

CHEM 5361/6361, Fall 2023

Advanced Inorganic Chemistry – Materials for Contemporary Research

Dr. Harish Banda, hbanda1@utep.edu

Department of Chemistry, University of Texas, El Paso

Class Details:

Days and times: Tuesday and Thursday, 10:30 – 11:50 AM
Location: CCSB 1.0204
Office: CCSB 2.0412
Office hours: Fridays 1:00 – 2:00 PM and by appointment
Course deadlines: <https://www.utep.edu/student-affairs/registrar/Academic%20Calendars/academic-calendar.html>

Email is the best way to reach the instructor. Please allow 24 hours for response, and then send a polite reminder.

Class Overview:

Principles of molecular structures of inorganic compounds; Molecular orbital theory and coordination chemistry; Emergence of metal organic frameworks and their properties; Applications of metal organic frameworks in problems related to areas of energy, water, and health

Learning Objectives:

This course is intended to develop students' understanding on the fundamentals and recent advances in inorganic chemistry. After mastering fundamentals, students will spend a significant part of the course in familiarizing themselves and learning about an emerging class of materials termed metal-organic frameworks. Students will identify societal and scientific problems in broad areas of energy, water, and health and discuss research related to the targeted design of materials for solutions.

This graduate level course is intended to develop students' aptitude in identifying research problems, analyzing reported literature, and presenting them to a knowledgeable audience. Students are expected to develop critical skills that can be applied toward their graduate thesis work.

Textbook & Supplemental Texts:

1. Inorganic Chemistry, Miessler & Tarr, 5th/6th edition
2. Inorganic Chemistry, Shriver & Atkins
3. Inorganic Chemistry - Principles of Structure and Reactivity, James E. Huheey, Ellen A. Keiter, Richard L. Keiter and Okhil K. Medhi
4. Introduction to Reticular Chemistry, Omar M. Yaghi

All class materials will be posted on Blackboard within 48 hours after each class.

Class materials and the discussed research articles are sufficient to score well in this course.

Syllabus Change Policy

This syllabus is a guide for the course and is subject to change without advance notice.

Class schedule:

Topics and their order of discussions are subject to change, but are likely to include:

Class	Date	General Topic	Lecture/Presentations Topic
1	08/29		Overview, syllabus, objectives, outcomes
2	08/31	Atoms and orbitals	Atom, History, Atomic orbitals, Quantum numbers,
3	09/05		Orbitals, electronic configuration, Slater's rules,
4	09/07	Molecules and bonding	Molecules: Chemical bond, Lewis Structures, VSEPR
5	09/12		MO Theory-1 Diatomic molecules
6	09/14		MO Theory-2 Multiatomic molecules
7	09/19	Acids & bases	Acids and bases – Models – Lewis's concept
8	09/21		Acids and bases – Metal acidity & Strength
9	09/26	Coordination compounds	Coordination chemistry – Intro, Geometries, Isomers
10	09/28		Coordination chemistry – Electronic structure/theories
11	10/03		Coordination chemistry – Ligand field, Jahn-Teller
12	10/05		Mid-term exam
13	10/10	Metal Organic Frameworks (MOFs)	Emergence of Metal Organic frameworks
14	10/12		Determination & Design of Porosity, Basics of gas sorption
15	10/17		Building units of MOFs & Functionalization
16	10/19	Articles on using porosity Presentation-1	Bio-mimetic & exotic active species (NO, O-O)
17	10/24		Catalysis, Liquid and gas-phase separations
18	10/26		Analytical chemistry – Extraction, purification
19	10/31		Capture of CO ₂ , NH ₃ , Hydrogen, Methane, VOCs
20	11/02		Water sorption – Harvesting
21	11/07		Water sorption – Heat pumps
22	11/09	2D MOFs	Conducting MOFs, polymers - Structure vs. property
23	11/14	Articles on using conductivity Presentation-2	Ways of enhancing conductivity
24	11/16		Chemiresistive sensing
25	11/21		Energy Storage, EDLC, Redox properties
26	11/28		Electrocatalysis, Water & CO ₂ reduction
27	11/30		Mixed conduction of ions and electrons
28	12/05		Final Exam
29	12/07		Last Day of Class

Grading Scheme:

Exams	Mid-term	20
	Finals	20
Class presentations	Presentation-1	20
	Presentation-2	20
Other activities	Class participation	20
	Assignments	
Total		100

Your grade in the course is based on your performance in the two exams, two presentations you will make, and the activities listed above. No additional work will be assigned for extra credit.

Mid-term (20 points): This exam will be entirely based on topics covered in classes 2 – 11.

Final exam (20 points): This exam will be entirely based on the research articles discussed in the second half of the semester.

Guidelines for class presentations (40 points):

In the second half of the semester, all students are expected to make two presentations based on contemporary research articles on Metal Organic Frameworks. Students will make one presentation related to an area of their research interest and another presentation on research unrelated to their current interests. Selection of the articles for both presentations will be made during one-on-one office hours and from a list of articles compiled by Dr. Banda. Both presentations, while giving a captivating understanding of the problem and research discussed, **must include elements** that clearly address the following questions;

What is the problem of interest?

What are the materials that are typically used to address this problem?

What fundamental merits can MOFs offer over previous materials in solving the problem?

What specific chemical features of MOF (structure/property/coordination) are being exploited?

If other MOFs were previously studied, how did this study make an improvement? (Presenters should talk briefly about at least one more paper related to this work)

Other activities (20 points):

Other activities in and outside the class can include surprise quizzes, assignments, and structured discussions in the class. All assignments, that will be in the form of written summaries/comments related to the research articles, will be collected at the beginning of class on the day they are due. Student audience is expected to participate and contribute extensively to the presentation and discussion of research articles.

Class policies:

Late assignments:

Assignments will be collected at the beginning of the class on the day they are due. Any assignments turned in beyond this point will be considered later and will receive a 20% deduction. An additional 20% will be deducted for each day the assignment is overdue. Late assignments will not be accepted 3 days past their due date.

Community Agreement

The expectation in this course is that learners participate in course activities and discussions with mutual respect. Participation in this course—whether as an individual or within team-based activities—will be expected to follow our mutually-agreed framework for how we would like to be treated by one another in this course. Examples of my expectations would be offering undivided attention to the person speaking, claiming, and distinguishing our opinions, sensitivity to sociocultural context, and disagreement without disrespect. Use of electronic devices is strictly limited to in-class activities.

Absences

Attendance in every class is expected and after 2 unexcused absences you will be asked to meet with Dr. Banda. After the 4th unexcused absence, you may be dropped from the course. If your absence is necessary, please contact Dr. Banda ahead of time to discuss. If you are late arriving to an in-person lecture, please enter quietly so as not to disturb others; any missed class engagement points are not available to make up.

Missing exams:

In circumstances where you miss the *mid-term exam*, evaluation of your case and qualification for a make-up exam will be made at my discretion. It is your responsibility to contact me at the email address listed above to schedule a re-take within 3 days of the original exam date. Otherwise, a failing grade of 0 will be automatically assigned. In any case, a valid and documented excuse must be provided (e.g., medical emergency). The make-up exam may mirror the original exam, be slightly altered, or altogether changes in form, format, and content at my discretion.

I will *not give make-up exam for the final exam*, but I will consider allowing students to take the exam early on a case-by-case basis, provided there is a legitimate reason.

Accommodations policy

Students requesting an accommodation based on a disability must register with the [UTEP Center for Accommodations and Support Services](#) (CASS). Contact the Center for Accommodations and Support Services at 915-747-5148, or email them at cass@utep.edu, or apply for accommodations online via the [CASS portal](#).

Scholastic integrity

Academic dishonesty is prohibited and is considered a violation of the UTEP Handbook of Operating Procedures. Any act of academic dishonesty attempted by a UTEP student is unacceptable and will not be tolerated. To learn more, please visit [HOOP: Student Conduct and Discipline](#). Technology resources at [Help Desk](#) and academic resources at [UTEP Library](#) available.