COURSE INFORMATION

Introductory Quantum Chemistry
CHEM 675 001 (3.0 Credits)
Fall 2018-2019 [1192]

Description
Basic principles of quantum chemistry, exactly solvable problems, angular momentum, approximation methods, applications to electronic structure. Enroll Info: Chem 562 or consent of instructor

Prerequisite(s)
CHEM 562 or graduate standing

Instruction Mode
Classroom Instruction

Department: CHEMISTRY
College: Letters and Science

Canvas Course URL
https://canvas.wisc.edu/

2018-2019 Fall [1192]
Term Start Date: Wednesday, 5-Sep-2018 Term End Date: Wednesday, 2-Jan-2019

Location and Schedule: Chemistry Building 8335 MWF 9:55 AM-10:45 AM
CRN: 224002847

How the Credit Hours are Met
This class meets for three 50-minute class periods each week over the semester and carries the expectation that students will work on course learning activities (reading, writing, problem sets, studying, etc) for about 2 hours out of classroom for every class period. The syllabus includes additional information about meeting times and expectations for student work.

INSTRUCTORS AND TEACHING ASSISTANTS

Instructor

EDWIN SIBERT
SIBERT@CHEM.WISC.EDU

Instructor Availability
Room: 8305c
Time: Mon. 1:30-2:30, Fri. 2:30-3:30

GRADING AND COURSE MATERIALS

Course Learning Outcomes (CLOs)
Apply the laws of quantum mechanics to solve a range of problems of chemical interest
[S5977]

Describe the energy levels of atomic systems using extensions of the quantum mechanical solutions to the hydrogen atom.
[S5978]

Solve a variety of problems using the method of separation of variables especially the hydrogen atom.
[S5979]

Justify the approximations that are made in order to obtain the quantum mechanical solutions for the electronic, vibrational, and rotational degrees of freedom of a diatomic molecule.
[S5980]

Apply the concept of basis set expansions to solve for eigenvalues and eigenfunctions using basis sets.
[S5981]

Apply perturbation theory appropriately to describe energy levels and wave functions of atomic and molecular systems.
[S5982]

Predict the time evolution of observables, given solutions to the time independent Hamiltonian.
[S5983]

Explain how one constructs both the time independent and time dependent Hamiltonian given the number of particles and the potential describing them.
[S5984]

Explain with equations how and why transitions take place in atoms and molecules.
[S5985]

Explain how normal modes are obtained and why they allow for a solutions of the molecular vibrations of polyatomic molecules.
[S5986]

Understand angular momentum and the commutation properties of angular momentum operators.
[S5987]

Grading

Your final course grade will be based on a 100 points scale. The total points are distributed as follows midterms (17 points each), problems sets (33 points), and final exam (33 points). If you receive 60 total points you will receive a B or better in this class. If obtain more than 75 total points you will receive an A. Your attendance in class is critical for success in this course, but is not part of your grade.

Required Textbook, Software, & Other Course Materials

The textbook for this course is the fifth edition of `Quantum Chemistry` by Ira N. Levine. You can get used copies on Amazon at a reasonable price. You can probably find copies around the chemistry building if you are resourceful.

EXAMS, QUizzes, PAPERS & OTHER MAJOR GRADED WORK

Exams, Quizzes, Papers & Other Major Graded Work

There are two in-class exams and a final. All exams are cumulative and are closed-book. The in-class exams are Wednesday on 10/17 and 11/14.

Homework & Other Assignments

There will be 11 homework assignments. These assignment can be viewed by clicking on the "assignment" tab to the left. Homework is the most important component of the class from a pedagogical point of view. Assignments will be posted on Wednesdays and are due on the following Wednesday during class period. You may discuss the homework with other students in the class, but you must turn in a single assignment for your group. Problems sets are not accepted after class time on the day that they are due, so that I can discuss the solutions that day. Some problems require the use of computer software. You may use the software of your choice. One of the choices is Excel.

OTHER COURSE INFORMATION

Other Course Information
Topics to be covered

1. Foundations of Quantum Mechanics and Particle in a Box (2 lectures) [Chapter 1-2]
2. Time Dependent Quantum Mechanics (1 lecture) [Chapter 2]
3. Piecewise Constant Potentials and Tunneling (2 lecture) [Chapter 2]
4. Operators, observables and a particle in a three-dimensional box (2 lectures) [Chapter 3]
5. The Harmonic Oscillator (3 lectures) [Chapter 4]
6. Central Force Problems and Angular Momentum (2 lectures) [Chapter 5]
7. Angular Momentum Operators (1 lecture) [Chapter 5]
8. Separation of Variables, center of mass variables, and the Hydrogen Atom (3 lectures) [Chapter 6]
9. More on the Foundations of Quantum Mechanics (2 lectures) [Chapter 7]
10. The Variational Principle (3 lectures) [Chapter 8]
11. He Atom and the Variational Principle (1 lecture) [Chapter 9]
12. He Atom and Time Independent Perturbation Theory (2 lectures) [Chapter 9]
13. Spin, the Pauli Principle, and Hartree-Fock Theory (3 lectures) [Chapter 10-11]
14. Molecular Structure and the Born-Oppenheimer Approx. (4 lectures) [Chapter 13]
15. Molecular Rotations and Vibrations of Diatomic Molecules (3 lectures) [Chapter 13]
16. Molecular Rotations and Vibrations of Polyatomic Molecules (3 lectures)
17. Time Dependent Perturbation Theory (2 lectures) [Chapter 9]
18. Molecular Electronic Transitions (2 lectures)

ACADEMIC POLICIES

ACADEMIC INTEGRITY

By enrolling in this course, each student assumes the responsibilities of an active participant in UW-Madison’s community of scholars in which everyone’s academic work and behavior are held to the highest academic integrity standards. Academic misconduct compromises the integrity of the university. Cheating, fabrication, plagiarism, unauthorized collaboration, and helping others commit these acts are examples of academic misconduct, which can result in disciplinary action. This includes but is not limited to failure on the assignment/course, disciplinary probation, or suspension. Substantial or repeated cases of misconduct will be forwarded to the Office of Student Conduct & Community Standards for additional review. For more information, refer to https://conduct.students.wisc.edu/academic-integrity/

ACCOMMODATIONS FOR STUDENTS WITH DISABILITIES

McBurney Disability Resource Center syllabus statement: “The University of Wisconsin-Madison supports the right of all enrolled students to a full and equal educational opportunity. The Americans with Disabilities Act (ADA), Wisconsin State Statute (36.12), and UW-Madison policy (Faculty Document 1071) require that students with disabilities be reasonably accommodated in instruction and campus life. Reasonable accommodations for students with disabilities is a shared faculty and student responsibility. Students are expected to inform faculty [me] of their need for instructional accommodations by the end of the third week of the semester, or as soon as possible after a disability has been incurred or recognized. Faculty [I], will work either directly with the student [you] or in coordination with the McBurney Center to identify and provide reasonable instructional accommodations. Disability information, including instructional accommodations as part of a student's educational record, is confidential and protected under FERPA.” http://mcburney.wisc.edu/facstaffother/faculty/syllabus.php

DIVERSITY & INCLUSION

Institutional statement on diversity: “Diversity is a source of strength, creativity, and innovation for UW-Madison. We value the contributions of each person and respect the profound ways their identity, culture, background, experience, status, abilities, and opinion enrich the university community. We commit ourselves to the pursuit of excellence in teaching, research, outreach, and diversity as inextricably linked goals.

The University of Wisconsin-Madison fulfills its public mission by creating a welcoming and inclusive community for people from every background – people who as students, faculty, and staff serve Wisconsin and the world.” https://diversity.wisc.edu/
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Room: 8305c
Instructor

Topics to be covered

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- Central Force Problems and Angular Momentum (2 lectures) [Chapter 5]
- Separation of Variables, center of mass variables, and the Hydrogen Atom (3 lectures) [Chapter 6]
- Piecewise Constant Potentials and Tunneling (2 lecture) [Chapter 2]
- He Atom and Time Independent Perturbation Theory (2 lectures) [Chapter 9]
- Molecular Rotations and Vibrations of Diatomic Molecules (3 lectures) [Chapter 13]
- Molecular Structure and the Born-Oppenheimer Approx. (4 lectures) [Chapter 13]
- Time Dependent Quantum Mechanics (1 lecture) [Chapter 2]
- Time Dependent Perturbation Theory (2 lectures) [Chapter 9]
- Molecular Electronic Transitions (2 lectures)

How the Credit Hours are Met

- 100 points are available
- Homework, Labs - 50 points
- 2 midterms - 50 points
- 1 final exam - 100 points

Grading:

- If you receive 45 total points you will receive a C or better in this class. If you obtain more than 60 total points you will receive an A or better in this class. If you obtain more than 75 total points you will receive an A or better in this class.

Course learning outcomes (CLOs)

1. Solve a variety of problems using the method of separation of variables especially the hydrogen atom.
2. Describe the energy levels of atomic systems using extensions of the quantum mechanical solutions to the hydrogen atom.
3. Justify the approximations that are made in order to obtain the quantum mechanical solutions for the electronic, vibrational, and rotational properties of atoms.
4. Apply the laws of quantum mechanics to solve a range of problems of chemical interest.
5. Explain how one constructs both the time independent and time dependent Hamiltonian given the number of particles and the potential.
6. Predict the time evolution of observables, given solutions to the time independent Hamiltonian.

Instructor Availability

This class meets for three 50-minute class periods each week over the semester and carries the expectation that students will work on course learning outcomes outside of class.

Instructor:

Access:

https://canvas.wisc.edu/

College: Chemistry
Department: Chemistry
Prerequisite(s):

Info: Chem 562 or consent of instructor

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Diversity & Inclusion

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Reasonable accommodations for students with disabilities is a shared faculty and student responsibility. Students are expected to inform the instructor of any accommodations needed.

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