CSI 783 *Computational Quantum Mechanics*
Crosslisted: **CHEM 736/PHYS 736**
Spring 2022

Classroom: Synchronous meetings on Zoom
Class time: Wednesdays, 4:30 pm - 7:10 pm
Class notes: distributed during the Zoom class time

Instructor Name: Estela Blaisten
Office location: Research Hall 221, Fairfax campus
Office hours: By appointment, will be through Zoom
Email address: blaisten@gmu.edu (preferred way of communication)

- ***This class is synchronous, online.*** *Activities and assignments in this course will regularly use web-conferencing software (Zoom). All students are required to have a laptop/desktop with a functional camera and microphone. In an emergency, students can connect through a telephone call, but video connection is the expected norm.*

- *Professor Blaisten does not authorize in anyway the recording of any lecture content in this course. Sharing of video lecture or lab content violates student privacy governed by the Family Education Rights and Privacy Act (FERPA). Additionally, any written, video, or audio content built by Prof. Blaisten for CSI 783/CHEM 736/PHYS 736 instruction that is shared online externally to GMU is a clear and punishable violation of GMU's Honor Code.*

- *All students taking courses with a face-to-face component are required to follow the university's public health and safety precautions and procedures outlined on the university Safe Return to Campus webpage (https://www2.gmu.edu/safe-return-campus). Similarly**, all students in face-to-face and hybrid courses must also complete the Mason COVID Health** every day they will be on campus. The COVID Health Check system uses a color code system and students will receive either a Green, Yellow, or Red email response. Only students who receive a "green" notification are permitted to attend courses with a face-to-face component. If you suspect that you are sick or have been directed to self-isolate, please quarantine or get testing. Faculty are allowed to ask you to show them that you have received a Green email and are thereby permitted to be in class.*

- *Students are required to follow Mason's current policy about facemask-wearing. As of August 11, 2021, **all community members are required to wear a facemask in all indoor settings, including classrooms**. An appropriate facemask must cover your nose and mouth at all times in our classroom. If this policy changes, you will be informed; however, students who prefer to wear masks consistently will always be welcome in the classroom.*

- *If the **campus closes**, or if a **class meeting needs to be canceled** or adjusted due to weather or other concern, **students should check the course website and their email for updates** on how to continue learning and for information about any changes to events or assignments. For university designated **snow days** the class adheres to the Mason instructions: (i) in-person classes are cancelled; (ii) hybrid classes are cancelled; (iii) uniquely online classes are not cancelled.*

- *If Professor Blaisten needs to quarantine, any in-person meeting will reverse to be online for the remaining of the semester.*

Course Description and Goals

- This is an introductory course for graduate students that includes computational techniques largely used by the quantum research community with emphasis on **molecular systems and quantum chemistry**. Each student will be responsible to cover the material in the textbook that supplements the class notes, develop a certain number of short computational projects leading to a final individual project. All projects will be using the package Gaussian09 installed in the lab workstations.

  There will not be midterm and/or final exams.

- Lectures will tend to be short for supplementing any assigned presentation from the textbook by students.

- By the end of this course, students will be able to
  1. Know how the quantum world works, be familiar with quantum mechanics terminology, solve simple problems.
  2. Appraise theoretical foundations of methods that can only be run in the computer.
  3. Learn to use a Quantum Chemistry software package which is extremely strong and recognized in the physical chemistry and physics based communities, worldwide.
  4. Perform elementary quantum mechanics atomistic simulations using the software.

Prerequisites: Calculus, introductory physics or physical chemistry, knowledge of a programming language (at the level of CSI 501 or better) and know or be able to learn on your own a few commands in linux.

Required textbook

- ***Quantum Chemistry*** by J. Lowe and K. Peterson, Academic Press 2005 (3rd edition).

A supplementary or alternative textbook is:

- *Quantum Chemistry* by Ira Levine, Prentice Hall 1998 (5^{th} - 7^{th} edition).

Extra references:

Introductory Quantum Chemistry by Frank Pilar, Mc Graw-Hill
Quantum Mechanics by L. Schiff, Mc Graw-Hill Co
Introduction to the Structure of Matter by J. J. Berehm, J. Wiley
Atoms and Molecules by Karplus and Porter, Benjamin

Online useful tutorials:

Introduction to quantum Chemistry using G09 software:

Gausian 09 keywords

Exploring Chemistry with electronic Structure Methods by J.B. Foreman and AE. Frisch

Evaluation

Grading scale (points): A (90-100), B (80-89), C (≤79) (with eventual slight variations)

Grading policy (may change slightly):

1) Homework (34%). Each of 8-10 homework will be graded between 1 and 10. Ten is the best. Present homework in a report-like fashion.
2) Individual project: project description (33%).
3) Class participation and attendance, including presentations by students on the material related to the textbook or class notes, on their advances in the individual project, or additional explanations on homework assignments. Additionally, participation includes a final presentation of the individual project to take place on the date of final exam that Registrar assigns to this course (33%).

Late assignments: Late assignments will not be accepted unless due to emergency or work-related compelling reasons for part-time students.

"Re-do" homework policy:

1) Homework graded and returned to you can be revised for a better grade with a penalty on its final grade of minus 1 point.
2) Redo homework should be turned in with the original handout containing the corrections.

Other considerations: If there are any obligations related to religious holidays, please inform the instructor the first week of class

Course schedule for Spring 2022 with tentative content

- 1. *Review of waves and the time independent Schroedinger wave equation*
- 2. *Quantum mechanics of simple systems* The particle in a box with infinite and finite wells in one dimension and generalization to 3D. Particle in a ring of constant potential
- 3. *The one-dimensional harmonic oscillator* Solution of the Schroedinger equation, Quantum mechanical average values. The model of vibrations in diatomic molecules
- 4. *The hydrogen-like ion, angular momentum* The Schroedinger equation for central-field problem. Separation of the central-field Schroedinger equation. Solution of the equation in R, Θ, an Φ coordinates. Angular momentum and spherical harmonics in real form. Solution of the radial equation for the Coulomb potential. The Laguerre polynomials. The wave functions of the one-electron atom. Orbital probability distributions functions.
- 5. *Introduction to the many-electron atom- approximate solutions to Schroedinger equation* The non-relativistic atomic Hamiltonian operator. Atomic units. The independent-particle model. The effect of electron repulsions on atomic energies. The mass-polarization effect. Scaling and the virial theorem. Self consistent field. Slater orbitals. Indistinguishability of identical particles: fermions and bosons. The antisymmetry principle. Spin angular momentum and their operators.
- 6. *Postulates and theorems of quantum mechanics.*

- 7. *The variation* method Linear and non-linear variation, hydrogen atom, helium atom. Linear combination of atomic orbitals (LCAO). Molecular orbitals. Basis sets. Numerical examples

- 8. *Matrix formulation of the linear variation method.* Review of matrices and vectors. Solving matrix equations. (this subject might be skipped depending upon the class composition).

- 9. *The SCF MO-LCAO method* The molecular Hamiltonian. The SCF total electronic energy. The Hartree-Fock limit. Correlation energy. Koopman's theorem. Configuration Interaction.

- 10. *Time independent perturbation theory* Perturbation method of Rayleigh- Shroedinger for non-degenerate and degenerate states. Selection rules in spectroscopy. Numerical examples.

- 11-12. *Topics on molecular structure.* The Born-Oppenheimer approximation. Solution of the nuclear equation. Selection rules for the molecular electronic transitions. Molecular HF calculations. Electronic transitions in molecules. The MO-LCAO approximation. The hydrogen molecule. Heteronuclear diatomic molecules. Linear polyatomic molecules. Molecular CI. The valence Bond method. Molecular perturbation calculations. Molecular symmetry. Elements of point groups: irreducible and reducible representations, direct-product, symmetry projection-operators. Point symmetry and molecular spectra. Numerical examples of SCF calculations using Gaussian.

- 13. Projects pre-presentations

Final exam day: Project presentations. Each student does a final presentation of his/her project. This meeting is not an exam, it is part of the individual project and your contribution to class participation.

Course Logistics

The course uses a password protected site for distributing lecture materials and study recommendations. Students access the site remotely with a browser (Firefox, Safari, etc).

ID/password instructions will be sent by email to your GMU email.

IT Requirements for the Course

Hardware: You will need access to a Windows, Macintosh, or Linux computer. The lab in RH 249 allows you to work in any of the 10 linux-servers, either in person or remotely through SSH (or Putty, or equivalent). You login with your Mason ID and password:

cdsXX.mesa.gmu.edu, where XX=15 through 24.

These RH 249 computers do not share the desktops. It is recommended that you take note on what computer you work the first time, and then keep working in that computer for the rest of the semester. To access these workstations you need the VPN (Virtual Private Network) and to be logged into it: https://its.gmu.edu/service/virtual-private-network-vpn/

Software: Computers in this lab have all the needed software and the package Gaussian 09. They have installed compilers for Fortran, C, c++. Python and MatLab. If computers in this lab are not used, students are expected to have access to a programming language software suitable for scientific calculations.

Course Policies: Student Responsibilities

Email: Students are responsible for reading and maintaining the content of university emails sent to their Mason email account. Therefore, students are required to activate their email account and check it regularly. All communications from this course will be sent to students solely through their Mason email account. Alternatively, students may set a "forward" for forwarding any Mason incoming email/message to your preferred email account.

Use of phones, cameras, recording, texting in class is not allowed. Students should turn off the ringing of smart devices (cell phone, alerts apps) while in the Zoom classroom.

- *The use of laptop or a desktop computer is required in this class. You will only be permitted to work on material related to the class, however. Engaging in activities not related to the course (e.g., gaming, email, chat, etc.) will result in a significant reduction in your participation grade.*
- *We will frequently be using the internet as a means to enhance our discussions. We will also be using computers for our in-class writing assignments. Please be respectful of your peers and your instructor and do not engage in activities that are unrelated to the class. Such disruptions show a lack of professionalism and may affect your participation grade.*

Academic integrity: Students are responsible for their own work and must take on the responsibility of dealing explicitly with consequences to any academic integrity violation. Students must adhere to the George Mason University **Honor Code** as it relates to integrity regarding coursework and grades. The Honor Code reads as follows:

"To promote a stronger sense of mutual responsibility, respect, trust, and fairness among all members of the George Mason University community and with the desire for greater academic and personal achievement, we, the student members of the University Community have set forth this: Student members of the George Mason University community pledge not to cheat, plagiarize, steal and/or lie in matters related to academic work."

This is very important now [See Academic Integrity website: https://oai.gmu.edu/].

Classroom Conduct: Students must adhere to the Mason Honor Code and be very respectful of all class co-participants. It is recommended that students select a static virtual background for joining the classes. This enhances privacy. It is helpful for the group if each student adds a photo (ID type of photo) to be visible when the conference video is off.

Academic honesty policy of the course: Students are expected to follow the Honor Code at all time and for all activities. Academic dishonesty will not be tolerated in this class. Exams, projects, and homework must reflect individual work. If you have difficulty with the assignments, discuss them with the instructor.

Students with disabilities: Students with disabilities who seek accommodations in a course must be registered with the George Mason University Office of Disability Services (ODS) and inform the instructor, in writing, at the beginning of the semester [See Office of Disability Services website: http://ods.gmu.edu/].

Students that become ill: Students that become ill due to the pandemic should follow the Mason health recommendations and steps to follow: https://shs.gmu.edu/ .

University policies: Students must follow the university policies [See University Policies website: http://universitypolicy.gmu.edu].

Responsible use of computing: Students must follow the university policy for Responsible Use of Computing [See University Policies website: http://universitypolicy.gmu.edu/policies/responsible-use-of-computing].

University calendar: Students should consult the current Academic Calendar: https://registrar.gmu.edu/calendars/.

University catalog: Students should use the current university catalog [See University Catalog website: http://catalog.gmu.edu].

Student Services

University libraries: University Libraries provide excellent resources for books and journal publications. In addition, there are resources for distance students [See Library website: http://library.gmu.edu/distance].

Writing center: The George Mason University Writing Center staff provides a variety of resources and services (e.g., tutoring, workshops, writing guides, handbooks) intended to support students as they work to construct and share knowledge through writing. (See Writing Center website: http://writingcenter.gmu.edu). ESL Help: The program was designed specifically for students whose first language is not English who feel they might benefit from additional, targeted support over the course of an entire semester.

Counseling and Psychological Services: The George Mason University Counseling and Psychological Services (CAPS) staff consists of professional counseling and clinical psychologists, social workers, and counselors who offer a wide range of services (e.g., individual and group counseling, workshops and outreach programs) to enhance students' personal experience and academic performance [See Counseling and Psychological Services website: http://caps.gmu.edu].

Family Educational Rights and Privacy Act (FERPA): The Family Educational Rights and Privacy Act of 1974 (FERPA), also known as the "Buckley Amendment," is a federal law that gives protection to student educational records and provides students with certain rights [See Registrar's Office website: http://registrar.gmu.edu/privacy].