

# Syllabus

## CHEM-GA 9668: Chemical Dynamics

### Spring 2024

#### Class Meetings

Lecture: Tuesday and Thursday, 8:15 am–9:30 am (1/22–5/10/2024), **Room N203**

Location: 567 West Yangsi Rd, Shanghai

Credits: 4 units

#### Instructor

Professor Xiang Sun

Email: xiang.sun@nyu.edu

Office hours: Tuesday, 2:00 pm–4:00 pm, **Room E621**

Location: 567 West Yangsi Rd, Shanghai

#### **Course Description**

This course will provide an introduction to chemical dynamics, especially in the condensed phase. Topics include classical molecular dynamics, quantum dynamics, rate theories, electron and energy transfer theories, mixed quantum-classical dynamics, semiclassical dynamics, and ultrafast spectroscopy.

#### **Course Learning Outcomes**

This course is intended to provide a balanced presentation of both classical and quantum mechanical descriptions of chemical dynamics. It is designed for introducing students to reactive and non-reactive dynamical methods with an emphasis on condensed-phase systems. Topics include classical mechanics, molecular dynamics, time-dependent classical and quantum statistical mechanics, time correlation functions, quantum dynamics, path integrals in quantum mechanics, Born-Oppenheimer approximation, quantum chemistry, transition state theory, electron transfer theory, quantum master equation, mixed quantum-classical dynamics, semiclassical dynamics, introduction to ultrafast spectroscopy. (4 units)

#### **Course Requirements**

##### Reference books

1. Herbert Goldstein, C. P. Poole, J. L. Safko, **Classical Mechanics** (3rd ed), Addison Wesley, 2001
2. Abraham Nitzan, **Chemical Dynamics in Condensed Phases**, Oxford University Press, 2006
3. Mark E. Tuckerman, **Statistical Mechanics: Theory and Molecular Simulation**, Oxford University Press, 2010
4. Volkhard May, Oliver Kühn, **Charge and Energy Transfer Dynamics in Molecular Systems** (3rd ed), Wiley-VCH, 2011

5. Shaul Mukamel, *Principles of Nonlinear Optical Spectroscopy*, Oxford University Press, 1999
6. J. J. Sakurai, Jim Napolitano, *Modern Quantum Mechanics* (3rd ed), Cambridge University Press, 2020
7. Claude Cohen-Tannoudji, B. Diu, F. Laloe, *Quantum Mechanics, (Volumes 1-3)*, Wiley-VCH, 2019
8. Ira N. Levine, *Quantum Chemistry* (7th ed), Prentice Hall, 2013
9. Literature references distributed throughout the course

### Software

**QChem, Spartan, Amber**, and packages will be accessible for computational needs in homework and the final project.

### Web access

Brightspace (<https://brightspace.nyu.edu/d2l/home>) serves as the electronic portal for this course. Please check it regularly for announcements, discussions, project guidelines, etc. Please familiarize yourself with how to post questions on the class forum (see Email policy below).

## Course Schedule

### Topics and Assignment

Week/Lecture	Topic	Due
Week 1	Review of Classical Mechanics, Lagrangian Hamiltonian	
Week1	Hamiltonian Mechanics	
Week 2	Molecular Dynamics Simulation	
Week 2	Force Field and Electrostatic Interactions	
Week 3	Time Correlation Functions	Homework 1
Week 3	Linear Response Theory	
Week 4	Quantum Dynamics in Hilbert Space	
Week 4	Density Operator and Quantum Dynamics in Liouville Space	
Week 5	Quantum Time Correlation Functions	
Week 5	Transport properties	Homework 2
Week 6	Path Integrals in Quantum Mechanics, PIMD	

<b>Week/Lecture</b>	<b>Topic</b>	<b>Due</b>
Week 6	Path-Integral Molecular Dynamics, Centroid MD, Ring-Polymer MD	
Week 7	Born-Oppenheimer Approximation, Introduction to Quantum Chemistry	
Week 7	Breakdown of Born-Oppenheimer Approximation, Adiabatic vs Diabatic representations	
Week 8	Transition State Theory, Reactive Flux Theory	Homework 3
Week 8	Electron Transfer Theory, Landau-Zener Model	
Week 9	Marcus Theory and Fermi's Golden Rule	
Week 9	Quantum Master Equations	
Week 10	Generalized Quantum Master Equation	
Week 10	Mixed Quantum-Classical Dynamics, mean-field Ehrenfest and Surface Hopping Dynamics	Homework 4
Week 11	Mixed Quantum-Classical Liouville	
Week 11	Quantum-classical correspondence and Wigner transform	
Week 12	Semiclassical Dynamics	
Week 12	Linearized Semiclassical Dynamics	
Week 13	Light-Matter Interaction	Homework 5
Week 13	Introduction to Ultrafast Spectroscopy	
Week 14	Optical Response in Nonlinear Spectroscopy	
Week 14	Liouville Pathways	
Week 15	<i>Students' presentations</i>	Final project

## Assessment, Measurement and Evaluation

### Rubrics for the entire course, i.e. how to be successful in this class

<b>Category</b>	<b>Excellent</b>	<b>Good</b>	<b>Average</b>	<b>Poor</b>	<b>Fail</b>
<b>Terminology</b>	Always able to use correct terminology,	Often able to use correct terminology,	Generally able to use correct terminology,	Seldom able to use correct terminology,	Rarely able to use correct terminology,

Category	Excellent	Good	Average	Poor	Fail
	notation, and units	notation, and units	notation, and units	notation, and units	notation, and units
<b>Scientific concepts</b>	Shows complete understanding of the scientific concepts	Shows substantial understanding of the scientific concepts	Shows some understanding of the scientific concepts	Shows limited understanding of the scientific concepts	Shows little understanding of scientific concepts
<b>Application of chemical principles</b>	Able to choose the most suitable chemical principle and apply it to solve problems	Able to choose a suitable chemical principle and apply it to solve problems	Able to choose a working chemical principle and apply it to solve problems	Able to choose a tangent chemical principle and apply it to solve problems	Unable to choose a chemical principle and have trouble of applying it to solve problems
<b>Mathematical accuracy</b>	All of the calculations have no mathematical errors	Almost all of the calculations have no mathematical errors	Most of the calculations have no mathematical errors	A minority of the calculations have no mathematical errors	Most of the calculations have mathematical errors
<b>Logic and reasoning</b>	Uses complex and refined scientific reasoning	Uses effective scientific reasoning	Some evidence of scientific reasoning	Little evidence of scientific reasoning	No evidence of scientific reasoning
<b>Connecting the dots</b>	Connect new knowledge or skills with previous one in an effective and organized manner	Connect new knowledge or skills with previous one in a clear manner	Connect new knowledge or skills with previous one in an acceptable manner	Connect new knowledge or skills with previous one in a passive manner	Unable to connect new knowledge or skills with previous one
<b>Communication</b>	Summarize, explain, articulate and exemplify concepts and ideas in a perfectly clear and efficient manner	Summarize, explain, express and exemplify concepts and ideas in a clear and efficient manner	Summarize, explain, express and exemplify concepts and ideas in an acceptable manner	Summarize, explain, express and exemplify concepts and ideas in a vague manner	Unable to summarize, explain, express and exemplify concepts and ideas
<b>Creativity</b>	Apply chemical principles and initiate new approaches of understanding nature in a proactive manner	Apply chemical principles and initiate new approaches of understanding nature in a proactive manner	Apply chemical principles and initiate new approaches of understanding nature in a passive manner	Able to apply chemical principles and understand nature in approaches taught in class	Unable to apply chemical principles and understand nature in approaches taught in class

### **Class Participation**

***Students are expected to attend all lectures.*** Important concepts will be presented during lectures and ***students are strongly encouraged to ask questions.*** You will get the most benefit from lectures if you complete the reading beforehand. If you have difficulty understanding a particular point presented during lectures, chances are other students feel the same. It is better to ask the instructor to clarify a point of confusion than get lost and not follow for the rest of the lecture. Lectures start promptly at the scheduled time, after which time the lecture room door is closed. Out of courtesy to your fellow classmates, and the instructor, late arrivals will not be admitted.

**Homework**

Homework will be problem sets and computer practicums for learning the basic usage of quantum chemistry software *QChem* via *Spartan* interface, as well as molecular dynamics software *Amber*. The homework should be announced and submitted via **Assignments** section in Brightspace site electronically. Write your **name** and NYU **NetID** at the top of the homework report and combine your homework report into a single **PDF** file before uploading. Problem sets are assigned to help you to deepen your understanding of the material. It is also important to show your approach to obtain the results, rather than just a final answer. No late work will be accepted, and there will be no make-up or rescheduled homework.

**Final Project**

There will be a final project serving as the final exam. Students are expected to select the final project topic and get approved by the lecturer before the midterm of the semester. The final project should be finished individually and **presented during the last week** of the semester to the class. **A complete project report in PDF format** should be submitted via the **Assignments** section in Brightspace electronically no later than the Monday of the final exam week. If there is a schedule conflict involving other courses or religious obligations, communicate with the instructor as soon as you are aware of the conflict and no later than one week prior to deadlines.

**Grading**

The grade for this course will be determined according to the following formula:

<b>Assignments/Activities</b>	<b>% of Final Grade</b>
Class participation	5%
Homework	45%
Final project	50%

**Grading Evaluation Scale**

NYU Shanghai follows the same grading practices as NYU New York. The following grades may be awarded: A, A-, B+, B, B-, C+, C, F. In general, A indicates excellent work, B indicates good work, C indicates satisfactory work, which is the lowest passing grade. F indicates failure. There are some additional grades—P for pass, W for Withdrawal—which are awarded administratively.

The final score will be scaled to a maximum of 100 points, and then assigned a letter grade according to:

<b>Letter Grade</b>	<b>Percent</b>
<b>A</b>	90.0% and higher
<b>A-</b>	85.0% – 89.99%
<b>B+</b>	80.0% - 84.99%

Letter Grade	Percent
B	75.0% - 79.99%
B-	70.0% - 74.99%
C+	65.0% - 69.99%
C	60.0% - 64.99%
F	49.99% and lower

## Course Policies

### Laptop and mobile device policy

Laptops or tablets are permitted in lecture and recitation but may be used only for legitimate classroom purposes, such as taking notes, translating words, or accessing information from NYU Classes. Email, social media, browsing, reading the news, or playing games are not considered legitimate classroom purposes; such inappropriate laptop use is distracting to those seated around you and is unprofessional. The first one or two rows of seats in lecture and recitation will be reserved for students who do not wish to use a laptop/tablet.

***Cellphones must be switched off or made silent, and put away.***

### Email Policy

For Course-related questions, avoid emailing the instructors and instead ***please post to the class forum any questions related to the course*** (logistics, or material covered in lecture/recitation) so that everyone has access to discussions pertinent to the entire class. Before posting, please first look at the class announcements and search the forum to see if your question has already been covered. For questions that would benefit the class to have answers to, please post them for all to see in Brightspace.

***E-mail correspondence to the Instructors is reserved for matters of a personal nature (non-Course-related), e.g. illness, religious observances, etc.*** The expected response time is 24 hours. We will not check and respond to emails after working hours on weekdays or anytime on weekends/holidays.

### Late Assignment

Assignments/Homework/Projects are due at the date and time indicated in the syllabus. Late assignments will be treated as missing assignments. Exceptions can be made only with the prior approval of the instructors.

### University Policy on Make-up of Absence from Class due to illness

When students are ill, they are expected to notify professors in advance of class, if at all possible. Students should negotiate with professors the time and place for make-up of assignments, tests and/or examinations missed. In cases where students are seriously ill and will miss more than a week of classes, the Office of Health and Wellness should be contacted so that the student's other professors may be contacted. The Office of Health and Wellness will not verify medical absences of under a week.

## Academic Honesty/Plagiarism

**NYU Shanghai has ZERO tolerance of any kind of cheating or plagiarism.** Behaviors that are in violation of NYU Shanghai's policies on academic integrity include, but are not limited to, bringing or accessing unauthorized materials during an exam or quiz, or verbatim copying homework. While you are encouraged to work in groups on problem sets, the answers you turn in must be written by you in your own words. When academic dishonesty is suspected, it will be dealt with in adherence to the official guidelines of NYU Shanghai. If you are found in violation of NYU Shanghai's policies on academic integrity you will receive an F in the course and you could be subject to additional sanctions, including academic dismissal. It is not worth risking your career over a few possible points. If you have any questions or doubts about plagiarism, please do not hesitate to come to my office hours or speak with your academic advisor.

Violations of Academic Integrity include, but are not limited to:

- Cheating: Intentionally using or attempting to use unauthorized materials, information, notes, study aids, or other devices in any academic exercise.
- Fabrication and Falsification: Intentional and unauthorized alteration or invention of any information or citation in an academic exercise. Falsification is a matter of inventing or counterfeiting information for use in any academic exercise.
- Multiple Submissions: The submission of substantial portions of the same academic work for credit (including oral reports) more than once without authorization.
- Plagiarism: Intentionally or knowingly presenting the work of another as one's own (i.e., without proper acknowledgment of the source).
- Abuse of Academic Materials: Intentionally or knowingly destroying, stealing, or making inaccessible library or other academic resource materials.
- Complicity in Academic Dishonesty: Intentionally or knowingly helping or attempting to help another to commit an act of academic dishonesty.

Plagiarism includes, but is not limited to:

- Copying or borrowing liberally from someone else's work without his/her knowledge or permission; or with his/her knowledge or permission and turning it in as your own work.
- Copying of someone else's exam or paper.
- Allowing someone to turn in your work as his or her own.
- Not providing adequate references for cited work.
- Copying and pasting large quotes or passages without properly citing them.

## Disability Disclosure Statement

Academic accommodations are available for students with disabilities. Please contact the Moses Center for Students with Disabilities (212-998-4980 or [mosescsd@nyu.edu](mailto:mosescsd@nyu.edu)) for further information. Students who are requesting academic accommodations are advised to reach out to the Moses Center as early as possible in the semester for assistance.

NYU is committed to providing equal educational opportunity and participation for students with disabilities. It is NYU Shanghai's policy that no student with a qualified disability be excluded from participating in any NYU Shanghai program or activity, denied the benefits of any NYU Shanghai program or activity, or otherwise subjected to discrimination with regard to any NYU Shanghai program or activity. Any student who needs a reasonable accommodation based on a qualified disability is required to register with the CSD for

assistance. Students can [register online](#) through the Moses Center and can contact the Director of the Academic Resource Center with questions or for assistance.

## **Title IX Compliance**

From the [NYU Title IX website](#): “Title IX of the Education Amendments of 1972 (Title IX) prohibits discrimination on the basis of sex in educational programs. It protects victims of sexual or gender-based bullying and harassment and survivors of gender-based violence. Protection from the discrimination on the basis of sex includes protection from being retaliated against for filing a complaint of discrimination or harassment. NYU is committed to complying with Title IX and enforcing University policies prohibiting discrimination on the basis of sex. Mary Signor, Executive Director of the Office of Equal Opportunity, serves as New York University’s Title IX Coordinator. The University’s Title IX Coordinator is a resource for any questions or concerns about sex discrimination, sexual harassment, sexual violence, or sexual misconduct and is available to discuss your rights and judicial options. University policies define prohibited conduct, provide informal and formal procedures for filing a complaint and a prompt and equitable resolution of complaints.

### **Links to the Policy and related documents:**

- [Sexual Misconduct, Relationship Violence, and Stalking Policy](#)
- [Procedures for Complaints Against Students](#)
- [Procedures for Complaints Against Employees](#)
- [Resource Guide for Students](#)
- [Resource Guide for Employees](#)

## **Religious Observances**

New York University, as a nonsectarian institution, adheres to the general policy of including in its official calendar only certain legal holidays. However, it has also long been NYU policy that members of any religious group may, without penalty, excuse themselves from classes when compliance with their religious obligations requires it. In 1988, the University Senate affirmed this policy and passed the following resolution:

1. Students who anticipate being absent because of any religious observance should, whenever possible, notify faculty in advance of such anticipated absence;
2. Whenever feasible, examinations and assignment deadlines should not be scheduled on religious holidays. Any student absent from class because of religious beliefs shall not be penalized for any class, examination, or assignment deadline missed on that day or days.
3. If examinations or assignment deadlines are scheduled, any student who is unable to attend class because of religious beliefs shall be given the opportunity to make up that day or days.
4. No adverse or prejudicial effects shall result to any student who avails himself or herself of the above provisions.