

CHEM 532

Physical Chemistry II (Quantum Chemistry), 3 credit hours

Fall 2022

Catalog description:

Introduction to quantum mechanics; postulates of quantum mechanics; exact solutions and approximation methods. Recommended preparation: CHEM 332 or equivalent.

MWF 12:10-13:00 in Fulmer 124 (note the room change)

Instructor: Kirk Peterson (<https://chem.wsu.edu/faculty/peterson-kirk/>)

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Office Hours: by appointment

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Recommended Textbooks

Molecular Quantum Mechanics, 5th ed., by P.W. Atkins and R.S. Friedman (Oxford Univ. Press).

Quantum Chemistry, 3rd ed., by J.P. Lowe and K.A. Peterson (Elsevier)

Introduction to Quantum Mechanics in Chemistry, by G.C. Schatz and M.A. Ratner (Prentice Hall).

Evaluation

Homework (approx. weekly):	20% of grade (check website for assignments)
Hour exams (2)	60% of grade (check website for dates)
Final exam	20% of grade

Lecture Topics

I. Basic tools of quantum mechanics

Properties of operators, Dirac bra-ket notation, adjoint and Hermitian operators, eigenfunctions/eigenvalues, matrix formulations, the Uncertainty Principle, time evolution of observables

II. Postulates of quantum mechanics

The Born Interpretation, position and momentum representations, the time dependent and time independent Schrödinger Eqns., expectation values

III. Fundamentals: Exact solutions of the Schrödinger Eqn.

- a) free translation
- b) particle in a box
- c) harmonic oscillator
- d) particle on a ring of fixed radius
- e) particle on a sphere of fixed radius
- f) the hydrogen atom
- g) the H_2^+ molecular ion

IV. Things get difficult: Systems with 2 or more electrons

- a) The helium atom
 - 1) Introduction to spin
 - 2) indistinguishable particles, the Pauli Principle, Slater determinants
- b) Approximation methods
 - 1) variation method
 - b) perturbation theory

V. Many-electron atoms

- a) spin eigenfunctions for many electron wave functions, specifying states of the system: term symbols

X. Many-electron molecules

Hückel theory, the LCAO method, Gaussian basis sets, self-consistent field and density functional theories

State, Federal, and/or WSU Policy-related required statements

(taken from <https://syllabus.wsu.edu/required-syllabus-elements/>)

1. Reasonable Accommodation

Reasonable accommodations are available for students with documented disabilities or chronic medical or psychological conditions. If you have such a condition and need accommodations to fully participate in this class, please visit your campus' Access

Center/Services website to follow published procedures to request accommodations. Students may also contact their campus offices to schedule an appointment with a Access Advisor. All disability related accommodations are to be approved through the Access Center/Services on your campus. It is a university expectation that students connect with instructors (via email, Zoom, or in person) to discuss logistics within two weeks after they have officially requested their accommodations.

For more information, contact an Access Advisor on your home campus:

- Pullman, WSU Global Campus, Everett, Bremerton, and Puyallup: 509-335- 3417 [Access Center \(https://www.accesscenter.wsu.edu\)](https://www.accesscenter.wsu.edu) or email at access.center@wsu.edu

2. Academic Integrity Policy

Washington State University, a community dedicated to the advancement of knowledge, expects all students to adhere to high expectations of scholarship and the Standards of Conduct for Students. Potential violations of the Standards of Conduct for Students should be referred to the Center for Community Standards. The Center for Community Standards supports students, upholds their rights and responsibilities, and holds them accountable for behavior that doesn't meet our community expectations.

University instructors have the authority, and are expected to intervene, in all situations where students may have violated [academic integrity expectations](#). Where an instructor believes it is more likely than not that a student violated expectations, they have the authority to assign an academic consequence consistent with the academic integrity statement found in their course syllabus. The instructor is required to [report the violation to the Center for Community Standards](#) to provide an appropriate and fundamentally fair process for the student. More information regarding responding to academic integrity violations can be found at: <https://www.handbook.wsu.edu/academic-integrity-process/>.

Feel free to contact the Center for Community Standards if you would like more specific information about the process. The Center for Community Standards can be reached at 509-335-4532 or community.standards@wsu.edu.

The Writing Program (509-335-7959) can assist with proactive assignment design that minimizes the risk of academic dishonesty.

3. Policy Prohibiting Discrimination and Harassment (Executive Policy 15) This policy expresses WSU's commitment to maintaining an environment free from discrimination, including sexual harassment. This policy applies to all students, faculty, staff, or others having an association with the University.

Discrimination, including discriminatory harassment, sexual harassment, and sexual misconduct (including stalking, intimate partner violence, and sexual violence) is prohibited at WSU (See WSU Policy Prohibiting Discrimination and Harassment (Executive Policy 15) and WSU Standards of Conduct for Students).

If you feel you have experienced or have witnessed discriminatory conduct, you can contact the WSU Office of Compliance and Civil Rights (CCR) and/or the WSU Title IX Coordinator at 509-335-8288 to discuss resources, including confidential resources, and reporting options. (Visit <https://ccr.wsu.edu/> for more information).

Most WSU employees, including faculty, who have information regarding sexual harassment or sexual misconduct are required to report the information to CCR or a designated Title IX Coordinator or Liaison. Visit <https://ccr.wsu.edu/file-a-complaint/> for more information.

4. Class Attendance and Absences (Academic Regulation 72)

Class attendance is not mandatory for this class, although it is strongly encouraged.

- **University Sponsored.** Any student who is required to participate in off-campus, university-sponsored activities such as field trips, musical performances, judging teams, intercollegiate athletic events, etc., should obtain an official Class Absence Request form from the faculty or staff member supervising the on- or off-campus activity. The form must contain specific information concerning the activity and date, be signed by the supervising faculty or staff member, and be submitted by the student at least one week in advance to the individual instructors of the student's classes. Alternative forms of the Class Absence Request may also be provided by the supervising faculty or staff member and are acceptable for requesting university-sponsored absences. It is recommended, but not required, that a student not be penalized for absence from class provided a properly signed form has been filed with the instructor prior to the absence. These university-sponsored absences are subject to an instructor's attendance policy and are not intended to imply additional acceptable absences. In all instances, it is the student's responsibility to make up all work missed.
- **Military Service Members.** Students who are members of the National Guard or a reserve branch of a military service are occasionally required to miss class for weekend drills, active duty, and related responsibilities and are entitled to make up the class (RCW 28B.10.270). In such a case, instructors must not penalize students for the absences and must allow them to make-up the missed work. In each instance, it is the responsibility of the student to inform the instructor of the duty before the absence, provide appropriate documentation if requested, and complete the missed work as soon as reasonably possible.
- **Flexible Attendance as an Access Accommodation.** Some students have disabilities or chronic medical conditions of an episodic nature that may require flexibility regarding attendance. The Access Center recognizes that in some cases, allowing absences beyond those normally allowed in a course is a reasonable accommodation. However, there are courses in which a specified standard of attendance may be an essential part of the course. When the Access Center determines that flexible attendance may be a reasonable accommodation, instructors will receive notification of approved accommodations and procedures for their consideration. Final determinations regarding flexible attendance will be determined on a case-by-case basis. See the Flexible Attendance Guidelines at the Access Center website and Rule 83. NOTE: The Access Center does not provide accommodations for acute illnesses such as the common cold or flu. In these cases, students are to work with their instructors as indicated under c.6. Other Absences.

- Reasonable Religious Accommodation. Washington State University reasonably accommodates absences allowing for students to take holidays for reasons of faith or conscience or organized activities conducted under the auspices of a religious denomination, church, or religious organization. Reasonable accommodation requires the student to coordinate with the instructor on scheduling examinations or other activities necessary for course completion. Students requesting accommodation must provide written notification within the first two weeks of the beginning of the course and include specific dates for absences. Approved accommodations for absences will not adversely impact student grades. Absence from classes or examinations for religious reasons does not relieve students from responsibility for any part of the course work required during the period of absence. Students who feel they have been treated unfairly in terms of this accommodation may refer to Academic Regulation 104 - Academic Complaint Procedures. See also Rule 82, available at <https://registrar.wsu.edu/academic-regulations/>
- Any student seeking reasonable accommodations under this section must provide written notice to the instructor, within the first two weeks of the beginning of the course and include the specific dates for absences. Absence from classes or examinations for religious reasons does not relieve students from responsibility for any part of the course work required during the period of absence.
- The instructor shall inform the student of the decision in writing within seven calendar days of the receipt of the request.
- Approved accommodations for absences will not adversely impact student grades.
- The university provides notice to students of this policy on the university's web site and in course or program syllabi, including grievance procedures.

Any student who believes that she or he has not been appropriately accommodated under this policy may seek review of the decision by sending a written request to the chairperson of the department offering the course, as soon as possible and no later than seven days after learning of the instructor's decision. After the chair's decision, the student or the instructor may appeal to the dean's office. Appeals to the dean's office must be presented in writing within seven calendar days of the chair's decision. The decision of the dean or associate dean shall be made within seven calendar days and is final. The University Ombudsman is available at any stage for advice or assistance in resolving requests for accommodation. Students should understand that fairness in the examination process is an important consideration in the educational process and that they do have a duty to cooperate in making alternate arrangements.

- Adverse Weather Conditions. When appropriate campus authorities declare a "Yellow / Delayed or Limited Operations" or "Red / Closed" campus condition (BPPM 50.40 - 46), or travel to instructional locations is unsafe, classes may be cancelled or delayed. When a student does not attend due to adverse conditions, the instructor will not penalize the student. See the Inclement Weather Policy online at each campus website and at the Office of the Provost website.
- Other Absences. Students must sometimes miss class meetings, examinations, or other academic obligations affecting their grades due to extenuating circumstances. It is the responsibility of the student to provide a written explanation for the absence to the instructor as soon as it is reasonable to do so. When possible,

students should provide appropriate documentation for their absence but instructors cannot require written excuses from health care professionals.

- **Emergency Notifications**

While the Office of the Dean of Students does not excuse or verify student absences, in the event a student is going to be away from class for an extended period and is unable to contact the instructor in a timely manner, the Office of the Dean of Students may provide an emergency notification on the student's behalf to the instructors, informing them of the student's absence and the planned duration of the absence. An emergency notification should not be required or used to excuse a student's absence.

It is the responsibility of the student to make contact with their instructors as soon as possible to make arrangements for missed work. It is up to the instructor to determine what if any arrangements will be made for the student based upon the attendance policy as stated in syllabus.

- **Request for Consideration**

The Office of the Dean of Students and/or the Office of Civil Rights Compliance and Investigation may contact instructors on a student's behalf when the student's involvement in a matter implicating the WSU Policy Prohibiting Discrimination, Sexual Harassment, and Sexual Misconduct, Executive Policy #15 is having a significant impact on the student's academic progress.

In such cases, the instructor is strongly encouraged to work with the student to address the student's needs without compromising learning objectives. It is the responsibility of the student to contact the instructor to make these arrangements.

- **Complaints**

Students who wish to raise a concern about the instructor's arrangement regarding missed work may follow the Academic Complaint Procedure, Rule 104. (note: please first talk to the instructor)

5. Lauren's Promise – I will listen and believe you if someone is threatening you.

Lauren McCluskey, a 21-year-old honors student athlete, was murdered on October 22, 2018 on the University of Utah campus by a man she briefly dated. We must all take actions to ensure that this never happens again.

University Support and Response for Discrimination and Harassment

Discrimination, discriminatory harassment, sexual harassment, and sexual misconduct (including stalking, intimate partner violence, and sexual violence) are prohibited at WSU (see Executive Policy 15 - [WSU Policy Prohibiting Discrimination and Harassment](#), the [WSU Standards of Conduct for Students](#), and relevant employee manuals). WSU has instituted procedures to respond to violations of these laws and standards, programs aimed at the prevention of such conduct, and intervention on behalf of victims.

If you are in immediate danger, call 911.

If you are experiencing sexual assault, domestic violence, stalking, discrimination or harassment, **you have support and options**. If you share information with me, please know that I am required to reach out to the Title IX Coordinator in WSU Compliance and Civil Rights (CCR), and CCR will reach out to you with information about on and off campus reporting options and resources. CCR is a system-wide resource (all campuses) which is available for intake consultations for you to learn more about available support. You can reach them directly at 509-335-8288, ccr@wsu.edu, or [report online](#) (anonymous reports accepted).

You can also speak to a victim advocate, a medical provider, or counselor confidentially about your concerns. Advocates help survivors of crime determine their own needs in regards to their physical and emotional health, reporting options, and academic concerns. At no cost, advocates connect survivors to campus and community services, and provide accompaniment to important appointments (court, hospital, and police) and support throughout the process. For a list of confidential victim advocates and medical providers, please visit [CCR Resources](#).

WSU Police Department (WSU PD) officers and campus security will treat victims of sexual assault, domestic violence, stalking, hate crimes, and other crimes with respect and dignity. WSU PD, campus security departments, CCR, and victim advocates can also help you with safety planning.

6. Safety and Emergency Notification

Please sign up for emergency alerts on your account at MyWSU. For more information on this subject, campus safety, and related topics, please view the FBI's Run, Hide, Fight video and visit the classroom safety page <https://provost.wsu.edu/classroom-safety/>.