Fall 2024; Chemistry 16:160:471/571
ADVANCED INORGANIC CHEMISTRY
Syllabus & Schedule of Lectures

Schedule	Mondays and Thursdays, 12:10 PM - 1:30 PM; Room: ARC-108; Busch Campus
Instructors	Charles Dismukes (WL-113, 445-1489; 445-6786, dismukes@rutgers.edu) Tewodros (Teddy) Asefa (CBE-138, 445-2970, tasefa@chem.rutgers.edu)
Course Goals	Learn how to apply and interpret physical methods and quantitative reasoning to understand the current literature in inorganic chemistry.
Course Content	Survey of modern inorganic chemistry including: Electronic structures of atoms and molecules, Spectroscopy of optical transitions, DFT vs VB and MO methods, chemical bonding in coordination complexes, simple solids, and nanocrystalline solids, ligand field theory, electronic states and spectra, theory of catalysis, catalysis by organometallic complexes and nanocrystalline and inorganic materials, heterogeneous catalysis, and electrocatalysis
Textbook	"Inorganic Chemistry", 5th Ed., 2017, G. L. Miessler and D. A. Tarr. https://www.pearsonhighered.com/miessler5einfo/ "*Electronic Structure and Properties of Transition Metal Compounds. Introduction to the Theory*" 2010 Second Ed., by I. B. Bersuker; chapter 6 assigned and will be made available. + Multiple articles from the primary literature will be assigned and made available.
Lecture Notes	Lecture notes will be available and will be posted on the course website on Canvas. Access will be provided to all students enrolled in the course.
Problems	Assigned readings and homework from the textbook or other sources will be reviewed in class and problems solved. These will not be graded. These concepts will be evaluated in the quizzes and the two exams. In lieu of a written proposal used in previous years and to provide examples of how to apply the scientific method., examples of papers from the recent literature will be discussed and analyzed.
Quizzes/Attendance	Four pop-quizzes that are unannounced will be given from time to time. These will make up 20% of the overall grade (see below).
Attendance	Attendance in classes is expected. Unannounced attendance may be taken during lectures

Office Hours	By appointment and Wednesdays 1:30-2:30 pm (Asefa office, Dismukes office)
Review Report	Each student is expected to write and defend a review report using scientific methods in a current topic in an area of inorganic chemistry. Graded at 20%. (Due on Nov. 14, 2014 midnight as an e-mail attachment to both Profs. Asefa and Dismukes and late reports lose 20%).
Exams	Two exams. First and second half contents.
Grading Policy	There will be no make-up exams.

Exams (2)		2 x 30%
Literature review using the Scientific Method		2 x 10%
Attendance + Pop-quizzes	(4 x 5)	20%
Total		100%

Academic Integrity: Cheating, plagiarism, and academic dishonesty

Cheating and plagiarism will not be tolerated. Students caught cheating will fail the assignment (get 0 point on the specific assignment). University policy on academic dishonesty will be followed, and the student(s) will be referred to the appropriate university office for disciplinary action. A letter will be sent explaining the punishment to the Office of Student Conduct and Student Affairs in the Offices of the Dean of Students. If you have further complaints regarding the failed assignment and the letter, you must contact the Offices of the Dean of Students directly. Each student must turn in or present his or her own work. Copying is considered cheating and will be treated as stated above, with 0 points given for the exam and a letter to the Offices of the Dean of Students. If you let someone copy your exam and quiz from you, you will have 50% deduction from your grade and a letter sent to the Offices of the Dean of Students and persons in charge in your college describing these.

We will require students involved in this class to include the following statement in each literature review report using scientific methods that they write and submit for this course.

"*I certify that this assignment represents my own work. I have not used any unauthorized or unacknowledged assistance or sources in completing it including free or commercial systems or services offered on the internet or text generating systems embedded into software*."

New Rutgers Academic Integrity Policy & Procedures

The university academic integrity rules apply to students taking this course; see https://nbprovost.rutgers.edu/academic-integrity-students Students are *obligated* to tell the instructor if violation of academic integrity is observed. Communicating in any manner (texting etc.) during a quiz or exam will be treated as a violation of the honor code.

Lecture Etiquette

Please silence all pagers and cell phones prior to the start of lecture. If you come in late and lecture has already begun, please take a seat at the end of a row (and preferably near the back of the lecture hall) as a courtesy to those already seated, as coming into and going out of the lecture room during class is disruptive.

(Tentative Schedule, Fall 2024)

(Subject to minor changes depending on the discussion times some lectures may take due to additional explanation in class they may need or by popular request of students).

Class	Date	Ch. M&T or other	Topics
1	Sep 5	Literature	The Scientific Method
2	Sep. 9	2	Atomic Structure
3	Sep. 12	3	Simple Bonding Theory
4	Sep. 16	5	Molecular Orbitals (MO) and MO Diagrams
5	Sep. 19	Literature	X-Ray Photoemission Spectroscopy (XPS) and Energy Band Structure
6	Sep. 23	7	Crystalline Solid State and Solid-State Chemistry
7	Sep. 26	7 + Literature	Crystalline Solids, Solid-State Chemistry, and Effects of Doping
8	Sep. 30	Literature	Inorganic Nanocrystals and their Properties and Applications
9	Oct. 3	8	Main Group Chemistry
10	Oct. 7	8 + Literature	Main Group Chemistry (*Continued*) + Organometallic Chemistry: Introduction
11	Oct. 10	13 + Literature	Organometallic Chemistry: Synthesis
12	Oct. 14	13	Organometallic Chemistry: Properties
13	Oct. 17	15	Parallels Between Main Group and Organometallic Chemistry
14	Oct. 21	16	Inorganic Materials Chemistry
15	**Oct. 24**	**Lectures 1-12**	**Exam 1, lectures 2-14**
16	Oct. 28	10	TM Bonding
17	Oct. 31	10	TM Bonding σ-, π-, δ- Bonding Effects
18	Nov. 4	11	Many Electron States, Tanabe–Sugano Diagrams
19	Nov. 7	11	Electronic Spectroscopy Correlation Diagrams, Selection Rules
20	Nov. 11	12	TM Reactions & Mechanisms
21	Nov.14	12	TM Reactions & Mechanisms
22	Nov. 18	TBD	Magnetism & Electron Paramagnetic Spectroscopy
23	Nov. 21	TBD	Magnetism & Electron Paramagnetic Spectroscopy
24	Nov. 25	TBD	DFT and HF Computational Methods for Electronic States
25*	Nov. 26*	TBD	DFT and HF Computational Methods for Electronic States

	Nov. 28		*– No Class - Thanksgiving*
26	Dec. 2	Ertl & Samorjai	Heterogeneous Catalysis & Surface Science
27	Dec. 5	Bockris & Shao-Horn	Electro-catalysis
28	Dec. 9	**Exam 2**	**Covering lectures 16-27**
	Dec. 11		*Regular classes end*

* Thursday classes given on this date (as per RU policy)

+ indicates supplemental readings to be distributed in advance (Study Guides)
Other assigned readings to be covered in class:

Scientific methods readings:

Reading assignment:
http://teacher.pas.rochester.edu/phy_labs/appendixe/appendixe.html
This is a condensation of
Wilson, E. Bright. An Introduction to Scientific Research (McGraw-Hill, 1952). Available from Dover publications. https://store.doverpublications.com/products/9780486665450

Wilfred F. van Gunsteren, The Seven Sins in Academic Behavior in the Natural Sciences, Angew, Angew. Chem. Int. Ed. Volume 52, Issue 1, 3 DEC 2012. https://doi.org/10.1002/anie.201204076

VB, MO, XPS, and electronic structures readings:

Albert Haim, The Relative Energies of Molecular Orbitals for Second-Row Homonuclear Diatomic Molecules: The Effect of s-p Mixing, J. Chem. Educ.1991, 68, 737-738.

Fei Luo, George C. McBane, Geunsik Kim, Clayton F. Giese, W. Ronald Gentry, The Weakest Bond: Experimental Observation of Helium Dimer, J. Chem. Phys. 1993, 98, 3564-3567.

Yong-Feng Hu, G. Michael Bancroft, Zhifeng Liu, and Kim H. Tan, Comprehensive High Resolution Photoelectron Spectra of Metal Carbonyls Using Synchrotron Radiation, Inorg. Chem. 1995,34, 3716-3723.

Emil Roduner, Size Matters: Why Nanomaterials are Different? Chem. Soc. Rev., 2006, 35, 583-592.

Rongchao Jin, Quantum Sized, Thiolate-Protected Gold Nanoclusters, Nanoscale, 2010, 2, 343-362.

Xiaorong Li, G. Michael Bancroft, Richard J. Puddephatt, Yong-Feng Hu, Kim H. Tan, Variable-Energy Photoelectron Spectroscopy of $CpM(CO)_2$ (M = Co, Rh, Ir): Molecular Orbital Assignments and an Evaluation of the Difference in Ground-State Orbital Characters, Organometallics 1996, 15, 2890-2904.

Pekka Pyykko, Understanding the Eighteen-Electron Rule, J. Organometal. Chem., 2006, 691, 4336–4340.

C. C. Chusuei, M. A. Brookshier, and D. W. Goodman, Correlation of Relative X-ray Photoelectron Spectroscopy: Shake-up Intensity with CuO Particle Size, Langmuir 1999, 15, 2806-2808.

DFT vs MO methods:

G. Zhang and C. Musgrave, Comparison of DFT Methods for Molecular Orbital Eigenvalue Calculations. (2007) The Journal of Physical Chemistry A 111(8):1554-61.DOI:10.1021/jp061633o

Catalysis readings:

Gerhard Ertl, Reactions at Surfaces: From Atoms to Complexity(Nobel Lecture)
Angew Chemie, 2008; DOI: 10.1002/anie.200800480

Gabor A. Somorjai and Yimin Li, Impact of surface chemistry,
www.pnas.org/cgi/doi/10.1073/pnas.1006669107

Electrocatalysis readings:

J. O'M Bockris,A Primer on Electrocatalysis, *J. Serb. Chem. Soc. 70* (3) 475–487 (2005)

Jin Suntivich, Kevin J. May, Hubert A. Gasteiger, John B. Goodenough, Yang Shao-Horn. A Perovskite Oxide Optimized for Oxygen Evolution Catalysis from Molecular Orbital Principles ,*Science 9 December 2011: Vol. 334 no. 6061 pp. 1383-1385 ; DOI: 10.1126/science.1212858 ; read* Article + supporting material + this Perspective article:

A Vojvodic, J K Nørskov, On Discovering descriptors for catalyst performance. *Science* 2011;334:1355-1356.