

Elements of Computational and Quantum Materials Science

Rutgers University-Newark
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Syllabus

Overview

The goal of this 3 credit course for Chemistry graduate and undergraduate students is to provide basic knowledge of the theory of materials science and molecular quantum mechanics when it is applied to determine molecular properties (e.g., Photoelectron Spectroscopy, IR, UV/VIS, NMR, etc ...).

The lectures are scheduled for Wednesdays 6:00 to 8:50PM and will cover “Theory” and “Applications”. Theory lectures will treat the theoretical background (formal proofs, derivations and problem solving). “Applications” lectures will involve learning Linux, BASH scripting, basic Python and practicing concepts of computational chemistry on the provided computer and computer software (GAUSSIAN, NWChem, ORCA, GAMESS, QUANTUM-ESPRESSO, etc...).

The first part of the course (January-March) will be devoted to treating electronic and vibrational properties of ground electronic states of molecules (vibrations, photoelectron spectroscopy).

The second part of the course (March-May) will be devoted to the study of excited electronic states, and the molecular properties that become theoretically accessible if excited states are computed (NMR, EPR, UV/VIS, Fluorescence, etc...).

Timeline

Grade distribution

Item	Percentage
Homework	20%
Midterm	30%
Computational/Theoretical Project	50%
Total	100 %

Table 1: Schedule of classes

Lecture	Date	Topic	Assignments Due
1	1/20	Basic Quantum	
	1/26	Last day to Drop w/out W	
2	1/27	Linux, BASH	Ch. 1
3	2/3	Molecules and Materials	
4	2/10	Amarel Supercomputer	Ch. 2
5	2/17	Basic Python / Gaussian	
6	2/24	Many-electron systems	
7	3/3	Molecular Orbital Theory	Ch. 3
8	3/10	Midterm	Ch. 4
	3/17	Spring Break	
	3/22	Last day to Drop with W	
9	3/24	Periodic systems (crystals)	
10	3/31	Nuclear motion / Reactivity	Ch. 5
10	4/7	Excited states: TD-DFT	Ch. 6
11	4/11	Molecular Properties	Ch. 7
12	4/18	Presentations	
13	4/25	Presentations	

Grade cut-offs

Grade	Percentage
A	85–100
B	65–84
C	55–64

Homework rules

Homework assignments...

- ... are worth 20 points for each handout, and the total “Homework” grade percentage is calculated as the arithmetic mean of the grades of each assignment.
- ... will be handed out or posted on the course website (see below).
- ... are due in the beginning of the next class period according to the schedule in Table 1.
- ... can be worked on in a study group setting.
- ... will involve problem solving and might treat questions not directly tackled in class (either theoretical or computational)

Midterm and Final

The midterm exam will be one-hour long and will involve problem solving. It will concern the course material covered until the last lecture before the exam. *There will be no final exam for this class.*

Computational/Theoretical Project

This project will be either Computational or Theoretical. Title and abstract of the Project need to be agreed upon by Prof. Pavanello no later than lecture #4. The subject of the project should be formulated in collaboration with the student's research advisor.

Computational

will involve using an established computer software (such as GAUSSIAN) to study a chemical reaction or physical process. A 3–5 page report and a presentation on this project will be graded out of 50 points and will constitute the grade associated with the “Computational/Theoretical Project” grade item. Further instructions will be given later.

Theoretical

will involve coding from scratch in python one of the following features in a local orbital basis, or plane wave basis or finite differences basis:

- Ground state HF or DFT.
- Time-dependent HF or DFT in real time or Casida formalism*.
- Time-dependent current DFT in real time or Casida formalism*.
- Phonons / molecular vibrations using the Sternheimer equation*.
- RPA using the Sternheimer equation.

* can start from a python based DFT/HF code like PySCF, DFTpy or Psi4numpy.

This project also will involve a 3–5 page report preferably on a Jupyter notebook in markdown language, together with in-line examples of computations run with the computer code as well as a presentation. Alternative computer coding projects can also be considered.

Official Course Website

The official course webpage is

<https://rutgers.instructure.com/courses/116692>

On the website you will find resources relevant to the “applications” part of the course as well as lecture notes and homework assignments. The *announcements* window should be checked regularly as it will be updated frequently.

Disability Services

Rutgers University welcomes students with disabilities into all of the University’s educational programs. In order to receive consideration for reasonable accommodations, you must complete and submit the Registration Form, schedule and complete an intake meeting, and submit appropriate documentation. If your request for reasonable accommodations is approved, you will receive a Letter of Accommodations (LOA), which you should present privately to the instructor as early in the semester as possible. Accommodations are not retroactive and are effective only upon submission of the LOA to the instructor. Please begin the process by completing and submitting the Registration Form, Applying for Services, available at the website below.

- Applying for Services: <https://ods.rutgers.edu/students/applying-for-services>
- Documentation Guidelines: <https://ods.rutgers.edu/students/documentationguidelines>
- Letter of Accommodations (LOA): <https://ods.rutgers.edu/myaccommodations/letterof-accommodations>
- Office of Disability Services (ODS) Suite 219, Paul Robeson Campus Center (973) 353-5315 odsnewark@rutgers.edu

Religious Holiday Policy

Students are advised to provide timely notification to instructors about necessary absences for religious observances and are responsible for making up the work or exams according to an agreed-upon schedule.

Counseling Services

Counseling Center Room 101, Blumenthal Hall, (973) 353-5805 or <http://counseling.newark.rutgers.edu/>.

Students with Temporary Conditions/Injuries

Students experiencing a temporary condition or injury that is adversely affecting their ability to fully participate in their courses should submit a request for assistance at: <https://temporaryconditions.rutgers.edu>

Students Who are Pregnant

The Office of Title IX and ADA Compliance is available to assist students with any concerns or potential accommodations related to pregnancy: (973) 353-1906 or TitleIX@newark.rutgers.edu.

Gender or Sex-Based Discrimination or Harassment

Students experiencing any form of gender or sex-based discrimination or harassment, including sexual assault, sexual harassment, relationship violence, or stalking, should know that help and support are available. To report an incident, contact the Office of Title IX and ADA Compliance:

- (973) 353-1906 or TitleIX@newark.rutgers.edu.
- To submit an incident report: <http://tinyurl.com/RUNReportingForm>.
- To speak with a staff member who is confidential and does NOT have a reporting responsibility, contact the Office for Violence Prevention and Victim Assistance: (973) 353-1918 or run.vpva@rutgers.edu

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