Chem 529 – X-ray spectrometry: an introduction, applications and experiments, Spring 2015
3 credit hours
LECTURES: to be arranged
LOCATION: to be arranged
INSTRUCTOR: Ursula Fittschen, ChulHee Kang
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Office: Fulmer 264 **Phone:** 335-1409 **Email:** chkang@wsu.edu
PREREQUISITES: Basic math skills, general understanding of physical chemistry

COURSE STRUCTURE AND FOCUS: This is a three credit hour graduate level Chemistry course. The level of presentations will be such that upper division undergraduates should be able to handle the work. In this course, explorations of the fundamental nature of interaction of X-rays and matter will be discussed.
Besides X-ray absorption, significant focus will be on X-ray fluorescence and X-ray diffraction analysis, point group/space group symmetry. These concepts will be discussed within the general framework of instrumentation aspects of modern laboratory X-ray set ups e.g. sources, optics and detectors. Figures of merits of these analytical tools compared to other methods will be discussed. Attention will be given to experimental techniques for processing primary data and some exercise of data analysis methods. The course will also include a "hands on" work shop on a Total reflection X-ray fluorescence spectrometer and single crystal X-ray diffraction.
The course will touch on advanced instrumentation available at synchrotron facilities.
There is no single textbook that covers in the desired level of detail all of the material of interest, hence reading material will be provided either directly or through the use of library resources.

Bibliography (all are recommended for different purposes – excerpts from these materials (constituting required reading material) will be distributed as needed for reference/background):

Cantor, Charles R.; Schimmel, Paul R. (1980). Biophysical Chemistry - Part II: Techniques for the Study of Biological Structure and Function (1st ed.). W.H. Freeman & Co Ltd. ISBN 0716711907.

Bernhard Rupp, Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology, ISBN: 0815340818 / ISBN-13: 9780815340812 by

Total-Reflection X-Ray Fluorescence Analysis, 2nd Edition, Reinhold Klockenkamper, Wiley, ISBN: 978-1-118-46027-6, 552 pages December 2014

Theory of XRF: getting acquainted with the principles, Peter Brouwer, PANalytical B.V., 2003, ISBN 9090167587, 9789090167589, 71 pages

Handbook of X-ray spectrometry, Edition: 2nd ed., rev. and expanded, R Grieken (René); Andrzej Markowicz, New York : Marcel Dekker c2002, 983 pages ISBN: 0824706005

GRADING: There will be three modules each 100 points (33%). Module 1 and 2 will be finalized by an examination (33% each exam). Module 3 will be graded by a literature reading/research exercise (including a brief written report and discussion period in which all will participate – 10% of semester grade). Module 3 will also include a work shop with

hand on experience on TXRF (23% of semester grade). Cooperation and collaboration on reading and any homework assignments is encouraged. Class participation is important, as the preferred means of learning is dialog rather than the spewing of facts (and opinions) by the instructor. Class participation will also be given consideration in establishing semester grade.

Students with Disabilities:
Reasonable accommodations are available for students with a documented disability. If you have a disability and need accommodations to fully participate in this class, please either visit or call the Access Center (Washington Building 217; 509-335-3417) to schedule an appointment with an Access Advisor. All accommodations MUST be approved through the Access Center. For more information contact a Disability Specialist on your home campus:
Pullman or WSU Online: 509-335-3417 http://accesscenter.wsu.edu, Access.Center@wsu.edu

Spokane: http://spokane.wsu.edu/students/current/studentaffairs/disability/
Tri-Cities: http://www.tricity.wsu.edu/disability/
Vancouver: 360-546-9138 http://studentaffairs.vancouver.wsu.edu/student-resource-center/disability-services

Academic integrity statement:
Serious chemistry graduate students wouldn't contemplate cheating, as the principal harm would be self-inflicted wounds. The course will be structured such that cheating is virtually impossible – or (officially), *As an institution of higher education, Washington State University is committed to principles of truth and academic honesty. All members of the University community share the responsibility for maintaining and supporting these principles. When a student enrolls in Washington State University, the student assumes an obligation to pursue academic endeavors in a manner consistent with the standards of academic integrity adopted by the University. To maintain the academic integrity of the community, the University cannot tolerate acts of academic dishonesty including any forms of cheating, plagiarism, or fabrication. Washington State University reserves the right and the power to discipline or to exclude students who engage in academic dishonesty.*

Safety and emergency notification:
Pullman: "Washington State University is committed to enhancing the safety of the students, faculty, staff, and visitors. It is highly recommended that you review the Campus Safety Plan (http://safetyplan.wsu.edu/) and visit the Office of Emergency Management web site (http://oem.wsu.edu/) for a comprehensive listing of university policies, procedures, statistics, and information related to campus safety, emergency management, and the health and welfare of the campus community."

Student Learning Outcomes: This graduate-level chemistry course is designed to inform and educate graduate chemistry and material science students in the interaction of X-ray with matter and the analytical exploitation of the same e.g. absorption spectroscopy, fluorescence spectrometry and diffraction analysis. It is expected that successful participants will have gained insights into the field that are far above that of the general population. As prospective chemistry Ph.D. candidates, the overarching student learning outcome is for the students to begin to develop a more sophisticated approach to solving complex problems (which is what most Ph.D. scientists are expected to do) through the reading of descriptions of prior knowledge on the subject, in class discussions of these concepts, and through opportunities to critically evaluate and use information from the chemical literature. Progress will be evaluated in the two exams, written exercises, and group discussions.

The course features approximately 85% faculty lectures/15% student-centered discussions. Student performance will be judged based on their performance on mid-term and final examinations (33% each), 33% on planned exercises with adjustments made for active participation in class activities. Aside from the above mentioned exercises, no "homework" will be assigned aside from a considerable quantity of reading materials transmitted to the students electronically by the instructor.

Approximate Schedule Module 1 (100points): **Ursula Fittschen** -: Introduction and basics in X-ray – matter interaction
Week 1 Jan 13 – Introduction, Overview, arrangements ***Literature paper assignment***
Week 1 Jan 15 Radiation fundamentals absorption, refraction, diffraction, ionization, fluorescence, comparison Optical regime-X-ray regime
Week 2 Jan 20 X-ray Instrumentation, general set up, source optics detectors (same for mostly any experiment, XRF, XRD etc.) – functionality founds on X-ray interaction
Week 2 Jan 22 Interaction: absorption
Week 3 Jan 27 Interaction: Fluorescence, Auger and Photoelectron emission
Week 3 Jan 29 Interaction: Refraction, Total reflection, Reflectivity
Week 4 Feb 3 Interaction additions, repetitions
Week 4 Feb 4 Exam
Module 2 (100points): ChulHhee Kang: X-ray diffraction analysis, scattering theory, point group/space group symmetry, February 10th to March 13th
Week 5 Crystal, Lattice, Symmetry, Point group, Plane group, Space group
Week 5 Optical diffraction, Bragg's law, Laue equation, Superposition of waves
Week 6 Atomic scattering factor, Fourier transform, Reciprocal space
Week 6 Intensity measurement & Data reduction, Phase problem, Patterson function
Week 7 Isomorphous replacement, Heavy atom method
Week 7 Anomalous Scattering, Laue method, MAD method
Week 8 Model building & Structure Refinement
Week 8 Molecular replacement, Rotation and Translation Function, Direct method
Week 9 Mar 10: **Workshop on XRD** crystallization
Week 9 Mar 13 Exam
Module 3 (100points): Ursula Fittschen: Instrumentation, Quantification, Imaging and absorption spectroscopy **Work shop assignment (schedule individually with 2-3 students at each appointment for XRF)**
Week 10 Mar 24 Introduction to module 3, workshop assignments
Week 10 Mar 27 XRF quantitative, EDX, WDX, TXRF
Week 11 Mar 31 Imaging in general, scanning, transmission, confocal, tomography
Week 11 Apr 02 Paper presentation and discussion group 1 and 2
Week 12 Apr 14 Paper presentation and discussion group 3 and 4
Week 12 Apr 16 Paper presentation and discussion group 5 and 6
Week 13 Apr 21 X-ray-Optics ~~X-ray Sources and Detectors~~
Week 13 Apr 23~~5~~ X-ray Sources and Detectors ~~XANES (EXAFS) introduction~~
Week 14 Apr 28 XANES (EXAFS) introduction ~~XANES absorption/fluorescence/electrons~~
Week 14 Apr 30 XANES absorption/fluorescence/electrons ~~**Workshop on XRD** crystallization,~~
Week 15 Mai 5 **Workshop on XRD** X-ray diffraction data collection
Week 15 Mai 7 **Workshop on XRD** phasing

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