Quantum Chemistry, CHEM 743

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- **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; or instructor consent

- Classes will take place M,W 9:40-10:55 AM at Jones 101. We will work with Maple, Q-Chem, Spartan
  Class materials and assignments or links to them will be posted on **Blackboard** or on file system in Jones 101

  Computer and software support:
  Christian Price priceca@mailbox.sc.edu
  Jones 102

- The **required** textbook for the course is 'Quantum Chemistry' by D. McQuarrie, 2nd edition

  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. Another textbook on quantum mechanics and theoretical methods of chemistry is G. C. Schatz and M. A. Ratner "Quantum mechanics in chemistry" ($22.95 at Amazon, BN etc).

- **Other resources**

  "Physical Chemistry" by Atkins, "Mathematical Methods for Physicists" by Arfken; "Quantum Chemistry" by Levine

  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`
  various electronic resources and applets; let me know about any other useful/interesting 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 (20%)
  Midterm exam (25%)
  Final and computational/theoretical project (55%).

  There will be an opportunity to retake quizzes or the midterm; grade for the project will include a discussion of its final version.

  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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*Electronic address: `garashch@mailbox.sc.edu`
†Office hours: TBD. However, feel free to stop by my office whenever you want. I am mostly in the office every weekday 7:30-4:30

- *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.
- *Unusual molecules.* Study a molecule made of up to 6 main-group atoms that makes at least some chemical sense, but is not known to Wikipedia.
- *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: $A \geq 90 > B+ \geq 85 > B \geq 77 > C+ \geq 69 > C \geq 60 > D \geq 40$

- **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 normally 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 Office of Academic Integrity for possible further disciplinary action.
- **Hazardous Weather**: In case of emergency closure, assignments will be posted on Blackboard. Emergency closures are announced on the university's Carolina alert website `http://carolina alert.edu`
- **Accommodating Disabilities**: Reasonable accommodations are available for students with a documented disability. If you have a disability and may need accommodations to fully participate in this class, contact the Office of Student Disability Services: 777-6142, TDD 777-6744, email `sasds@mailbox.sc.edu`, or stop by LeConte College Room 112A. All accommodations must be approved through the Office of Student Disability Services.
- **Course principles**

– familiarize students with theory so they should be able to use modern electronic structure codes with confidence
– develop critical thinking and problem-solving skills
– improve computer literacy, develop research skills.

- **Content** (about 3 lectures per topic)
  - Course tools: Linux in command-line-interface (CLI), Maple, basics of linear algebra
  - Fundamentals of QM. Wavefunction, normalization, operator, inner product, hamiltonian.
  - Particle-in-a-box. Harmonic oscillator. Hydrogen atom. Angular momentum. Atomic orbitals, atomic units, basis sets.
  - Electron spin. Many-electron atoms, antisymmetry, Hartree-Fock model
  - Technical aspects: initial guess, convergence, stability.
  - Beyond Hartree-Fock: electron correlation, perturbation theory.
  - Model chemistries. Computation of molecular properties
  - Other correlated methods (configuration interaction, coupled cluster, density functional theory).
  - Time-dependent Schrodinger equation. Wavepackets, propagation, correlation functions.
- **Tentative lecture plan** (updated as we go)

1. 08/26 First class Computer accounts; Tools of the trade: Unix, Maple, Q-Chem, Spartan.
2. 08/28 Basic unix commands. Fundamentals of Maple.
3. 09/02 Labor Day. No class.
4. 09/04 Linear algebra review.
5. 09/09 Fundamentals. Wavefunctions and operators.
6. 09/11 Energy minimization. Derivation of the linear algebra equations for 1-e problem.
7. 09/16 Basis set. Orthogonality of solutions. Exact solutions.
8. 09/18 Formal study of harmonic oscillator. Numerical study of quartic oscillator. Classical limit. Steps of computational procedure.

9. 09/23 Morse oscillator, molecular vibrations.
10. 09/25 Particle-in-a-box. Multidimensional case, separation of variables.
11. 09/30 Polar coordinates. 2D and 3D rotations, spherical harmonics. Hydrogenic functions.
12. 10/02 Exact hydrogenic solutions.
13. 10/07 Commutators. Non-orthogonal bases.
14. 10/09 Perturbation theory. First look at molecules, 1-e part.
15. 10/14 Running a calculation in Spartan and in Q-Chem.
16. 10/16 Electron spin. $\hat{S}^2$ and $\hat{S}_z$ operators, and their eigenfunctions in multi-electron case.
17. 10/21 Many-electron systems: antisymmetry and Slater determinant.
18. 10/23 Expectation value of Slater determinant. Coulomb and exchange. Fock operator.
19. 10/28 Midterm exam. Project selection is due.
20. 10/30 AO representation. Running Hartree-Fock calculations. Initial guess, convergence methods.
21. 11/04 Orbital energies. Standard basis sets. Effective core potentials.
22. 11/06 Geometry optimization. PES scans.
23. 11/11 Limitations of Hartree-Fock, post Hartree-Fock, UHF and RHF
24. 11/13 Density Functional Theory.
25. 11/18 Møller-Plesset Perturbation Theory, (MPn, n=2,3,...); CI
26. 11/20 Properties of correlation methods. Size-consistency, Coupled-Cluster, types of calculations.
27. 11/25 IR/Raman and UV/Viz spectra, charge distributions, solvation models.
28. 11/27 Work on projects.
29. 12/02 Quantum dynamics.
30. 12/04 Correlation functions and spectra.
31. 12/09 Final exam. Projects are due. Doing both early is welcome!