

# Syllabus

## CHEM-SHU 651 Physical Chemistry: Quantum Mechanics & Spectroscopy

Fall 2023

### Class Meetings

Lecture: Tuesday and Thursday, 8:15 am–9:30 am (8/28–12/8/2023), **Room EB122**

### Instructor

Professor Xiang Sun,

Email: xiang.sun@nyu.edu

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

### Course Learning Outcomes

An introduction to quantum mechanics—general principles and applications to important model systems. Covers electronic structure of one- and many-electron atoms, theory of chemical bonding in diatomic and polyatomic molecules. Includes principles and applications of molecular spectroscopy: rotational, vibrational, electronic, and nuclear magnetic resonance. Elements of photochemistry are also included.

Prerequisites: PHYS-SHU 12 General Physics II OR PHYS-SHU 93 Foundations of Physics II Honors, and CHEM-SHU 126 Foundations of Chemistry II. Fulfillment: Chemistry additional required course.

### Course Requirements

#### Textbook

Required:

- Donald A. McQuarrie and John D. Simon, ***Physical Chemistry: A Molecular Approach***, University Science Books (1997).

Recommended reading:

- Claude Cohen-Tannoudi, *et al*, ***Quantum Mechanics, Volume I*** (2<sup>nd</sup> ed), Wiley-VCH (2020).
- Thomas Engel, ***Physical Chemistry: Quantum Chemistry and Spectroscopy*** (4<sup>th</sup> ed), Pearson (2019).
- Andrew Cooksy, ***Physical Chemistry: Quantum Chemistry and Molecular Interactions***, Pearson (2014).
- Ira N. Levine, ***Quantum Chemistry*** (7<sup>th</sup> ed), Pearson (2014).
- Gilbert Strang, ***Introduction to Linear Algebra*** (5<sup>th</sup> ed), Wellesley-Cambridge Press (2016).

**Materials**

Required: Non-programming scientific calculator. Your calculator must have the following capabilities: logarithms, exponentiation, and trigonometric functions. It must have at least an eight-digit display and you must be able to switch manually between scientific and decimal notation. Typically, these are standard features.

**Web access**

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

**Assessment, Measurement, and Evaluation****Rubrics for the entire course, i.e. how to be successful in this class**

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

Category	Excellent	Good	Average	Poor	Fail
<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

### In-class Quizzes

During lectures, we may have quizzes, which will be designed for probing the understanding of the assigned reading sections and the knowledge from the previous lectures and assigned readings. We may use multiple-choice questions, calculation/derivation questions, or conceptual questions. Quizzes will be **closed book**. The quizzes may happen anytime during some lectures, but not in all lectures. We won't have make-up quizzes.

### Homework

Homework will be assigned after the second lecture of the week and will be due at the beginning of the second lecture the following week, and no late homework will be accepted. The homework should be announced in the "**Assignments**" section in Brightspace.

- Students should submit Homework as a **combined single PDF** file from a digital scan of their handwritten work. Please make sure the scanned PDF is legible.

Ensure your **name** and NYU **NetID** is written clearly at the top of the homework.

Problem sets are assigned to help you pace your learning and for you to gauge your own understanding of the material, and **you should finish the homework on your own**.

Homework will probably be related to Quizzes and Exams and serves as evidence of your progress in the course. It is also important to show your approach to the problems, rather than just the final answer. No late work will be accepted without a valid and documented excuse and there will be no make-up or rescheduled homework.

### Exams

There will be one midterm and one final exam. Exams are mandatory. If you have 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 the exam. Any missed exams will result in a zero grade for that particular exam unless there are serious extenuating personal circumstances that are immediately brought to the attention of the course instructor. The midterm exam will cover lecture materials for the first half semester. The final exam is comprehensive but will be weighed more heavily on material not

covered by the midterm exam. Only non-programming calculators will be allowed during the exams.

Exams will be **closed book**. Laptops, mobile devices, notes, books, or any other material will not be allowed during testing periods.

### **Grading**

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

<b>Assignments/Activities</b>	<b>% of Final Grade</b>
In-class Quizzes	10%
Homework	20%
Midterm Exam	30%
Final Exam	40%

### **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, C-, D+, D, F. In general, A indicates excellent work, B indicates good work, C indicates satisfactory work, and D indicates passable work and 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%
<b>B</b>	75.0% - 79.99%
<b>B-</b>	70.0% - 74.99%
<b>C+</b>	65.0% - 69.99%
<b>C</b>	60.0% - 64.99%
<b>C-</b>	55.0% - 59.99%
<b>D</b>	50.0% - 54.99%
<b>F</b>	49.99% and lower

The instructor reserves the right to give extra bonus of up to 10% based on the overall excellent performance during the entire course (see Rubrics).

## Course Policies

### Class Attendance and Participation

**Students are expected to attend all lectures.** Important concepts will be presented during the lecture and students are strongly encouraged to ask questions. **You need to complete the relevant reading before the lecture, otherwise, you won't be able to follow the lecture.** If you have difficulty understanding a particular point presented during a lecture, 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.

### Laptop and mobile device policy

Laptops or tablets are permitted in lectures 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; inappropriate laptop use distracts those seated around you and is unprofessional. **Cellphones must be switched off or made silent and put away.** The use of any electronic device is forbidden during exams, with the exception of an approved calculator.

### Email Policy

E-mail correspondence to the Instructor or RI 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 in weekdays or anytime on weekends/holidays.

For Course-related questions, avoid emailing the instructor 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.

### Late Assignment

Assignments are due at the date and time indicated in the Brightspace. Late assignments will be treated as missing assignments. Exceptions for up to 3 days can be made once only with the prior approval of the instructor.

### 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 finished on your own. 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 from online resources; or with his/her knowledge or permission and turning it in as your own work.
- Copying of someone else's homework, code, data, 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.

## Course Schedule

### Topics and Assignments

Week	Topic	Reading	Assignment Due
W1, 8/29	#1: Introduction to quantum theory – failures of classical physics	Ch 1, MCh A&C	

Week	Topic	Reading	Assignment Due
W1, 8/31	#2: Postulates of quantum mechanics, vector space, ket, inner product	Ch 4.1, MCh E&F	
W2, 9/5	#3: Operator	Ch 4.2, MCh B	
W2, 9/7	#4: Matrix form of operators, change of basis	Ch 4.3, MCh E&F	
W3, 9/12	#5: Measurement postulate, eigenvector and eigenvalue	Ch 4.3	
W3, 9/14	#6: Eigen basis of Hermitian operators, Common eigenstates	Ch 4.4, 4.5	
W4, 9/19	#7: Expectation and Time-dependent Schrödinger equation	Ch 4.6	
W4, 9/21	#8: Quantum particle in a box	Ch 3	
W5, 9/26	#9: Quantum harmonic oscillator 1, Eigenvalue problem	Ch 5.1-5.4	
W5, 9/28	#10: Quantum harmonic oscillator 2, creation and annihilation operators	Ch 5.6-5.7	
9/29-10/6	<b>National Day Holiday (no class)</b>		
W6, 10/10	#11: Quantum harmonic oscillator 3		
W6, 10/12	#12: Rigid rotator and microwave spectroscopy	Ch 5.8-5.9, MCh D	
W7, 10/17	<b>Midterm Exam</b>		
W7, 10/19	#13: Angular momentum: quantization	Ch 6.1-6.3	
W8, 10/24	#14: Angular momentum: wavefunction	Ch 6.4-6.5	
W8, 10/26	#15: Hydrogen atom, orbital	Ch 6.6-6.7	
W9, 10/31	#16: Spin, many-electron atoms	Ch 8.1-8.6	
W9, 11/2	#17: Addition of angular momentum	Ch 8.9	
W10, 11/7	#18: Atomic spectroscopy	Ch 8.8-8.11	
W10, 11/9	#19: Variational principle, Hatree-Fock method, Perturbation theory	Ch 7.1-7.4	
W11, 11/12 Legislative day	#20: Chemical bonding in diatomic molecules	Ch 9	



Week	Topic	Reading	Assignment Due
W11, 11/14	#21: Polyatomic molecules	Ch 10	
W11, 11/16	#22: Intro to group theory	Ch 12	
W12, 11/21	#23: Molecular symmetry, Point groups	Ch 12	
W12, 11/23	<b>Thanksgiving Holiday (no class)</b>		
W13, 11/28	#24: Molecular spectroscopy	Ch 13	
W13, 11/30	#25: Molecular spectroscopy	Ch 13	
W14, 12/5	#26: Nuclear magnetic resonance	Ch 14	
W14, 12/7	#27: Review		
W15	<b>Final Exam</b>		

## Exam Schedule

Midterm Exam: during lecture, TBA

Final Exam: TBA

*Note: If exam arrangement is updated or changed, please follow instructions from Brightspace announcement.*

## Resources

- **Access your course materials:** [Brightspace](https://brightspace.nyu.edu) (brightspace.nyu.edu)
- **Obtain 24/7 technology assistance:** [IT Help Desk](https://nyu.edu/it/servicedesk) (nyu.edu/it/servicedesk)
- **Academic Support.** The Academic Resource Center (ARC) provides free tutoring and support to students looking to reach their highest academic potential. Students can schedule a meeting, or drop by, for any of the following:
  - Individual and small-group tutoring with the class Learning Assistant (LA)
  - Individual writing consultations at any stage of the writing process
  - Academic coaching in areas such as time management, reading & note-taking strategies, exam preparation, and goal setting
  - Workshops on writing, academic skills, and technologies
  - Group study and conversation circles
- **Library and Research Services.** The Library is available to support your research needs. They have access to 14,000 print resources, 2,000 DVDs, and 1,000 databases (including over a million e-books, as well as streaming audio and video and image databases). Librarians with expertise in Business, Economics, Humanities, Science (STEM), and Social Sciences are available in-person and online to help. Services include:
  - One-to-one consultations to help you with your research projects

- Reference Desk hours for immediate help with finding and using resources
- Workshops throughout the semester on research strategies, special databases, academic integrity, and using citation tools.
- Visit the Library on the 4th floor, or go to [shanghai.nyu.edu/library](https://shanghai.nyu.edu/library) to learn more