



PHYS 6/8540: Structure, Defects, and Diffusion CHEM 4/6/8810: Materials Science 1

The University of Toledo
College of Natural Sciences and Mathematics
PHYS 6540 – 001 CRN 40844
PHYS 8540 – 001 CRN 40847
CHEM 4810 – 001 CRN 47569
CHEM 6810 – 001 CRN 40845
CHEM 8810 – 001 CRN 40846

Instructor:	Nikolas Podraza	Offered:	Fall 2021
Email:	Nikolas.Podraza@utoledo.edu <i>(Email is Preferred Means of Communication)</i>	Course Website:	https://blackboard.utdl.edu/
Office Hours:	Tuesday 2:00-4:00 PM (R1) Wednesday 2:00-4:00 PM (R1) Thursday 2:00-4:00 PM (MH)	Class Location:	Health Sciences and Human Services (HH) Room 3318 Also See Teaching Methodology and Course Location Below
Office Location:	McMaster Hall (MH) Room 4023 R1 Room 2100E	Class Day/Time:	Tuesday and Thursday 10:00-11:50 AM
Instructor Phone:	419 530 4905	Credit Hours:	4

SPECIAL COURSE EXPECTATIONS DURING COVID-19

Maintaining a safe campus during the ongoing COVID-19 pandemic remains a top priority. UToledo continues to follow the guidance of the U.S. Centers for Disease Control and Prevention and Ohio Department of Health to keep our campus safe.

ATTENDANCE

The University of Toledo has a missed class policy. It is important that students and instructors discuss attendance requirements for the course. Before coming to campus each day, students should take their temperature and complete a self-assessment for symptoms of COVID-19, such as cough, chills, fatigue or shortness of breath. Anyone with a temperature at or above 100.0 degrees Fahrenheit or who is experiencing symptoms consistent with COVID-19 should not come to campus and contact their primary care physician or the University Health Center at 419.530.5549. For more information on the symptoms of COVID-19, please go to <https://www.cdc.gov/coronavirus/2019-ncov/symptoms-testing/symptoms.html>

COVID-19 testing for sick students is available on both Main Campus and Health Science Campus. Call 419.383.4545 for an appointment. Absences due to COVID-19 quarantine or isolation requirements are considered excused absences. Students should notify their instructors and follow the protocols summarized in this document on [Navigating COVID-Related Course Concerns](#).

In the event that you have tested positive for COVID-19 or have been diagnosed as a probable case, please review the [CDC guidance](#) on self-isolation and symptom monitoring, and report the disclosure to the Division of Student Affairs by emailing StudentAffairs@utoledo.edu or by connecting with their on-call representative at 419.343.9946. Disclosure is voluntary and will only be shared on a need to know basis with staff such as in the Office of Student Advocacy and Support, The Office of Residence Life, and/or the Office of Accessibility and Disability Resources to coordinate supportive measures and meet contact tracing requirements.



FACE COVERINGS

Face coverings are required while on campus, except while eating, alone in an enclosed space, or outdoors practicing social distancing. Students will not be permitted in class without a face covering. If you have a medical reason preventing you from wearing a face covering due to a health condition deemed high-risk by the CDC, submit an [online application](#) to request an accommodation through the Office of Accessibility and Disability Resources. Students will need to provide documentation that verifies their health condition or disability and supports the need for accommodations. Students already affiliated with the Office of Accessibility and Disability Resources who would like to request additional accommodations due to the impact of COVID-19, should contact their accessibility specialist to discuss their specific needs. You may connect with the office by calling 419.530.4981 or sending an email to StudentDisability@utoledo.edu.

VACCINATION

Doctors and other health care professionals agree that the best way to protect ourselves and each other is to get vaccinated. Case data clearly show that vaccines remain highly effective at preventing serious illness from COVID, including the highly contagious delta variant. If you have not yet received your COVID vaccine, the University encourages you do so as soon as possible. No appointment is needed to get the shot at the UTM Outpatient Pharmacy, University Health Clinic or Main Campus Pharmacy. Once you receive the COVID vaccination, please register on the COVID Vaccine Registry site at: <https://utvaccinereg.utoledo.edu/>.

SPECIAL NOTES

It's important to note, that based on the unpredictability of the COVID-19 virus, things can change at any time. So please be patient and understanding as we move through the semester. I also ask that you keep me informed of concerns you may have about class, completing course work/assignments timely and/or health concerns related to COVID.

CATALOG/COURSE DESCRIPTION

A generic materials science approach to the study of crystalline structure and defects (point, line and planar) in crystalline materials. The mechanisms and kinetics of diffusion in the condensed state.

COURSE OVERVIEW

Survey of topics relevant to Materials Science. This course is the first in a two semester sequence surveying topics in materials science for undergraduate (CHEM 4810) and graduate (CHEM 6180, CHEM 8810, PHYS 6540, PHYS 8540) students in physics, chemistry, or related fields.

Topical Outline:

- 1) Interatomic Bonding
- 2) Crystallography
- 3) Crystal Structures
- 4) Structure Determination
- 5) Structural Disorder
- 6) Point Defects
- 7) Line Defects
- 8) Planar Defects
- 9) The Effects of Defects on Structural, Electrical, and Optical Properties
- 10) Fundamental Equations of Diffusion
- 11) Mechanisms of Diffusion
- 12) Kinetics of Diffusive Processes
- 13) Structure Sensitive Diffusion Processes
- 14) Surface Diffusion
- 15) Experimental Methods

Assume about 1/3 of the semester for topics 1-5, 1/3 for topics 6-9, and 1/3 for 10-15.



TEACHING METHODOLOGY AND COURSE LOCATION

Teaching Methodology: Course notes, pre-recorded lectures, and recommended reading materials are available via Blackboard. To access the course content, log into Blackboard. Course notes (PDF format, no audio), recommended reading materials, and exam review materials for each part of the course can be accessed by going to “start here” for the course. Course notes with audio (PPTX format) can be accessed by going to “Lecture Capture (Echo360)” then “Echo 360.” Students are expected to review the course notes and / or pre-recorded lectures prior to the corresponding regularly assigned class time (10:00-11:50 AM, Tuesdays and Thursdays). During the regularly assigned class time, we will discuss questions contained within the course notes and any other questions generated during your review of the lecture material. The homework problem corresponding to a given lecture will be due before 5:00 PM the day following the regularly assigned class time. Students are strongly encouraged to ask questions during the regularly assigned class time and during office hour appointments. Engaging in discussion of the course material is vital in preparation for the exams. The exams will be oral and recorded with the exam grade based on your demonstrated understanding of the topics covered on that exam.

Course Location: Room 3318 Health Science and Human Services (HH) Building during regular class time, 10:00-11:50 AM on Tuesdays and Thursdays. Since the primary use of the scheduled class time is to discuss the course material, sometimes we will have class outdoors when the weather is favorable. For outdoor classes, a map will be emailed before 5:00 PM on the day prior to the scheduled class meeting. If you receive no email, assume classes will be inside in 3318 HH.

STUDENT LEARNING OUTCOMES

The students will learn about the structure of condensed matter systems, the defects present in real materials, and how impurities can diffuse within condensed matter.

PREREQUISITES AND COREQUISITES

For PHYS 6540, PHYS 8540, CHEM 6810, and CHEM 8810 the student must be enrolled in a graduate program.

TEXTS AND ANCILLARY MATERIALS

There is no required text. Course notes, pre-recorded lectures, and recommended reading materials are provided on Blackboard via <https://blackboard.utdl.edu/> or the myUT portal at <https://myut.utoledo.edu/>. After entering the portal, click on Blackboard in the UT Online panel.

TECHNOLOGY REQUIREMENTS

Access to a computer and internet.

ACADEMIC POLICIES

[Undergraduate Policies: http://www.utoledo.edu/policies/academic/undergraduate/](http://www.utoledo.edu/policies/academic/undergraduate/)

[Graduate Policies: http://www.utoledo.edu/policies/academic/graduate/](http://www.utoledo.edu/policies/academic/graduate/)

COURSE EXPECTATIONS

Attendance and Participation: You are expected to attend regularly assigned classes, read or review any required materials prior to class, and participate in discussions. You are highly encouraged to consider how the topic matter applies to your own areas of interest. All regularly assigned class times and corresponding lecture discussion topics are noted on the Tentative Schedule at the end of this syllabus. Specific pre-class topics are noted for the given lecture.

Before Each Lecture: You should read through the course notes provided for that lecture and / or listen to the pre-recorded presentation for that lecture. You may also wish to review the recommended reading for each of the



topics provided. If there is a specific pre-class topic listed, for example: "Identify the crystal structure of a material of your own interest," please be ready to discuss it during class.

During Each Lecture: You should participate in the discussion. Any questions you have about the topic in general or how it relates to materials of your interest are welcome and will likely benefit your and your classmates' understanding for the exams.

After Each Lecture: You will complete the homework problem corresponding to the lecture. These problems are designed to take about 10 minutes, used to test your understanding of the material, and due by 5:00 PM on the day following class.

Office Hours: I will be available from 2:00-4:00 PM on Tuesdays and Wednesdays in R1 and 2:00-4:00 PM on Thursdays in McMaster Hall (MH). These are normally "open" times where you can come by to ask any questions. You can schedule an appointment within these times or others throughout the week to ensure my availability via email. I am also available to meet via teleconferencing. If you make an appointment with me, please suggest three time windows in which you are available so that we can find an option which fits both our schedules.

Participation and Your Grade: There are 12 weeks of lecture classes (not counting Thanksgiving week) and 3 weeks of exams throughout the semester. If I see you at least once during each of those 12 weeks of lecture classes either (1) in class, (2) in office hours, or (3) in a separate teleconference equivalent to an office hour visit, you will earn 0.5 points per week up to a maximum of 5 points contributing to your final grade (equivalent to the 5% of your final grade). If you are present at least once for at least 10 of those 12 weeks, you will earn the full points for attendance. Attending less than 10 of the 12 weeks will reduce your maximum obtainable grade.

Homework Problems: At the end of Lectures 1 through 22, there is a problem. You should spend about 10 minutes addressing this problem and email me your answer no later than 5:00 PM the day following the corresponding regularly assigned class. All homework problem due dates are noted on the Tentative Schedule at the end of this syllabus. There are 22 homework problems, one corresponding to each lecture (excluding Lecture 0) throughout the semester. You will be responsible for emailing me your response to those problems by 5:00 PM on the day following the lecture class. The subject lines of your emails should state: "Problem, Lecture X," where "X" is the lecture number. Answers are expected to be brief. If you were to write your answer it should be no more than the size of a 3 inch by 5 inch index card. Problems will be graded and assigned a point value of 1 or 0, with 1 indicating an answer that is correct or demonstrated substantive understanding (even if not correct). Each homework problem should take less than 10 minutes to complete. You will earn 1 point for each successfully answered problem up to a maximum of 20 points contributing to your final grade (equivalent to the 20% of your final grade). If you answer at least 20 of those 22 problems satisfactorily, you will earn the full points for homework problems. Answering less than 20 of the 22 problems will reduce your maximum obtainable grade.

Exam Review Days: Prior to each exam, we will have a review day during the assigned in class time. The dates will be 9/28 for Exam 1 (Structure: Interatomic Bonding, Crystallography, Crystal Structures, Diffraction; Lectures 1-8), 10/28 for Exam 2 (Defects: Point, Line, and Plane Defects; Impact on Properties; Lectures 9-14), and 12/9 for Exam 3 (Diffusion: Drift and Diffusion, Mechanisms, Characterization; Lectures 15-22). During these review days, you should ask any questions you have on the course material covered in that exam. We will also review pertinent homework problems and related questions relevant to the exam material. Students may be assigned a problem to present/review to the class and give their explanation to start the class discussion on the topic.

Exams: Each exam will be oral, by teleconferencing, and recorded. The exams will last 30 minutes, and we will discuss questions relevant to the topic matter of that exam. A week prior to each exam, I will assign each of you an example material which we will discuss as part of the content of your oral exam. You do not need to perform outside research on this material, but you may want to consider how the course topics may apply to it. Your exam time will be scheduled two weeks prior to the exam days noted on the Tentative Schedule at the end of this syllabus. The two exams on which you earn your highest grade will be weighted equally and contribute to 30% of your final grade each



(30% for highest exam + 30% for second highest exam). The exam with the lowest score will be weighted half the value of the other two and only contribute 15% to your final grade. Combined, all three exam scores will be account for 75% of your final grade.

OVERVIEW OF COURSE GRADE ASSIGNMENT

Grades will be based on homework problems, three exams, and attendance weighted as:

Participation:	5%
Homework Problems:	20%
Highest Exam Score:	30%
Second Highest Exam Score:	30%
Third Highest Exam Score:	15%

Participation: There are 12 weeks of lecture classes (not counting Thanksgiving Week) and 3 weeks of exams throughout the semester. If I see you at least once during each of those 12 weeks of lecture classes either (1) in class, (2) in office hours, or (3) in a separate teleconference equivalent to an office hour visit, you will earn 0.5 points per week up to a maximum of 5 points contributing to your final grade (equivalent to the 5% of your final grade). If you are present at least once for at least 10 of those 12 weeks, you will earn the full points for attendance. Attending less than 10 of the 12 weeks will reduce your maximum obtainable grade.

Homework Problems: There are 22 homework problems, one corresponding to each lecture (excluding Lecture 0) throughout the semester. You will be responsible for emailing me your response to those problems by 5:00 PM on the day following the lecture class. The subject lines of your emails should state: "Problem, Lecture X," where "X" is the lecture number. Answers are expected to be brief. If you were to write your answer it should be no more than the size of a 3 inch by 5 inch index card. Problems will be graded and assigned a point value of 1 or 0, with 1 indicating an answer that is correct or demonstrated substantive understanding (even if not correct). Each homework problem should take less than 10 minutes to complete. You will earn 1 point for each successfully answered problem up to a maximum of 20 points contributing to your final grade (equivalent to the 20% of your final grade). If you answer at least 20 of those 22 problems satisfactorily, you will earn the full points for homework problems. Answering less than 20 of the 22 problems will reduce your maximum obtainable grade.

Exams: The two exams on which you earn your highest grade will be weighted equally and contribute to 30% of your final grade each (30% for highest exam + 30% for second highest exam). The exam with the lowest score will be weighted half the value of the other two and only contribute 15% to your final grade. Combined, all three exam scores will be account for 75% of your final grade.

Letter grade scale is:

A:	93-100%	C:	73-76%
A-:	90-92%	C-:	70-72%
B+:	87-89%	D+:	67-69%
B:	83-86%	D:	63-66%
B-:	80-82%	D-:	60-62%
C+:	77-79%	F:	0-59%

Midterm Grading

The university has set a midterm grade deadline of 10/24. Your midterm grades will be calculated based on attendance, homework problems, and exams up to that point weighted according to:

Participation (Weeks 1-7):	5%
Homework (Problems 1-12):	20%
Exam 1 Score:	75%



Note that only the final grading metric (below) accounts for all attendance, homework problems, and the three exams throughout the semester, therefore the midterm grade is only reflective of an estimation of performance up to 10/24.

Final Grading

At the end of the semester will be calculated according to:

Participation:	5%
Homework Problems:	20%
Highest Exam Score:	30%
Second Highest Exam Score:	30%
Third Highest Exam Score:	15%

UNIVERSITY POLICIES

Institutional Classroom Attendance Policy Please be aware that the university has implemented an attendance policy, which requires faculty to verify student participation in every class a student is registered at the start of each new semester/course. For this course, if you have not attended/participated in class (completed any course activities or assignments) within the first 14 days, I am required by federal law to report you as not attended. Unfortunately, not attending/participating in class impacts your eligibility to receive financial aid, so it is VERY important that you attend class and complete course work in these first two weeks. Please contact me as soon as possible to discuss options and/or possible accommodations if you have any difficulty completing assignments within the first two weeks.

Policy Statement on Non-Discrimination on the Basis of Disability (ADA) The University is an equal opportunity educational institution. Please read [The University's Policy Statement on Nondiscrimination on the Basis of Disability Americans with Disability Act Compliance](#). Students can find this policy along with other university policies listed by audience on the [University Policy webpage](#) (<http://www.utoledo.edu/policies/audience.html/#students>).

Academic Accommodations The University of Toledo embraces the inclusion of students with disabilities. We are committed to ensuring equal opportunity and seamless access for full participation in all courses. For students who have an Accommodations Memo from the Office of Accessibility and Disability Resources, I invite you to correspond with me as soon as possible so that we can communicate confidentially about implementing accommodations in this course.

For students who have not established accommodations with the Office of Accessibility and Disability Resources and are experiencing disability access barriers or are interested in a referral to health care resources for a potential disability, please connect with the office by calling 419.530.4981 or sending an email to StudentDisability@utoledo.edu.

ACADEMIC AND SUPPORT SERVICES

Please follow this link to view a comprehensive list of [Student Academic and Support Services](#) (<http://www.utoledo.edu/studentaffairs/departments.html>) available to you as a student.

SAFETY AND HEALTH SERVICES FOR UT STUDENTS

Please use the following link to view a comprehensive list [Campus Health and Safety Services](#) available to you as a student.

INCLUSIVE CLASSROOM STATEMENT

In this class, we will work together to develop a learning community that is inclusive and respectful. Our diversity may be reflected by differences in race, culture, age, religion, sexual orientation, gender identity/expression, socioeconomic background, and a myriad of other social identities and life experiences. We will encourage and



appreciate expressions of different ideas, opinions, and beliefs so that conversations and interactions that could potentially be divisive turn, instead, into opportunities for intellectual and personal development.



TENTATIVE COURSE SCHEDULE

Dates by topic and learning objective. Assessment methods (exams and homework problems) are listed.

Before 8/31: Lecture 0: Course Syllabus and Introduction—introduction to course objectives, format, and expectations.

Part 1: Structure (Lectures 1-8)

- 8/31: Lecture 1: Interatomic Bonding—bonding types and fundamentals.
Problem 1 due before 5:00 PM on 9/1.
- 9/2: Lecture 2: Interatomic Bonding—bonding types and fundamentals.
For Class: Identify and justify the bond types you suspect to be in a solid of your choice.
Problem 2 due before 5:00 PM on 9/3.
- 9/7: Lecture 3: Crystallography—lattice systems, point groups, space groups, symmetry.
For Class: Identify the Bravais Lattice for a solid of your choice.
Problem 3 due before 5:00 PM on 9/8.
- 9/9: Lecture 4: Crystallography—lattice systems, point groups, space groups, symmetry.
For Class: Identify the space group for a solid of your choice. Is it symmorphic?
Problem 4 due before 5:00 PM on 9/10.
- 9/14: Lecture 5: Crystal Structures —bases and common structure types.
For Class: Identify the crystal structure for a solid of your choice.
Problem 5 due before 5:00 PM on 9/15.
- 9/16: Lecture 6: Crystal Structures —bases and common structure types.
For Class: Determine the approximate packing density for a solid of your choice.
Problem 6 due before 5:00 PM on 9/17.
- 9/21: Lecture 7: Diffraction—characterization of crystal structures by diffraction methods.
For Class: For solid of your choice, what diffraction method is most used?
Problem 7 due before 5:00 PM on 9/22.
- 9/23: Lecture 8: Diffraction—characterization of crystal structures by diffraction methods.
For Class: For solid of your choice, what x-ray diffraction measurement is most used?
Problem 8 due before 5:00 PM on 9/24.
- 9/28: Exam 1 Review Day (Structure: Interatomic Bonding, Crystallography, Crystal Structures, Diffraction).
- 9/29-10/4: Exam 1 (Structure: Interatomic Bonding, Crystallography, Crystal Structures, Diffraction) exam times scheduled by appointment.

Part 2: Defects (Lectures 9-14)

- 10/5: Lecture 9: Point Defects—types and stability in crystal structures; impact on properties.
For Class: For solid of your choice, what point defects are most common?
Problem 9 due before 5:00 PM on 10/6.



- 10/7: Lecture 10: Point Defects—types and stability in crystal structures; impact on properties.
For Class: For solid of your choice, why may the defect concentration vary among samples?
Problem 10 due before 5:00 PM on 10/8.
- 10/12: Lecture 11: Line Defects—types and stability in crystal structures; impact on properties.
For Class: Identify a solid with line defects present.
Problem 11 due before 5:00 PM on 10/13.
- 10/14: Fall Break: No Class
- 10/19: Lecture 12: Line Defects—types and stability in crystal structures; impact on properties.
For Class: Identify a solid with planar faults likely to be present.
Problem 12 due before 5:00 PM on 10/20.
- 10/21: Lecture 13: Plane Defects—types and stability in crystal structures; impact on properties.
For Class: Identify a polycrystalline material with either larger or small grain boundaries.
Problem 13 due before 5:00 PM on 10/22.
- 10/26: Lecture 14: Plane Defects—types and stability in crystal structures; impact on properties.
For Class: For your polycrystalline material, what are the interface coherencies and energetics like?
Problem 14 due before 5:00 PM on 10/27.
- 10/28: Exam 2 Review Day (Defects: Point, Line, and Plane Defects; Impact on Properties).
- 10/29-11/3: Exam 2 (Defects: Point, Line, and Plane Defects; Impact on Properties) exam times scheduled by appointment.

Part 3: Diffusion (Lectures 15-22)

- 11/4: Lecture 15: Drift and Diffusion—theoretical formalism of how defects and impurities propagate within crystal structures.
For Class: Is drift or diffusion more relevant for your material of interest?
Problem 15 due before 5:00 PM on 11/5.
- 11/9: Lecture 16: Drift and Diffusion—theoretical formalism of how defects and impurities propagate within crystal structures.
For Class: Qualitatively, what traps may occur in a material of your interest?
Problem 16 due before 5:00 PM on 11/10.
- 11/11: Veterans Day: No Class
- 11/16: Lecture 17: Drift and Diffusion—theoretical formalism of how defects and impurities propagate within crystal structures.
For Class: Does diffusion have a directional dependence in a material of your interest?
Problem 17 due before 5:00 PM on 11/17.
- 11/18: Lecture 18: Diffusion Mechanisms—types of diffusion involving specific defects.
For Class: What is the most likely diffusion mechanism in a material of your interest?
Problem 18 due before 5:00 PM on 11/19.
- 11/23: Lecture 19: Diffusion Mechanisms—types of diffusion involving specific defects.
For Class: What is the most likely means of decreasing diffusion by the previous mechanism?
Problem 19 due before 5:00 PM on 11/29.



- 11/25: Thanksgiving: No Class
- 11/30: Lecture 20: Low Dimensional Diffusion—diffusion along line and plane defects.
For Class: Do grain boundaries increase or decrease diffusion in your material?
Problem 20 due before 5:00 PM on 12/1.
- 12/2: Lecture 21: Low Dimensional Diffusion—diffusion along line and plane defects.
For Class: How might the presence of grain boundaries impact other properties related to diffusion?
Problem 21 due before 5:00 PM on 12/3.
- 12/7: Lecture 22: Diffusion Characterization—experimental methods of tracking diffusion.
For Class: Does would you measure diffusion in a material of your interest?
Problem 22 due before 5:00 PM on 12/8.
- 12/9: Exam 3 Review Day (Diffusion: Drift and Diffusion, Mechanisms, Characterization).
- 12/13-12/17: Exam 3 (Diffusion: Drift and Diffusion, Mechanisms, Characterization) exam times
Finals week scheduled by appointment.