CHEM 743 "Quantum Chemistry" S'15

Instructor: Sophya Garashchuk*
Dept of Chemistry and Biochemistry, University of South Carolina, Columbia †
(Dated: January 7, 2015)

Syllabus

- **Learning outcomes**: (i) the students will gain theoretical knowledge in quantum mechanics and computer skills enabling them to use modern electronic structure codes and simulations with confidence and intelligence to better understand chemical processes; (ii) the students will be able to set up their own input files and interpret/visualize output files for standard quantum chemistry programs/packages that might be relevant to their research; (iii) the students will improve general critical thinking and problem-solving skills as well as improve their skills of independent computer-aided research through extensive use of electronically available resources.

- **Prerequisites**: CHEM 542 or equivalent, i. e. Physical Chemistry - Quantum Mechanics and Spectroscopy

- Classes will take place MW 9:40-10:55 AM at PSC 101. We will work with Maple, Q-Chem, Spartan, ADF
  Class materials and assignments or links to them will be posted on **Blackboard**
  Computer and software support:
  Jun Zhou
  zhouj@mailbox.sc.edu
  Ph: (803) 777-5492
  College of Arts & Sciences
  Sumwalt College 228

- Office hours: Tue 10-11 am, GSRC 407. I am generally available Mon-Fri 9:00 AM – 5PM. You can just drop by, call or e-mail to check if I am available, or if you have difficulty reaching me, make an appointment.

- The **suggested** general quantum chemistry textbook is "Introduction to Quantum Mechanics in Chemistry", by M. A. Ratner and G. C. Schatz, Prentice-Hall, New Jersey, 2001. Used copies are available through BN.com. The textbook is on reserve at Thomas Cooper library. Another textbook on quantum mechanics and theoretical methods of chemistry (highly recommended) is G. C. Schatz and M. A. Ratner "Quantum mechanics in chemistry" ($22.95 at Amazon, BN etc). Some **other books**: "Physical Chemistry" by Atkins, "Mathematical Methods for Physicists" by Arfken, "Quantum Chemistry" by Levine. Another resource is a **free downloadable text** "Quantum mechanics in chemistry" by Simons and Nichols
  `http://simons.hec.utah.edu/TheoryPage/BookPDF/TableofContents.html` Also use resources onf Jack Simons' webpage http://simons.hec.utah.edu/TheoryPage/

  There are many useful guides and texts on the web, particularly with respect to UNIX, linear algebra, and general aspects of computational chemistry. On-line manuals for all software packages are very useful and often outline the theory. In addition, **electronic wiki-book** is a useful resource:
  `http://en.wikipedia.org/wiki/Book:Electronic_structure_methods`

  "Quantum Chemistry" libguide `http://guides.library.sc.edu/qchem` has various electronic resources and applets. Let me know about any other useful or fun stuff that can be added!

- The best way to study is active participation during class (ask a lot of conceptual and specific questions!) and working through the homework problems to develop your skills and to test your knowledge. By far the most important part of learning in science is **not** memorization of facts, principles, and laws, but comprehension of the larger picture. This is **especially true** of quantum mechanics. Also, **notation** is one of the most difficult aspects of learning electronic structure theory. Use it and get comfortable with it as soon as possible.

- **Required work**: homework problems (15%), midterm exam (20%) a computational chemistry project (50%) approved by the instructor and, in lieu of the final, a short in-class computational task (15%). You can use any sources (except people) for the latter. The project can be related to your research area or chosen from instructor's suggestions; full information will be given in class. Some examples are:

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- *Isomers of triatomic molecule made of* Li, C, *and* N. Find the absolute minimum and the metastable isomer(s) in linear configuration. Calculate force constants for each minimum, and calculate the isomerization barrier. Compare your results using different levels of theory.
- *Study of valency.* Calculate bond energies of the XH_{n-1}-H bond in molecules where X is Be, C, O, and n takes all possible values yielding stable molecules. Use different levels of theory and different basis sets. Find the average bond energy for each X.
- *How does benzene crystallize?* Examine the benzene dimer to predict the arrangement of molecules in the solid state.

Attendance above 80% is expected.

The grading scale: $A \geq 90 > B+ \geq 85 > B \geq 77 > C+ \geq 69 > C \geq 60 > D \geq 40$

Modification for undergraduate students: instead of the independent research-related project (50% of the grade) you will choose one well-defined computational Spartan lab offered by the instructor. Homework problems will be simplified.

- **Academic Conduct**: Cheating, plagiarism, copying from old reports, and other forms of academic dishonesty in connection with any portion of this course is a serious infraction and will result in failure of the course. Assisting or knowingly cooperating in academic dishonesty will also result in failure in the class. All incidents of academic dishonesty will be reported to the Academic Integrity Office.

Timeline

- 01/12 First class
- 01/19 MLK day, no class
- 02/18 CHEM 749/CHEM 649 join in
- 03/08-03/15 Spring break, no classes
- 03/18-25 Choose and verify your project selection with the instructor
- 04/27 Last class
- 04/29 Turn in your projects and final

Content (by week)

1. 01/12: CHEM 743 "Quantum chemistry" begins. Computer accounts; Tools of the trade: Unix, Maple, Q-Chem, Spartan
2. 01/19: Fundamentals of QM; Wavefunction, normalization, operator, inner product, Hamiltonian.
3. 01/26: Separation of variables; Time-dependent and time-independent Schrodinger equation; The variation principle
4. 02/02: Harmonic oscillator; Particle in a box.
5. 02/09: Basis representation of a wavefunction; Review of linear algebra; Vectors, matrices, eigenvalues; Hermitian and unitary matrices
6. 02/16: Variation principle for a wavefunction represented in a basis; Example – anharmonic oscillator
   02/18: CHEM 743 Midterm exam
   02/18: CHEM 749/649 "Computational chemistry" begins. Computer accounts; Tools of the trade: Unix, Maple, Q-Chem, Spartan.
7. 02/23: Atomic units. Hydrogen atom; Angular momentum; Atomic orbitals.
8. 03/02: Electron spin and the Pauli principle. Variation principle and perturbation theory. Helium example.
9. 03/09-03/15 Spring break.
10. 03/16 Basis representation of a wavefunction and basis sets. Energy minimization as a linear algebra problem: vectors, matrices, eigenvalues.

11. 03/23 The Hartree-Fock model. Technical aspects: initial guess, convergence, stability. Energy calculation, geometry optimization.

12. 03/30 Post-Hartree-Fock (electron correlation, perturbation theory). Barriers to the reactions; vibrational spectra; isotope effect.

13. 04/06 Model chemistries. Other correlated methods (configuration interaction, coupled cluster, density functional theory).

14. 04/13 Computation of molecular properties, visualization in Spartan, energy profiles. Polarizability, properties in solutions.

15. 04/20 In-class work on the projects; Calculation of excited electronic states and electronic spectra.

16. 04/27 Finish the projects.

17. 04/29 Final: independent projects are due; in-class computational tasks are completed.

CHEM 649 "Computational Chemistry" Spring 2012

- ***Instructor*** : Sophya Garashchuk; GSRC 407, phone # 777–8900, sgarashc@mail.chem.sc.edu

  This is a ***2 credit-hour*** course for undergraduate and graduate students "Computational Chemistry". Prerequisite: undergraduate quantum mechanics, such as CHEM 542 or consent of the instructor. For a ***3-credit hour*** option contact the instructor.

  Late start: first day of class is 02/27/2012. The classes are scheduled MWF 10:10-11:00 am in the LINUX computer lab at PSC 101.

- ***Topics and skills***

(i) you will learn basic concepts and gain computer skills enabling you to use electructure codes and simulations with confidence and intelligence for better anding of the chemical processes (such as computation of stationary geometries, , electrostatics and polarizability, properties in solutions, IR and UV spectra)
(ii) you will be able to set up their own input files and interpret/visualize output files for standard quantum chemistry programs/packages that might be relevant to their research
(iii) we will cover the basics of LINUX, computational chemistry programs (Spartan, QChem, MOPAC etc.), using a computer cluster

- ***No required textbook***, extensive class notes and electronic resources will be provided. The suggested quantum chemistry textbook is "Introduction to Quantum Mechanics in Chemistry", by M. A. Ratner and G. C. Schatz, "Physical Chemistry" by Atkins; "Quantum mechanics in chemistry" by Simons and Nichols http://simons.hec.utah.edu/TheoryPage/BookPDF/TableofContents.html