## CHM 6470: Chemical Bonding and Spectra

# Fall 2014 (3 credits)

Instructor:	Nick Polfer, Chemistry Lab Building (CLB) 311C, polfer@chem.ufl.edu
Dr Polfer Office hours:	ТВА
Lectures:	T, R <b>2<sup>nd</sup>-3<sup>rd</sup></b> period (8:30-10:25 am) UST 104
Aims:	To provide students with a solid background in the concepts of quantum mechanics, to provide a deeper understanding of computational chemistry and relating these insights to spectroscopy.
Text book:	Molecular Quantum Mechanics, by Atkins & Friedman (Oxford University Press)
Home work:	Problem sets will be made available throughout the semester, which will be graded.
Exams:	The course consists of one in-class exam during the semester as well as a comprehensive final. The exams will cover homework problems and will emphasize understanding of the lecture material and problem solving. All exams will be <u>closed</u> <u>book</u> . <b>Exam I</b> Oct 14
	Final comprehensive exam Dec 16

**Grading:** The grade consists of four different types of assessments: exams (during-term and final), homework, attendance, and a project. The during-term exam is worth 20%. The final comprehensive exam is also worth 20%. The total points for the homework assignments are 35% (5x7%). Attendance and active participation in class will be monitored for a score of 5%. A project is allocated a max of 20%.

Total = 20 + 20 + 35 + 5 + 20 = 100%

#### **Proposed Grade Levels:**

- A: 92-100 A-: 88-91.9 B+: 84-87.9 B: 80-83.9 76-79.9 B-: C+: 72-75.9 C: 68-71.9 C-: 64-67.9 D+: 60-63.9 D: 56-59.9 D-: 52-55.9
- E: < 52
- **Course policies:** Attendance in this course is expected. Any request for make-up exams should have a legitimate excuse, and be made to Dr. Polfer as far in advance as possible.

Students should also familiarize themselves with the UF Student Honor Code posted on the web at <u>www.chem.ufl.edu/~itl/honor.html</u>.

Students with disabilities must first register with the Dean of Students Office, see http://www.chem.ufl.edu/~itl/disabilities.html;

the Dean of the Students Office will provide documentation to the student who must then provide this documentation to the instructor when requesting accommodation.

For counseling, students should consult the webpage:

http://www.chem.ufl.edu/~itl/counseling.html

#### Advice: We will cover a lot of material in a short period of time. It is hence essential that you keep up-to-date with the lecture material and do your homework assignments.

The lecture, homework exercises, example tutorial notebooks can be found on Sakai (<u>https://lss.at.ufl.edu/</u>) under the *Resources* tab. Lectures are named as follows, including the title: e.g. Lecture\_1\_Wave\_Particle\_Duality.pdf

### **Tentative Lecture Schedule CHM 6470**

Lecture	Date	Торіс	нพ
1	<b>T</b> 08/26	Wave particle duality	
2	<b>R</b> 08/28	Dirac notation	
3	<b>T</b> 09/02	Commutators	
	<b>R</b> 09/04	No class	
4	<b>T</b> 09/09	Uncertainty principle	
5	<b>R</b> 09/11	Schrödinger equation	
6	<b>T</b> 09/16	Particle in a 1 D box	H1
7	<b>R</b> 09/18	Harmonic oscillator	
8	<b>T</b> 09/23	Angular momentum	
9	<b>R</b> 09/25	The hydrogen atom	
10	<b>T</b> 09/30	Coupled 2-state system	
11	<b>R</b> 10/02	Spin and coupling of angular	H2
10		, momenta	
12	10/07	Approximation methods: variational	
10	<b>D</b> 10/00	theorem	
13	<b>R</b> 10/09	Approximation methods:	
		perturbation theory &	
		time-dependent	
	<b>T</b> 10/14	EXAM I	
	<b>R</b> 10/16	Exam review	
14	<b>T</b> 10/21	Molecules: Born-Oppenheimer	H3
		approx.	
15	<b>R</b> 10/23	Molecular orbitals, energy diagrams	
16	<b>T</b> 10/28	Group theory	
17	<b>R</b> 10/30	Spectroscopy & rotations	
18	<b>T</b> 11/04	Vibrational spectroscopy	H4
19	<b>R</b> 11/06	Electronic spectroscopy	
20	<b>T</b> 11/11	Calculations in quantum chemistry	
21	<b>R</b> 11/13	MP2, DFT, CNDO	
22	<b>T</b> 11/18	MP2, DFT, CNDO	
23	<b>R</b> 11/20	Comparison of theory and expt	H5
	<b>T</b> 11/25	Presentation of projects	
	<b>R</b> 11/27	Thanksgiving (No class)	
	<b>T</b> 12/02	Presentation of projects	
	<b>R</b> 12/04	Presentation of projects	
	<b>T</b> 12/09	Reading days (no class)	
	<b>T</b> 12/11	Reading days (no class)	
	<b>T</b> 12/16	FINAL EXAM (in-class)	