

CHM 6580: Special topics: Advanced electronic structure

Term: Spring 2022

Instructor: Ramón Alain Miranda Quintana

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Class schedule: Tuesday (Period 2), Thursday (Periods 2-3)

Books:

Required book: Molecular Electronic-Structure Theory; Helgaker, Jorgensen, Olsen.

For some particular topics we will also use the auxiliary text:

- Robert G. Parr and Weitao Yang, “Density-functional theory of atoms and molecules”, Oxford University Press, (1989)

Course objective and goals:

This course will give a self-contained exposition of different topics on advance electronic structure, from density functionals, to wavefunctions for strongly correlated systems.

Course Outline:

- Density Functional Theory.
- Reduced Density Matrices.
- Second quantization.
- Configuration Interaction.
- Coupled Cluster.
- Geminals.
- Perturbation Theory.
- FANCI.
- FANPT.
- Embedding.

*NOTE: The course is designed to be flexible and adaptive. As we progress, we can discuss about touching on some particular topics depending on your particular interests.

Grading:

Projects-----40%

Homework----40%

Class participation will also be taken into account (20%).

Letter grade	From	To
A	90	100
A-	84	89.99
B+	81	83.99
B	78	80.99
B-	75	77.99
C+	72	74.99
C	69	71.99
C-	66	68.99
D+	63	65.99
D	60	62.99
D-	50	59.99
E	0	49.99

More information on current UF grading policies for assigning grade points can be found at: [link to the university grades and grading policies](#).

Accommodations for students with disabilities: Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center. [Click here to get started with the Disability Resource Center](#). It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.

Homework:

Homework due date will be announced in class. Late homework will not be accepted. Each problem will have to show the full derivation. It is expected that the students will collaborate on some of the problems but, unless otherwise indicated, the homework must be delivered individually.

Honor code:

The student honor code can be found at: www.dso.ufl.edu/sccr/honorcodes/honorcode.php. The students and instructor are honor bound to comply with the Honors Pledge: We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

CampusResources:

Health and wellness:

U Matter, We Care: If you or someone you know is in distress, please contact umatter@ufl.edu, 352-392-1575, or visit [U Matter, We Care website](#) to refer or report a concern and a team member will reach out to the student in distress.

Counseling and Wellness Center: [Visit the Counseling and Wellness Center website](#) or call 352-392-1575 for information on crisis services as well as non-crisis services.

Student Health Care Center: Call 352-392-1161 for 24/7 information to help you find the care you need, or [visit the Student Health Care Center website](#).

University Police Department: [Visit UF Police Department website](#) or call 352-392-1111 (or 9-1-1 for emergencies).

UF Health Shands Emergency Room / Trauma Center: For immediate medical care call 352-733-0111 or go to the emergency room at 1515 SW Archer Road, Gainesville, FL 32608; [Visit the UF Health Emergency Room and Trauma Center website.](#)

Academic Resources:

E-learning technical support: Contact the [UF Computing Help Desk](#) at 352-392-4357 or via e-mail at helpdesk@ufl.edu.

Career Connections Center: Reitz Union Suite 1300, 352-392-1601. Career assistance and counseling services.

Library Support: Various ways to receive assistance with respect to using the libraries or finding resources.

Teaching Center: Broward Hall, 352-392-2010 or to make an appointment 352- 392-6420. General study skills and tutoring.

Writing Studio: 2215 Turlington Hall, 352-846-1138. Help brainstorming, formatting, and writing papers.

Student Complaints On-Campus: [Visit the Student Honor Code and Student Conduct Code webpage for more information.](#)

On-Line Students Complaints: [View the Distance Learning Student Complaint Process.](#)