PHYS-6120: Molecular Physics Fall 2024

Credit hours:	3
Prerequisites:	PHYS 6110 (Atomic Physics). Students who are interested in taking PHYS-6120, but have not taken PHYS-6110, should contact Dr. Le to discuss.
Instructor:	Dr. A.T. Le, GS-313G, E-mail: thu.le@uconn.edu
Class time & place:	3:30-4:45pm TuTh, GS-119
Office hours:	4:45-6:00pm Thursday or by appointment
Main textbook:	I.V. Hertel and C.P. Schulz, *Atoms, Molecules and Optical Physics 2: Molecules and Photons – Spectroscopy and Collisions,* Springer, 2015th edition

Additional textbooks:

1. W. Demtröder, *Atoms, Molecules and Photons: An Introduction to Atomic, Molecular- and Quantum Physics,* 1st (or 2nd) edition.
2. H. Haken and H.C. Wolf, *Molecular Physics and Elements of Quantum Chemistry*
3. B.H. Bransden, C.J. Joachain, *Physics of Atoms and Molecules* (1st or 2nd Edition).

The course will not always follow these books. Class attendance is important.

Course Objective: To achieve clear understanding of the basic concept of molecular structure, spectra, and atomic collisions. To get familiar with typical modern quantum chemistry software and be able to calculate, visualize, and understand the output for electronic and vibrational structure of molecules.

Description: Fundamental concepts and methods of quantum mechanics applied to molecular structures and spectra, atomic collisions, and interaction with lasers will be covered. Topics include Born-Oppenheimer approximation, Heitler-London and molecular orbital theories for diatomic and polyatomic molecules, Hartree-Fock equations, symmetry in molecules, rotational, vibrational and electronic spectra, potential scattering, atomic collisions, photoionization, ultracold molecules, time-resolved spectroscopy, intense laser-molecule interaction.

Grading:

Attendance & in-class participation:	25%
Problem sets:	25%
Midterm exam:	25%
Project & in-class presentation:	25%

Attendance: The course will not always follow the textbooks. Class attendance is important (250 points).

Homework: There will be five problem sets. Each problem set will be worth 50 points, so a total of 250 points may be earned. Late assignments will not be accepted. ***Guidelines for homework:***

- Discussions among the students are strongly encouraged.
- Try to always check your final answer to see if it makes sense.
- Students should document the intermediate steps so that partial credit can be given.
- Each student should write his/her own report. Report will not be accepted after the due date.
- Computational exercises are a part of this course. Computational software *Gamess* and visualization software *GabEdit* (or *Molekel*) will be used. These programs are free and can be downloaded and installed on student's personal computers.

Exam: There will be one mid-semester open-book exam (250 points).

Project & Presentation: The project will be worth 250 points. You will work on one project in the second half of the semester. You will be able to choose from several topics. Each project will involve either reviewing research papers, book chapters, or performing some computational/data analysis. You can also propose a project on the topic of your own interest (an approval by the instructor and possible adjustment will be needed). The project will require a written report and a presentation at the end of the semester. The grade will be based on the clarity of the discussion, the coverage of essential elements that will be determined by the student's choice of presentation topic, and the legibility and clarity of the PowerPoint file.

Make-up policy: There are no make-ups for homework assignments, exam, or project. Students who anticipate being away from a class for a legitimate reason, should inform the instructor *by e-mail* ahead of class and give the reason for absence.

Topics to be covered (tentative):

I. Introduction (2 lectures)

1. Brief review on atomic physics
2. Brief introduction to molecular physics

II. Molecular structures and spectra: Diatomic molecules (8-9 lectures)

1. Born-Oppenheimer approximation
2. Hydrogen molecular ion and molecular orbitals

3. H_2 molecule: molecular orbitals approximation, Heitler-London method; Valence bond (VB) theory; Molecular diagrams: bonding and anti-bonding
4. Electronic structure of diatomic molecules: Hartree-Fock & Density Functional Methods.
5. [*Computation/Practice*] Brief introduction to computational chemistry: *Gamess* & *Gaussian*
6. [*Computation/Practice*] Basis sets: Slater- & Gaussian-types orbitals, polarization and diffuse functions, effective core potentials
7. Vibration and rotation of diatomic molecules
8. Hund cases & Nuclear spin
9. Spectra of diatomic molecules
   a) Pure rotational transition
   b) Vibration-rotational transition
   c) Electronic transition and Franck-Condon principle
10. [*Computation/Practice*] Single energy calculation, geometry optimization, potential energy curves

III. Molecular structures and spectra: Polyatomic molecules (7-8 lectures)
1. Symmetry in molecules, Mulliken symbols, and character tables
2. Valence bond (VB) theory for polyatomic molecules
3. Molecular orbitals (MO) and Hartree-Fock, closed shell and open-shell
4. Rotation of polyatomic molecules
5. Vibration of polyatomic molecules and normal coordinates
6. Spectra of polyatomic molecules
7. [*Computation/Practice*] Single energy calculation, potential energy surface, intrinsic reaction coordinate

IV. Basic concepts of atomic collisions (5 lectures)
1. Collisions: introduction
2. Potential scattering, partial waves and phase shifts
3. Coulomb potential & modified Coulomb potential scattering
4. Integral equation for scattering
5. Born approximation
6. Electron-atom collisions
7. Resonance in scattering and photoionization
8. Atom-atom collisions
9. Inelastic collisions

V. Modern topics (4-5 lectures)
1. Laser spectroscopy
2. Time-resolved spectroscopy and coherent control
3. Formation of ultracold molecules and molecular quantum gases
4. Multiphoton processes and tunneling ionization
5. High harmonic generation and attosecond physics