CHEM 26800/36800 AND MENG 25510/35510

Quantum Molecular and Materials Modeling

Instructors: Laura Gagliardi and Matthew Hennefarth

TAs:
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Lectures: Tue/Thu 11:00 am - 12:20 pm (Kent 101)

Textbooks: There is no required textbook. Daily class lectures will be distributed on the class website as pdf files. Some material will be taken directly from articles. O*ptional* books are:

Modern Quantum Chemistry: Introduction to Advanced Electronic Structure
(Dover Books on Chemistry) Reprint Edition by Attila Szabo (Author), Neil S. Ostlund (Author)
ISBN-13: 978-0486691862
ISBN-10: 0486691861

Molecular Electronic-Structure Theory
by Trygve Helgaker, Poul Jorgensen, Jeppe Olsen
ISBN-13: 978-1118531471
ISBN-10: 9781118531471.

Density Functional Theory, An Advanced Course Eberhard Engel · Reiner M. Dreizler Springer-Verlag Berlin Heidelberg 2011.

Electronic Structure: basic theory and practical methods: Richard M. Martin, 1st or second edition, Cambridge University Press

Coursework: The class is lecture-like in format, with the anticipated topics to be covered outlined below. Students are expected to keep up with posted class readings (they'll be made available at least a few days in advance) and to work on assigned homework problems (see below). Our intent is to spend the first 10 minutes of each lecture going over a previously assigned problem, and the remainder on lecture/demonstration of new material. Classroom attendance is not required, but you are likely to have a ***much*** more difficult time if you fail to attend classes.

Some of the lectures will be taught in an experimental style emphasizing class discussion. Students should prepare for these lectures accordingly. The material to be emphasized in each class will be announced beforehand, for example, at the previous lecture.

Homework: At the end of most of the lectures some homework problems will be assigned. The problems should be turned in once a week, as described in the outline, and discussed

with the instructor. The solution to the problems will also be discussed at the start of the following lecture. Students should be prepared to participate actively into the discussion. Homework also consists of preparing for class discussion of the readings. Homework may be done in groups, if desired.
You can consult any material available, when solving the homework problems. However, you are supposed to elaborate your problems on your own. If some homework appears to be copied verbatim from any existing source, it will receive zero points.

Exams: There will be one midterm exam cumulative on all class materials up to that point. The final exam consists of writing a simple Hartree-Fock or DFT code that will be presented by the students at the end of the course. Details will be given during the course.

Grading: Problem sets (10%), participation to the discussion (20%), midterm exam (30%) and final exam (40%). The class will be graded on a **semi-absolute scale**.

Preparing for Exams: The most effective method to prepare for an exam is to study the lecture notes, the assigned problems, and the textbook. We are happy to discuss any of these items during office hours, as are the TAs, if you need feedback.

Office Hours:
Matthew Hennefarth:
Office: Searle 105
Thursday, 12:30 pm – 1:30 pm
Also By Appointment
Bhavnesh Jangid
Office: Searle 105
Monday, 2:00 pm – 3:00 pm
Jiawei Zhan:
Office: ERC 351
Tue/Thu, 4:00 pm – 5:00 pm
Jacob Wardzala:
Office: Searle 105
Wednesday, 2:00 pm – 3:00 pm

Date	Instructor	Topic
3/19	Hennefarth	L1 Born-Oppenheimer Approximation, Many-electron Wave functions, Variational Principle
3/21	Hennefarth	L2 Examples of variational calculations. The helium atom. The hydrogen atom. Gaussian basis sets.
3/26	Hennefarth	L3 Antisymmetry. Fermions and bosons. Spin.
3/28	Gagliardi	L4 Two-electron wave functions. Hartree products. The Slater determinant. **Return HW1**

4/2	Gagliardi	L5 The Hartree-Fock Method I
4/4	Gagliardi	L6 The Hartree-Fock Method II **Return HW2**
4/9	Gagliardi	L7 Exact and approximate wave functions: the exact wave function; the variational principle; size-extensivity; Configuration-Interaction Theory CASSCF and RASSCF.
4/11	Hennefarth	L8 Many-Body Perturbation Theory. **Return HW3**
4/16	Gagliardi	L9 Catch up and review
4/18	Gagliardi	L10 Midterm
4/23	Gagliardi	L11 Coupled Cluster Theory
4/25	Gagliardi	L12 Quantum Computers for Quantum Chemistry
4/30	Gagliardi	L13 KS-DFT
5/02	Hennefarth	L14- First Derivative Properties, Hellman-Feynman Theorem **Return HW4**
5/07	Hennefarth	L15 Analytical Nuclear Gradients
5/09	Hennefarth	L16 Applications of Nuclear Gradients: *ab initio* Molecular Dynamics and Geometry Optimizations **Return HW5**
5/14	Hennefarth	L17 Excited States, Decay Pathways, Breakdown of Born-Oppenheimer Approximation
5/16	Hennefarth	L18 Review

Final Exam: Date to be determined.