

CHM 6470: Chemical Bond and Spectra

“When historians pick up their pens to write the story of the 21st century, let them say that it was your generation who laid down the heavy burdens of hate at last and that peace finally triumphed over violence, aggression and war.” (John Lewis 1940-2020)



This class focus on fundamental concepts of quantum chemistry with applications to spectroscopy

Instructor: Professor Valeria Kleiman. mail: kleiman@chem.ufl.edu

Class Schedule: Spring Semester 2021: January 11th – April 21th. T, R 8:30- 10:30 am online.

Office Hours: This is a very small class, so you can email me anytime to request a zoom meeting.

Textbook: The material we cover is available on any Quantum Chemistry textbook for graduate level students. I will provide notes through the class web site (CANVAS). You can use the notes to see the topics we cover and go to ANY graduate level book for more "in-depth" reading. From time to time I will provide some additional reading too.

List of Possible Books

Molecular Quantum Mechanics by P.W.Atkins and R.S. Friedman

Quantum Chemistry by Ira N. Levine

Elements of Quantum Mechanics by M. Fayer

Attendance: Attendance to lectures is required. In addition to the 4 hrs class a week, ~8-10/week of reading, homework and general study are required.

Course Site: We have a course workspace (<http://lss.at.ufl.edu>). it contains grade information. If you are register for the course, you are automatically registered in CANVAS. NOT THIS SEMESTER

Homework: Homework due date is posted on the class calendar. Late homework (if it is turned in on the same day, but after deadline) will have a **20% deduction on the grade**. Each homework problem has to show the **full derivation**, using SI units. **No points will be given for a final result without justification**. If you need help with the HW, or think you cannot finish it by the deadline, contact the instructor BEFORE the deadline to request a potential accommodation

Graphing Software: This must be done professionally and formatted for presentation in an ACS journal. You will learn to use Jupyter Notebooks (Python), thus it is the first choice to use, but you can also use Matlab (free in UF comp. labs and as an [App](#)), Origin, Igor, GRACE (free), gnuplot (free), or any other software of your choice. You will need time to learn to use it, so plan ahead. You must be able to have full control of axis, symbols, lines, and colors, be able to do linear fitting, learn to plot multiple dataset on the same graph, multiple graphs printed in a single page, etc.

During the course of the class we will introduce Jupyter Notebooks as a resource for calculations and graphs.

Course Grading: The grade will be determined by homework (35%), projects (50%) and in-class participation (15%).

*Although material for the class can be worked “in groups” and some information is always found online, the submitted homeworks and projects must be **your individual** work. If any assignment is suspect, a grade of zero will be given for that assignment.*

Information on current UF grading policies for assigning grade points is available at <https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx>

Evaluations: Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at <https://gatorevals.aa.ufl.edu/students/>. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via <https://ufl.bluera.com/ufl/>. Summaries of course evaluation results are available to students at <https://gatorevals.aa.ufl.edu/public-results/>.

Students with Disabilities

Students requiring special accommodations should register with the Dean of Students Office (<http://www.dso.ufl.edu/>, 352-392-1261) and the Disability Resource Center (DRC, <https://www.dso.ufl.edu/drc>, 352-392-8565, email: accessUF@dso.ufl.edu), and present documentation from that office to the instructor.

U-matter We care

Your well-being is important to the University of Florida. The U Matter, We Care initiative is committed to creating a culture of care on our campus by encouraging members of our community to look out for one another and to reach out for help if a member of our community is in need. If you or a friend is in distress, please contact umatter@ufl.edu so that the U Matter, We Care team can reach out to the student in distress. A nighttime and weekend crisis counselor is available by phone at 352-392-1575. The U Matter, We Care team can help connect students to the many other helping resources available including, but not limited to, Victim Advocates, Housing Staff, and the Counseling and Wellness Center. Please remember that asking for help is a sign of strength. In case of emergency, call 9-1-1.

The University of Florida provides counseling services for students, staff, and faculty. See <http://www.counseling.ufl.edu/cwc/>. If you or a friend are in distress, call (352) 392-1575 (available 24/7), email umatter@ufl.edu, or walk in for an emergency consultation during regular service hours (8:00am – 5:00pm) at the Radio Road Site, 3190 Radio Rd., or the Peabody Hall Site, on the 4th floor of Peabody Hall, adjacent to Criser Hall. For other hours or weekends, call the Alachua County Crisis Center, (352) 264-6789. For sexual assault recovery services call the Student Health Care Center at (352) 392-1161. For life-threatening emergencies always call 911.

Emergency Numbers and Web Sites

UFPD (UF Police Department): In case of emergency dial 911. The UF campus police non-emergency number is (352) 392-1111. Their web site: <http://www.police.ufl.edu/>,

UF Emergency management: (352) 273-2100. <https://emergency.ufl.edu/>,

Infirmery (student health center): (352) 392-1161, <http://shcc.ufl.edu/>.

EH&S (Environmental Health & Safety): (352) 392-1591, <http://www.ehs.ufl.edu/>.

Other Academic Resources

UF provides several other resources for students, such as

Library Support can be obtained here: <http://cms.uflib.ufl.edu/ask>, where you can find various ways to receive assistance with respect to using the libraries or finding resources.

The Career Resource Center is located on level One in the Reitz Union, (352) 392-1601, and provides career assistance and counseling. Refer to <http://www.crc.ufl.edu/> for further info.

The Teaching Center is located in Broward Hall, main phone (352) 392-2010 or appointment phone (352) 392-6420, and provides students with tutoring services and counseling regarding general study skills. Refer to <http://teachingcenter.ufl.edu/> for further info. It may also provide employment opportunities as tutors for well qualified students.

The Writing Studio is located at 302, Tigert Hall, (352) 846-1138, and provides help with brainstorming, formatting, and writing papers, see: <https://writing.ufl.edu/writing-studio/>.

The Ombuds Office is located at 31 Tigert Hall, (352) 392-1308, and provides students assistance in resolving problems and conflicts that arise in the course of interacting with the University of Florida. By considering problems in an unbiased way, the Ombuds works to achieve a fair resolution and works to protect the rights of all parties involved. For further information go to <http://www.ombuds.ufl.edu/> or refer to the official complaints policy here: https://www.dso.ufl.edu/documents/UF_Complaints_policy.pdf.

Netiquette: All members of the class are expected to follow rules of common courtesy in all email messages, threaded discussions, and chats. When attending Zoom meetings, please come prepared. Be presentable: clothing is not optional. You must be seated (not lying down or reclining). Make sure not to show any personally identifiable information and/or other items that you do not wish others to see. Let others finish what they are saying and only speak when it is your turn. Be present: you can check your email and work on other tasks after the meeting. Turn off all notifications and make sure your cell phone does not ring. Being online is equivalent to being in a classroom, where the focus is in the chemistry and the interactions are only among member of the class (no outside conversations with friends, family or pets).

Honor Code This class will operate under the policies of the student honor code which can be found at: <https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/>. The students, instructor, and TAs 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.** You are expected to exhibit behavior consistent with this commitment to the UF academic community, and on all work submitted for credit at the University of Florida, the following pledge is either required or implied: *"On my honor, I have neither given nor received unauthorized aid in doing this assignment."* It is assumed that you will complete all work independently in each course unless the instructor provides explicit permission for you to collaborate on course tasks. Furthermore, as part of your obligation to

uphold the Honor Code, you should report any condition that facilitates academic misconduct to appropriate personnel. It is your individual responsibility to know and comply with all university policies and procedures regarding academic integrity and the Student Honor Code. Violations of the Honor Code at the University of Florida will not be tolerated. Violations will be reported to the Dean of Students Office for consideration of disciplinary action. For more information regarding the Student Honor Code, please see: <https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/>.

If you have further questions, please contact me. Have a great semester!



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TENTATIVE Schedule of Classes

CHM 6470 FALL 2021

January

Tuesday	Thursday
12 Introduction to Jupyter Notebooks	14 Mathematical Review: Differential equations. Homogeneous, inhomogeneous, Boundary Conditions (Levine Chp 2 pg 23-24). Diff equation of a wave. Its solutions (Euler equation). Superposition of waves. Standing waves.
19 Superposition of waves. Standing waves. Matrices	21 Matrices, eigenvalues and eigenvectors (Levine Molec Spec. Chp 2)
26 Operators (Chp 3 Levine Quantum CHEM)	28 Dirac Notation. Operators, Commutators, Stern-Gerlach Experiment (app) Quantum Behavior/Wave Particle duality (ppt)

February

Tuesday	Thursday
2 Uncertainty Principle. Born Interpretation. Free particles, Localization of wavepackets.	4 Schrodinger and Heisenberg Representations Particle in a box
9 Particle in a box (infinite, finite)	11 1-D 2-D finite potentials
16 Harmonic Oscillator (ladder operators)	18 Harmonic oscillator functions, graphics, calculation of observables. Ang. Momentum
23 Angular Momentum (with algebra of Operators) Particle in a RING	25 Rigid Rotors. Schrödinger equation, separation of variables, Functions, degeneracy, Solutions (graphical and in particular)

March

Tuesday	Thursday
<p style="text-align: right;">2</p> <p>The H atom (SOLVING THE DIFFERENTIAL EQUATION)</p>	<p style="text-align: right;">4</p> <p>H-atom: THE SOLUTIONS</p>
<p style="text-align: right;">9</p> <p>Approximation Methods: Variational Theorem</p>	<p style="text-align: right;">11</p> <p>Approximation Methods: Perturbation Theory</p>
<p style="text-align: right;">16</p> <p>Approximation Methods: Perturbation Theory (excited state of He)</p>	<p style="text-align: right;">18</p> <p>Time dependent Perturbation Theory: Spectroscopy</p>
<p style="text-align: right;">23</p> <p>SPIN 2-state coupled system Coupling of angular momenta. ?)</p>	<p style="text-align: right;">25</p> <p>Molecules, LCAO-MO, Valence Bond theory</p>
<p style="text-align: right;">30</p> <p>Diatomic Molecules(homonuclear) intro to symmetry (reflection and inversion operators)</p>	

April

Tuesday	Thursday
	<p style="text-align: right;">1</p> <p>Diatomic Molecules (Terms, Bond Order, Heteronuclear) Hartree-Fock Self Consistent Field</p>
<p style="text-align: right;">6</p> <p>Semiempirical (Hückel)</p>	<p style="text-align: right;">8</p> <p>Ab-initio methods and DFT</p>
<p style="text-align: right;">13</p> <p>GROUP THEORY (spectroscopy)</p>	<p style="text-align: right;">16</p> <p>GROUP THEORY (spectroscopy)</p>
<p style="text-align: right;">20</p> <p>Project presentation</p>	