Chemistry 8201/4201 Materials Chemistry Fall 2023 11:15–12:30 h Tuesdays/Thursdays Smith Hall 231

- Instructor: Andreas Stein; 219 Smith; 612-624-1802, <u>a-stein@umn.edu</u>, <u>http://stein.chem.umn.edu</u> Office hours: Tue 12:30–13:30 h, Thu 16:30–17:30 h; or by appointment.
- TA:Gabrielle (Gabby) Vandendries; 34 Smith; vand1854@umn.eduOffice hours: Mon 13:00–14:00 h, Wed 12:00–13:00 h, 3rd-floor Kolthoff lounge

The Course: This course is scheduled as an in-person course. I intend to hold all class sessions in-person except if situational factors arise, such as personal illness of the instructor, when the class may be held synchronously via Zoom or recorded for later viewing. This is a survey course of materials chemistry/solid-state chemistry. Lectures will be based on the themes in Smart & Moore's text, *Solid State Chemistry* (structure and bonding, solid state synthesis, structure-property relationships), supplemented by materials from other texts (especially Rao & Gopalakrishnan and West) and from the more recent literature. Some specific course topics include: crystal systems/unit cells, structure types, porous materials, nanostructured materials, liquid/molecular crystals, powder X-ray diffraction, electronic structure, magnetic properties, solid state synthesis, and thin film preparation. Other topics will be introduced through student presentations, including selected topics from the following list: defects/interfaces, optical/dielectric properties, electrical/thermal conductivity, optical materials, piezoelectric materials, biomedical materials, catalysts. Chemistry graduate students should enroll in Chem 8201, undergraduate students in Chem 4201. Graduate students from other departments should discuss their enrollment choice with the instructor.

Required Text: Smart, L. E.; Moore, E. A. Solid State Chemistry, 5th ed., CRC Press, 2021.

Supplementary Texts:

A. R. West, *Solid State Chemistry and Its Applications*, 2nd ed. (student edition), Wiley: Chichester, 2014 (the UMN Library provides online access).

C. N. R. Rao, J. Gopalakrishnan, *New Directions in Solid State Chemistry*, 2nd ed., Cambridge University Press: Cambridge, 1997 (the UMN Library provides online access).

Reading Assignments: These include chapters from the text and supplementary material on the Canvas course site. They should be read in advance so that they can be discussed during the lectures.

Course Web Page: The course Canvas site will be used for posting the syllabus, lecture notes, grades, and other course-related material. Please ignore any letter grades listed on the Canvas site. These are automatically generated by Canvas but will not be used during the course.

Clickers: Clickers will be used for in-class responses. The required device is the iClicker2, and I will lend these to you. You must properly register your clicker to receive credit. Registration is done through the course Canvas site. On the Canvas page for CHEM 8201 or 4201, click on the entry with the title "iClicker registration" on the left-hand side bar and follow the instructions.

Course software: Throughout the course, we will use CrystalMaker software and the associated programs CrystalDiffract and SingleCrystal to visualize structures and their diffraction patterns. This software will also be needed for some of the homework assignments. The Chemistry Department has a software license for these programs for students in Chem 4201/8201 (both Mac and Windows). You will need to download the program files and manuals using the following link: https://drive.google.com/drive/folders/1zjRP7iBk7QAkbGfhPUiCaBJQnRZZXfC1?usp=sharing You have to have to sign in with your U of M Gmail account when you access this folder on Google Drive.

Online resources: We will also use several online resources during the course. The most important ones are listed below:

Symmetry and point groups: https://symotter.org

Space groups: http://img.chem.ucl.ac.uk/sgp/mainmenu.htm

Lattice planes and Miller indices: http://www.doitpoms.ac.uk/tlplib/miller indices/index.php Library of crystallographic prototypes: http://aflowlib.org/CrystalDatabase/space groups.html Solid state structure types: http://www.chemtube3d.com/solidstate/ table.htm Zeolite structures: http://www.iza-structure.org/databases/

Electronic structure: https://materialsproject.org (requires sign-in with your UMN Gmail account)

Grading:

	Chem 8201	Chem 4201
Quizzes:	5%	5%
Assignments:	25 %	35 %
Group presentation:	10 %	n/a†
Midterm exam 1* (Tue, Oct. 3):	20 %	20 %
Midterm exam 2* (Thu, Nov. 2):	20 %	20 %
Final exam (Sat., Dec. 16, 8:00–10:00 a.m.):	20 %	20 %

Cham 8201

*These exam dates are tentative and may be changed, if necessary, but they will be during class time. †Students in Chem 4201 may participate in the group presentations for extra credit.

NOTE ABOUT THE FINAL: DRC Testing Center Finals Scheduling Deadline: The DRC has set deadlines for scheduling exams in the Testing Center during the University's official finals week (December 15-21): November 21: priority deadline, space guaranteed

November 27: final deadline, dependant on space availability

This means that students need to schedule final exams about FOUR WEEKS IN ADVANCE!

During the course, all grades will be scored on a percentage basis. Final letter grades will be assigned based on the overall cumulative score. The following cut-offs will be used for letter 1. 87% grades:

A. 20170
A-:>85%
B+: >82%
B:>72%
B-:>67%
C+: >62%
C:>55%
C-:>50%

Note that at the end, I may opt to adjust these cutoffs such that it will be possible to get a particular letter grade with a score that is lower than the range indicated above. But in no case will this adjustment hurt your grade. That is to say, any adjustments, if applied, will only be used to improve your grade, not lower it.

If you are registered for this course on an S/N basis, a grade equivalent to C- or better on the A–F scale will be required to receive an "S". A D+ or below will receive an "N". Many programs or transfer courses do not like S/N grades or will assume that they are the minimum possible grade. Requests to change grading basis after the University deadline will not be approved. An *I* grade will be assigned only to students who have received passing grades on all work up to the final exam. If this occurs, you are responsible for contacting me before the end of finals week. Otherwise, a grade of F will be entered on the grade report.

If you need to use the Disability Resource Center (DRC, <u>https://disability.umn.edu/</u>), please contact DRC AS SOON AS POSSIBLE, to ensure your accommodations are in place at the beginning of the semester. You can do this by emailing <u>drc@umn.edu</u> or calling and leaving a message at 612-626-1333. If you already have an assigned access consultant and need modifications, please contact that person via email to address new access issues. Also let me know about any needs for accomodations at the beginning of the course.

University-wide **policies** on the following topics

- Student Conduct Code
- Use of Personal Electronic Devices in the Classroom
- Scholastic Dishonesty
- Makeup Work for Legitimate Absences
- Appropriate Student Use of Class Notes and Course Materials
- Grading and Transcripts
- Sexual Harassment
- Equity, Diversity, Equal Opportunity, and Affirmative Action
- Disability Accommodations
- Mental Health and Stress Management
- Academic Freedom and Responsibility

can be found at this webpage: <u>https://policy.umn.edu/education/syllabusrequirements-appa</u>

Important: In this course, you will have access to electronic material, including lecture notes, assignments, examinations, solution sets, video recordings of lectures etc. You are NOT ALLOWED to share this material with anyone who is not currently enrolled in this class and you are NOT ALLOWED to upload any of this material to any website, including but not limited to online "study sites" at any time (even after this course is finished). Violation of this rule constitutes a violation of the Student Conduct Code.

You are expected to do your own academic work and cite sources as necessary. Failing to do so is scholastic dishonesty. Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work, including the posting of student-generated coursework on online learning support and testing platforms not approved for the specific course in question; taking, acquiring, or using course materials without faculty permission, including the posting of faculty-provided course materials on online learning and testing platforms; ..."; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering, forging, misrepresenting or misusing a University academic record; or fabricating or falsifying data, research procedures, or data

analysis. If it is determined that a student has cheated, the student may be given an "F" or an "N" for the course, and may face additional sanctions from the University.

Artificial intelligence (AI) language models, such as ChatGPT, and online assignment help tools, such as Chegg®, are examples of online learning support platforms: they cannot be used for course assignments except as explicitly authorized by me, the instructor. The following actions are prohibited in this course:

- Submitting all or any part of an assignment statement to an online learning support platform;
- Incorporating any part of an AI generated response in an assignment;
- Using AI to brainstorm, formulate arguments, or template ideas for assignments;
- Using AI to summarize or contextualize source materials;
- Submitting your own work for this class to an online learning support platform for iteration or improvement.
- If you are in doubt as to whether you are using an online learning support platform appropriately in this course, I encourage you to discuss your situation with me.

Any assignment content composed by any resource other than you, regardless of whether that resource is human or digital, must be attributed to the source through proper citation. Unattributed use of online learning support platforms and unauthorized sharing of instructional property are forms of scholastic dishonesty and will be treated as such.

Tentative Course Outline

Introduction to course and to solid-state chemistry

Structure (Chpt. 1 Smart & Moore, Chpt. 1 West, Chpt. 1 Rao & Gop.)
Point groups and space groups
Crystal systems and unit cells
Close packing and space filling polyhedra approaches
Structure types
Special topics (silicates, carbon, amorphous materials, liquid crystals)
(Chpts 7, 11 in 5th ed. or Chpts. 6, 10 in 4th ed. Smart & Moore, Chpts. 4.12, 4.13, 4.14, 6.11, 6.12, 8.7, 8.9, Rao & Gop.)

Characterization (Chpt. 2 Smart & Moore, Chpt. 5 West, Chpt. 2 Rao & Gop.) X-Ray diffraction (powder methods, PDF files, indexing, identification of unknowns)

Electronic structure of solids (Chpts. 4, 11.4 (5th ed)/10.4 (4th ed) Smart & Moore, Chpt. 8, West, Chpt 6 Rao & Gop., E. Canadell, "Electronic Structure of Solids" in R. B. King (ed.) *Encyclopedia of Inorg. Chem.* vol. 3, Chichester N.Y., Wiley 1984, pp. 1173-1189, QD148.E53, 1994)

Band diagrams Effects of nanostructure and quantum size effects Conductive polymers

Synthetic methods in solid-state chemistry (Chpt. 3 Smart & Moore, Chpt. 4 West, Chpt. 3 Rao & Gop.)

Bulk methods for powders: high temperature and low temperature syntheses Single crystal growth Thin films and surfaces Nanomaterials

Magnetic properties (Chpt. 9 Smart & Moore, Chpt. 9 West)

Defects and nonstoichiometry (if time permits)

Structure-property relations and materials design (most of these topics may be covered as **student group presentations**)

Chemistry 8201

Materials Chemistry

Fall 2023

Student group presentations will be given in December during class (tentatively Dec. 5, Dec. 7). As a group of 3–4 graduate students, give a 30-minute presentation (plus 5 minutes for questions and answers) on one of the following topics and prepare one assignment question to be completed by everybody.

Student Presentation Topics

- Materials for molecular electronics
- Luminescent and laser materials
- Materials for piezo-electric devices
- Ferroelectric materials
- Thermoelectric materials
- Superhard materials
- Electrical energy storage materials
- Materials for solid state sensors
- High temperature superconductors
- Optical properties of hybrid organic-inorganic materials (luminescence, photochromism, nonlinear optics, plasmonics)
- Photonic crystals
- Magnetically responsive nanostructures
- Another materials chemistry topic approved by the instructor

The topics will be assigned on a first-come-first-served basis.

You can start your presentations with some basic background from general textbooks and review articles, but you should also include at least one or two examples from the recent primary literature in your discussions.

For the topic you select, provide the necessary background information, explain typical methods of synthesis, structural and compositional aspects, any special characterization techniques (if applicable), and how the structure-property relationships associated with the material(s) lead to their applications. You should also discuss the relevance of the work and possible future directions (you can be creative here).

You should use a lecture/teaching style, incorporating class interaction, rather than a straight seminar style. Make good use of the board, PowerPoint, and/or other media that you might find suitable. Divide your work equally among the group members. Make sure to practice your presentation as a group so that you stay within the allotted time.

One week before your presentation, hand out the assignment question, based on one of the references cited in your presentation, to the rest of the class (including both Chem 4201 and Chem 8201 students). The questions are meant to give your classmates an opportunity to read the article before class and to introduce them to the topic. Hopefully this will prepare everyone for better participation during your presentation. The questions are due at the beginning of your presentation and will be graded by your group. At least **two days before your presentation**, send me the PowerPoint file of your presentation so that I can post it on Canvas. Please do not

use a dark background, in case students want to print out the slides to take notes. Include appropriate references on slides in the format used by *Chem. Mater*. (For example: Mann, A. K. P.; Skrabalak, S. E. Synthesis of Single-Crystalline Nanoplates by Spray Pyrolysis: A Metathesis Route to Bi₂WO₆. *Chem. Mater*. **2011**, *23*, 1017-1022.).

Please check your topic selection with me by October 31. Meet with me by Nov. 16 to discuss the outline of your presentation. You should have a detailed outline prepared for this meeting. All group members are expected to be present for the meeting.

The information presented by the students is fair game for the final exam.

Evaluation of Oral Presentations

The oral presentations will be graded according to the following criteria:

	(Dutstanding	Very Good	Good	Fair	Poor
Background information:	15 pts. 6	G ()	()	()	()	()
Structural features:	15 pts. 6	G ()	()	()	()	()
Synthetic methods:	15 pts. 6	G ()	()	()	()	()
Structure-property relationships:	15 pts. 6	G ()	()	()	()	()
Future outlook:	15 pts. 6	б ()	()	()	()	()
Understanding of material presented:	15 pts. I	()	()	()	()	()
Overall organization:	15 pts. 6	б ()	()	()	()	()
Clarity of presentation (delivery):	15 pts. I	()	()	()	()	()
Graphics:	15 pts. 6	б ()	()	()	()	()
Response to oral questions:	15 pts. I	()	()	()	()	()
Homework question:	15 pts. 6	б ()	()	()	()	()
References in proper format:	$5\ pts.\ G$	()	()	()	()	()
Consulted with professor on time:	5 pts. G	()	()	()	()	()
Submitted files to professor on time:	5 pts. G	()	()	()	()	()
Kept to allotted presentation time:	5 pts. G	()	()	()	()	()

Total: 185 pts.

Note: G = group grade, I = individual grade

Comments: