Advanced Physical Chemistry I

CHEM 5351/ 6351 (CRN: 16714/16715)

Fall 2024

Instructor:

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Office hours: Fridays 10:00 am to 12:00 pm *(prior appointment is necessary)*

I. Textbook: No textbook is required for this course. Homework, related literature, and additional activities will be posted on the course Blackboard site.

II. Course Objectives:

a. Develop a comprehensive understanding of the historical development, significance, and advanced physical chemistry principles underlying Metal-Organic Frameworks (MOFs).
b. Acquire in-depth knowledge of coordination chemistry, reticular chemistry, crystal symmetry, and the thermodynamic and kinetic principles governing the synthesis and stability of MOFs.
c. Master the physical basis of various advanced characterization techniques to analyze the chemical and physical properties of MOFs and interpret the insights these techniques provide regarding structure-function relationships.
d. Survey the diverse applications of MOFs in catalysis, gas storage, sensing, environmental remediation, energy storage, etc., and explore their application in electrochemical energy conversion technologies in detail, focusing on understanding their functional properties and potential for innovation in these fields.

III. Course Description:

- This course is designed to provide a comprehensive understanding of MOFs through an interactive classroom.
- We will explore the foundations of MOFs, including their historical development, significance, and the fundamental physical chemistry principles that underpin their structure and function.
- Characterization techniques and theoretical approaches, including X-ray diffraction, spectroscopy, thermal analysis, microscopy, and density functional theory (DFT), will be covered to thoroughly understand the forefront activities in MOF research.
- The course will discuss the potential applications of MOFs in diverse fields.
- In-class and homework assignments will be given to reinforce understanding and ensure students are prepared for the lecture contents.
- Students will be required to give oral presentations to familiarize themselves with the latest literature.

- The mid-term and final exams will assess your ability to assimilate the information provided in the course and apply it to contemporary research and applications in MOF.
- Attendance and active participation in class will count towards your final grade, highlighting the importance of engagement in all class activities.

IV. Course Evaluation:

You will be evaluated based on your overall grasp of the skills, concepts, and participation. Your overall grades will depend on:

Grade Breakdown

Grade % **100 -------- 88 ------- 78 ------ 68 ------- 58 ----- 0**
A B C D F

AssessmentItems	Points Percent
a) Assignments	15 %
b) Oral presentations	25 %
c) Mid-Term Exam	20 %
d) Final Exam	30 %
e) Attendance	5 %
f) In-class participation	5%

a) **Assignments (on Blackboard or In-Class)-** Assignments will be available on Blackboard or distributed during class sessions. These assignments are designed to test your understanding of specific content covered in the lectures. You are expected to submit your completed assignments on Blackboard by the specified due date. No late submissions will be accepted, and if a late submission is accepted, grade points will be adjusted at the instructor's discretion.

b) **Oral presentations:** The instructor will select a set of papers, which will be assigned randomly to each group. Each group will be expected to critically analyze their assigned paper, highlighting key findings, methodologies, and potential implications for the field. Presentations will be 15-20 minutes long, followed by a round of questions and discussion. All students are expected to actively participate in both the preparation and delivery of the presentation, and each group member should be fully knowledgeable about the entire content, even if they are not presenting a specific section. This will be a peer-reviewed session where your classmates will also contribute to the scoring. More details about the presentation organization and group assignments will be provided in class.

c) **Mid-Term Exam**: The mid-term exam will cover content from Module 1 and Module 2. It will assess your understanding of MOFs' foundational principles and

characterization techniques. More details about the exam format and topics will be provided in class.

d) **Final Exam:** The final exam will cover all the content from the entire course and will comprehensively test your knowledge. However, at least 75% of the questions will focus on topics covered after the midterm. The exam will include fundamental questions and practical assessments to ensure a thorough understanding of the material. More details about the exam format and topics will be provided in class.

e) **Attendance:** Attendance is crucial and will count towards your final grade.

f) **In-class participation:** Active participation and engagement in all class activities, including lectures, presentations, and assignments, are essential for success in this course.

V. Course Policies:

- **Minor modifications to the syllabus and calendar** could be made during the semester. The instructor will inform the student about any change by announcing it in class and on the Blackboard course site. However, ***it is the student's responsibility to attend class and/or check the course site to keep up to date with any information provided to him/her and to use it responsibly***.

- **Academic honesty:** Materials (assignments, quizzes, exams, or otherwise) submitted to fulfill academic requirements must represent a student's own efforts. Any academic dishonesty attempted by a UTEP student is unacceptable and will not be tolerated.Academic dishonesty is prohibited and is considered a violation of the UTEP Handbook ofOperating Procedures. It includes, but is not limited to, cheating, plagiarism, and collusion.Violations will be taken seriously and referred to the Dean of Students Office for possible disciplinary action. Students may be suspended or expelled from UTEP for such actions.

- **Incomplete Grade Policy:** Incomplete grades may be requested only in exceptional circumstances after you have completed at least half of the course requirements. Talk to the instructors immediately if you believe an incomplete is warranted. If granted, we will establish a contract to complete the work with deadlines.

- **Accommodations Policy:** The University is committed to providing reasonable accommodations and auxiliary services to students, staff, faculty, job applicants, applicants for admissions, and other beneficiaries of University programs, services, and activities with documented disabilities in order to provide them with equal opportunities to participate in programs, services, and activities in compliance with sections 503 and 504 of the Rehabilitation Act of

1973, as amended, and the Americans with Disabilities Act (ADA) of 1990 and the Americans with Disabilities Act Amendments Act (ADAAA) of 2008. Reasonable accommodations will be made unless it is determined that doing so would cause undue hardship on the University. 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, email them at cass@utep.edu, or apply for accommodations online via the CASS portal.

- **Guidance on Artificial Intelligence:** The use of generative AI tools such as Chat GPT is permitted in this course for the following activities, which must be noted or cited:
  - Language correction
  - Grammar check

  However, you may not use AI tools to complete the following activities:
  - Write a part or the entire assignment.
  - Find ideas or anything that is not mentioned above.

  Students must cite any borrowed content sources to comply with all applicable citation guidelines, copyright law, and avoid plagiarism. Instances that violate these guidelines will be referred to the Office of Student Conduct and Conflict Resolution.

  **** AI detection software may be used, and grades will be adjusted accordingly.***

VI. Course Withdrawal Policy

Classes dropped before the official census date **(09/11/2024)** will be deleted from the student's semester record. After this date, the University permits any student to drop with an automatic "W" by the course dropping deadline **(11/01/2024).** After this date, students who withdraw must receive an "F" grade.

VII. Course Calendar:

The content is tentative and subject to change. Any changes will be announced in advance.

Week		Date	Lecture/Presentations Topic
1.		08/26	Overview, syllabus, objectives, outcomes
	Module 1: Foundations of MOFs	08/28	Introduction to MOFs - Historical Development, Significance, and Fundamental Physical Chemistry Principles
2.		**09/02**	**Labor day**
		09/04	Building and Designing MOFs: Coordination Chemistry, Reticular Chemistry, and Crystal Engineering

3.		09/09	Synthesis and Properties of MOFs: Thermodynamic and Kinetic Principles in Conventional and Advanced Methods. Conductivity, Band Gap, Adsorption, Functionalization, Magnetism, etc.
		09/11	**Students Presentation**
4.		**09/16**	
	Module 2: Characterization Techniques	09/18	Characterization Techniques for MOFs: XRD, XPS, XAS, FTIR, and UV-Vis for Chemical Composition Analysis.
5.		09/23	Surface Measurements and Microscopic Techniques: TGA, DSC, BET, BJH, SEM, STEM, and TEM Methods with Thermodynamic Context
		09/25	Advanced Microscopy Techniques and Spectroscopic Characterization for MOF - AFM, KPFM STM, NMR, EPR, and Quantum Chemistry Concepts
6.		09/30	Reserved for Schedule Adjustments
		10/02	**Students Presentation**
7.		**10/07**	
		10/09	**Mid-term exam**
8.	**Module 3: Theoretical and Computational Chemistry**	10/14	Introduction to Density Functional Theory (DFT) for MOFs
		10/16	Setting Up DFT Calculations for MOFs
9.		10/21	Geometry Optimization for Gas Separation in MOFs
		10/23	Geometry Optimization for Catalysis in MOFs
10.		10/28	Electronic Density of States (DOS) for MOFs
		10/30	Case Studies: Catalysis in MOFs
11.		11/04	Case Studies: Gas Separation in MOFs
		11/06	Combining DFT Results with Experimental Data
12.		11/11	MOFs for Gas Storage and Separation: Thermodynamic and Kinetic Aspects of Hydrogen, Methane, and Carbon Dioxide Storage
	Module 4: Applications and Functional Properties	11/13	Sensing Applications of MOFs: Chemical and Biosensors, Surface Chemistry, and Signal Transduction
13.		11/18	Environmental Applications of MOFs: Water Purification, Pollutant Removal, and Green Chemistry Principles
		11/20	Photocatalytic Applications of MOFs: Mechanisms, Properties, and Practical Uses in Solar Cells
14.		11/25	Energy-related Applications of MOFs: Batteries, Supercapacitors, Fuel Cells, and Electrochemical Energy Storage and Conversion
		11/27	Quantum Science in MOFs: Qubits, Information Storage and Transmission, and Supercomputers
15.		**12/02**	**Students Presentation**
		12/04	
16.		**12/09**	Reserved for Schedule Adjustments
		12/11	**Final Exam**