Chemistry 8201/4201 Materials Chemistry Fall 2021
11:15–12:30 h Tuesdays/Thursdays
Smith Hall 331

Instructor: Andreas Stein; 219 Smith; 612-624-1802, a-stein@umn.edu, http://stein.chem.umn.edu
Office hours: Tue 12:30–13:30 h, Thu 16:30–17:30 h; or by appointment.

TA: Yevedzo Chipangura; Kolthoff 366; 612-626-8036 chipa007@umn.edu
Office hours: Mon 11:00–12:00 h, Fri 11:00–12:00 h (lobby of 3rd floor Kolthoff)

The Course: 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, selected characterization techniques, 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, ceramics, liquid/molecular crystals, X-ray diffraction, bonding in solids, electronic structure, 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, magnetic/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, Zoom links for office hours and lectures (if applicable), 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.

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* (Tuesday, Oct. 19, 11:15 a.m.–12:30 p.m.):	20 %	20 %
Midterm exam 2* (Thursday, Dec. 2, 11:15 a.m.–12:30 p.m.):	20 %	20 %
Final exam (Friday, Dec. 17, 8:00–10:00 a.m.):	20 %	20 %

*These exam dates are tentative and may be changed, if necessary, but they will be during class time.

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 grades:

A: >87%
A-: >85%
B+: >82%
B: >72%
B-: >67%
C+: >62%
C: >55%
C-: >50%

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.

The Disability Resource Center (DRC) continues to hold all appointments and meetings remotely by phone or video conference (Zoom or Google Hangout). If you need to use the DRC, 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 drc@umn.edu 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.

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: https://policy.umn.edu/education/syllabusrequirements-appa

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; taking, acquiring, or using course materials without faculty permission; 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.

Tentative Course Outline

Introduction to course and to solid-state chemistry

Structure (Chpt. 1 Smart & Moore, Chpt. 1 West, Chpt. 1 Rao & Gop.)

- Crystal systems and unit cells
- Close packing and space filling polyhedra approaches
- Structure types
- Factors that influence crystal structure
- 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., Chpts. 1 & 2, Weller)

- X-Ray diffraction (powder methods, PDF files, indexing, point groups, space groups, identification of unknowns)
- Neutron diffraction
- Small-angle X-ray scattering (from H. Schnablegger, Y. Singh, A Practical Guide To SAXS, Anton Paar: 2006) (Order a newer version of The SAXS Guide at this website (free): https://www.anton-paar.com/corp-en/saxs-guide (Do this right at the beginning of the semester to receive it on time.)

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

Defects and nonstoichiometry (if time permits)
Phase diagrams (if time permits)

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

Student group presentations will be given in December during class (tentatively Dec. 7, Dec. 9). As a group of 4 graduate students, give a 40-minute presentation on one of the following topics and prepare one assignment question to be completed by everybody. The material presented by the students is fair game for the final exam.

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

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 or overhead projector, and/or other media that you might find suitable. You should also provide the class with handouts in the form of a pdf file, which must include a list of relevant references or recent reviews. (Send me that file *at least two days before* your presentation, so that I can distribute it to the other class members.) Divide your work equally among the group members. Please allow time for questions in class.

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.

The information presented by the students is fair game for the final exam. Please check your topic selection with me by November 4. Meet with me by Nov. 18 to discuss the outline of your presentation. You should have an outline prepared for this meeting. All group members are expected to be present for the meeting.

Evaluation of Oral Presentations

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

		Outstanding	Very Good	Good	Fair	Poor
Background information:	15 pts. G	( )	( )	( )	( )	( )
Structural features:	15 pts. G	( )	( )	( )	( )	( )
Synthetic methods:	15 pts. G	( )	( )	( )	( )	( )
Structure-property relationships:	15 pts. G	( )	( )	( )	( )	( )
Future outlook:	15 pts. G	( )	( )	( )	( )	( )
Understanding of material:	15 pts. I	( )	( )	( )	( )	( )
Organization:	15 pts. G	( )	( )	( )	( )	( )
Clarity of presentation (delivery):	15 pts. I	( )	( )	( )	( )	( )
Graphics:	15 pts. G	( )	( )	( )	( )	( )
Response to oral questions:	15 pts. I	( )	( )	( )	( )	( )
Questions:	15 pts. G	( )	( )	( )	( )	( )
Answers to questions:	15 pts. I	( )	( )	( )	( )	( )
Consulted with professor on time:	5 pts. G	( )	( )	( )	( )	( )
Submitted files to professor on time:	5 pts. G	( )	( )	( )	( )	( )
Total:	190 pts.					

Note: G = group grade, I = individual grade

Comments: