

Syllabus

Chemistry 626

Selected Topics in Inorganic Chemistry: Crystallography and X-ray Diffraction

Tuesday and Thursday

09:30-10:45

SA 125

Winter 2020

Prof. Michelle Dolgos

Required Textbooks: NONE

Recommended for those with further interest in diffraction:

- 1) Introduction to Crystallography Donald E. Sands
- 2) X-ray Diffraction B.E. Warren
- 3) X-ray Diffraction in Crystals, Imperfect Crystals, and Amorphous Bodies A. Guinier
- 4) Introduction to the Theory of Thermal Neutron Scattering G.L. Squires
- 5) The Rietveld Method R.A. Young
- 6) Structure of Materials Marc De Graef
- 7) Underneath the Bragg Peaks Takeshi Egami and Simon Billange
- 8) Elements of X-ray Diffraction B.D. Cullity
- 9) The Basics of Crystallography and Diffraction, Third Edition Christopher Hammond

Office Hours: By appointment, SB 323.

Course Objectives and Goals: X-ray diffraction (XRD) is a tool for the investigation of crystal structures of materials. It is an extremely important analytical tool for researchers in materials-related disciplines. This class is intended to provide students with knowledge of XRD and its applications. The course will include an in-depth exploration of both the practical and theoretical methods commonly used for structural determinations using XRD. However, because of time constraints, a deep study of the mathematics behind some of the diffraction theory is not possible.

By the end of this course, you should be able to:

Understand how to use the International Tables of Crystallography

Identify the symmetry elements in space groups

Understand how diffraction works

Derive Bragg's Law

Index simple unit cells

Recognize what structural features contribute to the peak positions and intensities in an XRD pattern

Understand the different diffraction techniques available and when it is best to use them

Gain the knowledge to design and perform high quality XRD experiments during your own research experience at UofC

Homework: Homework will consist of take home problems, group discussions and laboratory assignments with corresponding questions or problems. Homework must be turned in on the due dates discussed in class. Late homework will **not** be accepted.

Midterm: There will be one in-class midterm examination based on lecture notes, homework problems, and additional reading assignments.

Presentation: You will give a 15 minute power point presentation to the class during the last week of the term. You will present in detail some background and 2-3 literature papers that are related to your final paper topic. You will be given the rubric used for grading far in advance of the presentation and I will also provide a handout with tips for putting together and delivering an effective presentation.

Final Exam: The final exam will consist of a term paper. There will be a list of topics to choose from or you can pick your own. I will provide a handout with tips for writing a good paper. You will be given the rubric used for grading far in advance of the due date. Plagiarism will result in zero credit for the final.

Topics Covered:

Properties of X-rays
Crystal Structures and Symmetry
Diffraction
Diffractometer Optics
Single Crystal Diffraction (Theory, lab, and hands on data analysis)
Powder Diffraction (Theory, lab, and hands on data analysis)
Thin Film Diffraction
PDF
SAXS and GIWAXS
Neutron Diffraction
Electron Diffraction

Department Approval _____ Electronically Approved _____ Date _____ January 6, 2020 _____