Quantum Chemistry and Advanced Statistical Mechanics

Instructors

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Office hours: Wed 2:00 pm – 3:00pm during 1/25 – 3/24, Room 1262-1

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Course Description

This course is intended to provide a balanced presentation in both quantum chemistry and statistical mechanics. Quantum chemistry part includes representation theory, many-electron atoms and molecules, electronic structure methods. Statistical mechanics part includes equilibrium and nonequilibrium statistical mechanics, path integrals, dynamical and statistical methods. This course will have project components that could be developed as a research or thesis topic.

Course Learning Outcomes

This course is intended to provide a balanced presentation in both statistical mechanics and quantum chemistry with application toward chemistry problems. It is intended for graduate students who already have grasped the fundamental theories of quantum mechanics and basic statistical mechanics. The first half of the course covers advanced topics in statistical mechanics, specifically (1) quantum equilibrium statistical mechanics and path integrals, (2) classical time-dependent statistical mechanics, (3) quantum time-dependent statistical mechanics and quantum dynamics, (4) theory of ultrafast spectroscopy, and (5) enhanced sampling methods for generating free energy landscapes. In the second half of the course on quantum chemistry, the contents are organized to contain three main parts: (1) separation of electronic and nuclear wavefunctions, (2) electronic structure theory and (3) quantum theory for nuclear dynamics. The final score is made of 50% each on two parts of the course with independent final exam or project for each part. (4 units)

Course Requirements

Reference books

1. *Quantum Chemistry*, Ira N. Levine.
2. *Essentials of Computational Chemistry: Theories and Models*, Christopher Cramer.
3. *Theory and Application of Quantum Molecular Dynamics*, John Zhang
4. *Statistical Mechanics: Theory and Molecular Simulation*, Mark E. Tuckerman

5. *Chemical Dynamics in Condensed Phases, A. Nitzan*
6. *Principles of Nonlinear Optical Spectroscopy*, S. Mukamel
7. Literature references, as indicated throughout the course

Software

Gaussian, VASP, Amber, and ***i-PI*** packages will be accessible for computational needs in homework/computer practicums and projects.

Web access

NYU Classes (https://newclasses.nyu.edu) serves as the electronic portal for this course. Please check it regularly for announcements, discussions, projects guidelines, 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
Terminology	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
Scientific concepts	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
Application of chemical principles	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
Mathematical accuracy	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
Logic and reasoning	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
Connecting the dots	Connect new knowledge or skills with	Connect new knowledge or skills with	Connect new knowledge or skills with	Connect new knowledge or skills with	Unable to connect new knowledge or

Category	Excellent	Good	Average	Poor	Fail
	previous one in an effective and organized manner	previous one in a clear manner	previous one in an acceptable manner	previous one in a passive manner	skills with previous one
Communica-tion	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
Creativity	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 lecture 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 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 a 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 **four computer practicums** for learning the basic usage of quantum chemistry software ***Gaussian*** and ***VASP***, as well as molecular dynamics software ***Amber*** and ***i-PI***, respectively. The homework should be announced and submitted via **Assignments** section in NYU Classes electronically. Write your **name** and NYU **NetID** at the top of the homework report and combine your homework report in to 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 like the commands/code you use, rather than just the final answer. No late work will be accepted, and there will be no make-up or rescheduled homework.

Midterm and Final Projects

There will be two projects for quantum chemistry and statistical mechanics parts, respectively. The statistical mechanics project will be due on the first lecture of Week 8, whereas the quantum chemistry project will be due on Monday of the final exam week.

Combined PDF file of the project report should be submitted via **Assignments** section in NYU Classes electronically. Students should discuss the selection of topics with instructors and complete two project reports independently. Presentations could be arranged. Both midterm and final projects weight equally to the overall grade. 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 deadlines.

Grading

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

Assignments/Activities	% of Final Grade
Class Participation	15%
Homework	15%
Project Statistical Mechanics (Midterm)	35%
Project Quantum Chemistry (Final)	35%

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:

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

The grades will not be curved, but the instructors reserve the right to give **extra bonus of up to 10%** based on the overall performance during the entire course (see Rubrics).

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 by logging on to classes.nyu.edu.

***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 in 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 off 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) 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/Lecture	Topic	Due
	Statistical Mechanics Part by Prof. Xiang Sun	
W1, 1/25, Lec 1	Review of classical mechanics	
W1, 1/27, Lec 2	Equilibrium statistical mechanics	
W2, 2/1, Lec 3	Quantum dynamics in Hilbert space	
W2, 2/3, Lec 4	Density operator and quantum dynamics in Liouville space	
W3, 2/8, Lec 5	Quantum-classical correspondence and Wigner transform	Homework 1
W3, 2/10, Lec 6	Path integrals in quantum mechanics	

Week/Lecture	Topic	Due
W4, 2/22, Lec 7	Path integral based approximations: PIMD, PIMC, Centroid MD, ring-polymer MD	
W4, 2/24, Lec 8	Linear response theory and time correlation functions	
W5, 3/1, Lec 9	Quantum time correlation functions and applications to transport properties, rates	
W5, 3/3, Lec 10	Quantum master equation	Homework 2
W6, 3/8, Lec 11	Mixed quantum-classical dynamics	
W6, 3/10, Lec 12	Light-matter interaction and theory of linear spectroscopy	
W7, 3/15, Lec 13	Theory of nonlinear spectroscopy: Liouville pathways	
W7, 3/17, Lec 14	Enhanced sampling and rare events	
W8, 3/22, Lec 15	Midterm student presentation	Midterm project
	Quantum Chemistry Part by Prof. John Z.H. Zhang	
W8, 3/24, Lec 16	Separation of Electronic and Nuclear Motions	
W9, 3/29, Lec 17	Born-Oppenheimer Approximation	
W9, 3/31, Lec 18	Hellmann-Feynman Theory	
W10, 4/5, Lec 19	Diabatic Representation	
W10, 4/7, Lec 20	Transformation between Representations	
W11, 4/12, Lec 21	Crossing of Adiabatic Potentials	Homework 3
W11, 4/14, Lec 22	Hartree-Fock Theory	
W12, 4/19, Lec 23	Restricted Hartree-Fock (RHF)	
W12, 4/21, Lec 24	Unrestricted Hartree-Fock (UHF)	
W13, 4/25, Lec 25	Koopman's Theorem (**Legislative Day**)	
W13, 4/26, Lec 26	SCF Solution of HF Equation	Homework 4
W14, 4/28, Lec 27	Electron Correlation and Multiconfiguration	
W14, 5/5, Lec 28	Perturbation Methods	

Week/Lecture	Topic	Due
W15, 5/10, Lec 29	Density Functional Theory (DFT)	
W15, 5/12, Lec 30	Rovibrational motions of molecules	
W16, 5/17, Monday		Final project

Project Deadlines

Midterm Project: Statistical Mechanics due on the first lecture of week 8.
Final Project: Quantum Chemistry due on 12:00 PM, Monday of final exam week.

Resources

- **Access your course materials**: NYU Classes (nyu.edu/its/classes)
- **Obtain 24/7 technology assistance:** IT Help Desk (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 to learn more