
Virtual: https://njit.webex.com/meet/shakibnjit.edu

Course Partitions:

Lectures/Lab sessions January 20 – March 10 (8 lectures)
Working on Projects March 31 – May 14

Office Hours: By email, can be arranged as in-person (Tiernan hall Rm 368) or through WebEx at the instructor's personal WebEx room (https://njit.webex.com/meet/shakibnjit.edu)

There is no textbook for this course.

University-wide Withdrawal Date: The last day to withdraw with a **W** is Monday, April 4, 2022. 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 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
- Carry out molecular dynamic's simulations
- Analyze the molecular dynamics trajectories
- Describe the essence of path integral formalism
- Simulate dynamics through path integral molecular dynamics
- Describe the essence of non-adiabatic quantum dynamics
- 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	20
Class Participation Solving problems in class, active role in asking and answering questions	25
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	**D**	55-59.9
B	70-77.9	**F**	< 55
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 Wednesday 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. **Note that the exam will be held online**. 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. A picture of this information sheet should be uploaded to Canvas along with the answers to the exam problems.

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/

Course Outline

Lecture	Date	Lecture	Lab
1	01/20/2022	Differential equations, Time-independent Schrödinger equation	Linux/Bash scripts/vi editor/gnuplot
2	01/27/2022	Hartree-Fock method, density functional theory	Creating input files with Avogadro
3	02/03/2022	Basis sets	Electronic structure calculations with Gaussian
4	02/10/2022	Molecular dynamics, periodic systems	Analysis of MD trajectories with VMD/Radial distribution function
5	02/17/2022	Potential energy surfaces, classical vs. ab initio molecular dynamics	Preparing input files with packmol, ab initio simulations with CP2K
6	02/24/2022	Force fields and how to create them using Antechamber, Ensembles	DL_POLY Quantum/water simulations
7	03/03/2022	Nuclear quantum effects, path integral formalism	PIMD vs. MD in DL_POLY Quantum
8	03/10/2022	Non-adiabatic dynamics	Assigning projects and groups
9	03/17/2022	Spring recess, no class	
10	03/24/2022	Exam on theoretical concepts	
11	03/31/2022	Working on projects	
12	04/07/2022	Working on projects	
13	04/14/2022	Working on projects	
14	04/21/2022	Final presentations	
15	04/28/2022	Final presentations	