CHEM 516 Physical Inorganic Chemistry

Spring 2023 – Tuesday & Thursday, 9:30 – 10:50 AM, 165 Noyes Lab

SYLLABUS

Instructor:	Prof. Benjamin Snyder (bsnyder@illinois.edu) *Office Hours: Thursday, 10:50-11:50, A406 CLSL* *or by appointment – schedule by e-mail*
Teaching Assistant:	Luke Westawker (lukepw2@illinois.edu) *Office Hours: Tuesday, 10:50-11:50, location TBD*
Website:	CHEM 516 Box Folder: https://uofi.box.com/s/kjhsp9xbfezdlh8hnt8oliqz7j0c0fqx
Course Materials	Textbooks and other useful PDFs are provided in the shared Box folder. At the beginning of each unit, references / readings for the upcoming lectures will be posted on the course calendar *which is a living document*. It is recommended that you read the listed references *before* the lecture.
Assignments & Grading:	5 problem sets (100 points each), final project (250 points), participation (100 points), in-class exercises (150 points) Due dates for assignments are indicated on the course calendar. Problem sets will be graded 40% for completeness, 60% for correctness. Hard copies of completed problem sets should be turned in to the TA at the start of lectures. Each student is entitled to a no-questions-asked 7-day extension on one problem set of their choice. We will strive to return graded problem sets one week after they are due. In-class exercises will be graded only on completeness. Hard copies of completed in-class work should be turned in to the TA. More information on problem sets, in-class exercises, and the final project is provided on the following page.
Academic Integrity:	It is the responsibility of each student to refrain from infractions of academic integrity, from conduct that may lead to suspicion of such infractions, and from conduct that aids others in such infractions.
Class Attendance:	Regular class attendance is expected. *Accommodations can be arranged for illness, family emergencies, and religious observance*.
Students with Disabilities:	To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact the course instructor and the Disability Resources and Educational Services (DRES) as soon as possible. To contact DRES, you may visit 1207 S. Oak St., Champaign, call 333-1970, e-mail disability@illinois.edu or go to the DRES website. If you are concerned you have a disability-related condition that is impacting your academic progress, you can talk with someone at the Counseling Center, McKinley Mental Health, or DRES about how to see a provider to obtain a diagnosis or get your questions answered.

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Learning Goals: The primary goal of this course is to develop a more sophisticated understanding of the 'routine' physical methods used in modern inorganic chemistry. This course is designed to help you read and critically evaluate inorganic literature, choose the right characterization methods in your own research, and maximize the amount of chemical insight that can be extracted from your spectroscopic and computational data. To this end, the course will focus on the geometric and electronic structure of transition metal ions, and their correlations to spectroscopic observables.

In-class Activities: At the beginning of some (many!) lectures, I will pass out a worksheet containing a few questions relevant to the day's material. These questions are active learning tools to be completed at specified times during the lecture, and will be graded on completeness alone. You should therefore feel safe giving 'wrong' answers, or even stating you don't know the answer. This will help me keep track of how we are all doing with the material.

Problem Sets: There will be five problem sets covering: 1) group & representation theory; 2) free ion electronic structure, crystal field theory, and ligand field theory; 3) magnetism & electron paramagnetic resonance; 4) vibrational and electronic absorption; 5) magnetic circular dichroism, X-ray absorption, and Mössbauer. Each problem set will include a computational component. You are welcome to discuss problem solving strategies together in small groups (two or three), but your written answers must be entirely your own. If you elect to work together, please list your teammates at the top of your assignment.

Final Project: A key goal of this course is to prepare you to read, understand, and critically evaluate modern research in physical-inorganic chemistry. To that end, each of you will choose one or two closely related papers that make heavy use of physical-inorganic methods – ideally, ones relevant to your own research. You will prepare a 30 min. PowerPoint presentation based on the paper(s) and present it to the class. In addition, you will supplement the results from the paper with your own computational studies on those systems. More details will be provided to you once you choose a topic and the relevant research article(s). The paper(s) and associated DFT calculations are to be of your choosing. You will be asked to outline your plan in a brief (300-500 word) project proposal, which I will review and approve before spring break. *It is recommended that you consult with your research advisor to pick out the appropriate paper(s) soon!* You are welcome to choose a paper or manuscript in progress from your current group, do a deep dive into the spectroscopy, and complement it with your own computational studies. Grading of the presentations will follow the template given midway through the semester.

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TENTATIVE COURSE CALENDAR

DATE	CLASS #	TOPIC	REFERENCES	NOTES
1/17	1	Group & Representation Theory 1	MT 4; D 1, 2, 10-5; C 2, 3, 9.7; handouts	HW1
1/19	2	Group & Representation Theory 2	D 2; C 4, 5; handouts	survey due
1/24	3	Group & Representation Theory 3	D 4; C 5; HB 2; CC 4.5	
1/26	4	Computational Chemistry 1	CC 4, 8; M 10	
1/31	5	Free Ion Electronic Structure 1	MT 2; M 7	HW2
2/2	6	Free Ion Electronic Structure 2	D 10; C 9; MT 11	
2/7	7	Crystal Field Theory	D 10; C 9; MT 10, 11	HW1 due
2/9	8	Ligand Field Theory 1	D 10; C 9; MT 10, 11	
2/14	9	Ligand Field Theory 2	D 10; C 9; MT 10, 11	
2/16	10	Computational Chemistry 2	CC 14	
2/21	11	Magnetism 1	D 11	HW3, HW2 due
2/23	12	Magnetism 2	D 11	
2/28	13	Electron Paramagnetic Resonance 1	D 9, 13-1,2; WB 1, 4	
3/2	14	Electron Paramagnetic Resonance 2	D 13-3,4,5; WB 2, 3, 5	
3/7	15	Electron Paramagnetic Resonance 3	D 13-3,5; WB 6, 8	proposal due
3/9	16	Computational Chemistry 3		
3/14		*Spring Break*		
3/16		*Spring Break*		
3/21	17	Vibrational Spectroscopy 1	D 6; HB 3; C 10	HW4, HW3 due
3/23	18	Vibrational Spectroscopy 2	D 6; HB 3; Q 2	
3/28	19	Electronic Absorption 1	Q 1; C 9.6; D 5.7-5.15	
3/30	20	Electronic Absorption 2	Q 1; C 9.6; D 5.7-5.15	
4/4	21	CD & MCD	Q 5	HW 5
4/6	22	Computational Chemistry 4		
4/11	23	X-Ray Absorption Spectroscopy	Q 9	HW4 due
4/13	24	Mössbauer and NRVS	Q 6; D 15	
4/18	25	Student Presentations		
4/20	26	Student Presentations		
4/25	27	Student Presentations		
4/27	28	Student Presentations		
5/2	29	Student Presentations		HW5 due

Readings (number = chapter): C = *Chemical Applications of Group Theory*, Cotton; **D** = *Physical Methods in Chemistry,* Drago; **MT** = *Inorganic Chemistry*, 5th Ed., Miessler, Fischer, & Tarr; **HB** = *Symmetry and Spectroscopy,* Harris & Bertolucci; **WB** = *Electron Paramagnetic Resonance*, Weil & Bolton; **CC** = *Essentials of Computational Chemistry*, 2nd Ed., Cramer; **M** = *Quantum Chemistry*, 2nd Ed., McQuarrie; **Q** = *Physical Methods in Bioinorganic Chemistry*, L. Que (ed)