Student Course Information
Quantum Chemistry
CHEM*3860
Fall 2015

Course Calendar Description: F. (3-1) [0.50 credit] This course provides an introduction to quantum chemistry and how it applies to the understanding of the electronic structure of atoms and molecules, as well as the geometric structure of molecules. The theoretical background needed to understand molecular spectroscopy is also provided. An integral part of this course is the use of commercial software for the computation of molecular properties. Prerequisite: CHEM*2070, (MATH*2170 OR MATH*2270)

Course Instructor: Prof. Dan THOMAS SCIE 2504 x53961 dfthomas@uoguelph.ca

Lectures: M, W, F, 10:30 – 11:20 MacKinnon 234. No class Monday, October 12 for Thanksgiving.

Tutorial: Friday 3:30 – 4:20 SSC 1303 (Tutorial material is examinable!)

Text: I.R. Levine *Quantum Chemistry* 7th Edition. In bookstore, but copies also on reserve.

Course Content:

Schrödinger Equation, wavefunctions, probability
Particle in a Box, Tunneling, Degeneracy
Operators, Eigenfunctions, Eigenvalues (light)
Harmonic Oscillator
Particle on a Ring, Sphere, Angular Momentum
Hydrogen Atom
Operators, Eigenfunctions, Eigenvalues (deeper)
Variation Method, Perturbation Theory
Many-Electron Atoms
Small Molecules
Molecular Orbital Calculations (Gaussian Software)

Evaluation:

Assignments (4 at 10% each) 40%
Mid-Term Exam Friday, October 30 in class (10:30 – 11:20) 25%
Final Exam Friday, December 11 (11:30 – 1:30) Location TBA 35%

And Now The Fine Print:

E-mail Communication

As per university regulations, all students are required to check their e-mail account regularly: email is the official route of communication between the University and its students.

When You Cannot Meet a Course Requirement

When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons, please advise the course instructor in writing, with your name, id#, and e-mail contact. See the undergraduate calendar for information on regulations and procedures for
Academic Consideration:
http://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-ac.shtml

Drop Date

The last date to drop one-semester courses, without academic penalty, is **Friday, October 31st, 2014**. For regulations and procedures for Dropping Courses, see the Undergraduate Calendar:
http://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-drop.shtml

Copies of out-of-class assignments

Keep paper and/or other reliable back-up copies of all out-of-class assignments: you may be asked to resubmit work at any time.

Accessibility

The University of Guelph is committed to creating a barrier-free environment. Providing services for students is a shared responsibility among students, faculty and administrators. This relationship is based on respect of individual rights, the dignity of the individual and the University community's shared commitment to an open and supportive learning environment.
Students requiring service or accommodation, whether due to an identified, ongoing disability or a short-term disability should contact the Centre for Students with Disabilities as soon as possible.
For more information, contact CSD at 519-824-4120 ext. 56208 or email csd@uoguelph.ca or see the website: http://www.csd.uoguelph.ca/csd/

Academic Misconduct

The University of Guelph is committed to upholding the highest standards of academic integrity and it is the responsibility of all members of the University community – faculty, staff, and students – to be aware of what constitutes academic misconduct and to do as much as possible to prevent academic offences from occurring. University of Guelph students have the responsibility of abiding by the University's policy on academic misconduct regardless of their location of study; faculty, staff and students have the responsibility of supporting an environment that discourages misconduct. Students need to remain aware that instructors have access to and the right to use electronic and other means of detection.
Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from responsibility for verifying the academic integrity of their work before submitting it.
Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor.
The Academic Misconduct Policy is detailed in the Undergraduate Calendar:
http://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-amisconduct.shtml

Recording of Materials

Presentations which are made in relation to course work—including lectures—cannot be recorded or copied without the permission of the presenter, whether the instructor, a classmate or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.

Resources

The Academic Calendars are the source of information about the University of Guelph's procedures, policies and regulations which apply to undergraduate, graduate and diploma programs:
http://www.uoguelph.ca/registrar/calendars/index.cfm?index

What can Quantum Chemistry tell us?

1. Explain spectroscopy
   CHEM*2070, CHEM*3870. Every type of spectroscopy requires quantum chemical calculations to explain the results.
2. Explain atomic trends
   CHEM*2060, CHEM*3640, CHEM*3650
3. Explain molecular nuclear and electronic structure
   CHEM*2060, CHEM*2070, inorganic, organic, etc.
4. Can investigate such things as
   - Molecular properties such as structure, bond strengths, vibrational frequencies, electronic distributions, dipole moments, polarizability, NMR chemical shifts, NMR J-couplings, excited states (photochemistry), internal rotation and inversion, intermolecular interactions such as hydrogen bonding and van der Waals complex formation.
   - Chemical Reactions: mechanisms, pathways, etc.
   - Solvent effects on molecular properties and reactions.
   - Thermodynamic properties such as ΔH, ΔG, and so forth.

Course Learning Objectives

1) Upon successful completion of this course, students should be able to:
2) Explain the differences between classical and quantum descriptions of matter.
3) Follow the process to solve the relevant differential equations and explain the meaning of the various solutions.
4) Demonstrate an ability to solve eigenvalue equations and explain the solutions in terms of atomic and molecular properties.
5) Demonstrate an understanding of model systems and show how they can inform our view of relevant molecular systems.
6) Solve quantum problems involving variational and perturbation methods and explain how the solutions are relevant to physical systems.
7) Become proficient in using the Gaussian 09 software package and use it explain the properties of molecular systems
8) Demonstrate proficiency in describing molecular systems in various representations: words, equations, drawings, and animations.