The University of Western Ontario
Chemistry 9754R, Fall 2024 (Oct 24 – Dec 5)

Powder Diffraction

Instructor:
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Description:

The course addresses structural characterization and quantitative analysis for solid crystalline materials by X-ray powder diffraction techniques. Topics include pattern processing and indexing, data mining, structural visualization, introduction to Rietveld refinement - theory and use of computer software for structural refinement on powder patterns.

Topics:

Week	Topic
1	Solid material classifications. Available structural characterization probes. Review of basics of space group and crystallography: definitions, symmetry elements, screw axis, glide plane, 230 space groups, matrix representations, Bravais lattices, reciprocal lattices, 32 crystallography point groups, equivalent sites, international tables for crystallography.
2	Introduction of powder x-ray diffraction. Diffraction theories. Single crystal vs. powder diffraction. Energy dispersive vs. angle dispersive. Instrumentation, pattern acquisition and processing.
3	Pattern indexing. Reflections, d-spacings and Miller indices. General techniques, indexing algorithms, data mining, use of software.
4	Introduction to Rietveld refinement. History and achievements. Principles, algorithms, parameters, quantitative analysis. Limitations.
5	Introduction to Rietveld refinement software: GSAS. Primer for EXPGUI and GSAS. File preparations and extraction of structure. Refinement parameters. Crystal structure visualization.
6	Hands on practice on refinement of powder patterns. Refinement of lanthanum hexaboride powder pattern. Multiple phases and quantitative analysis.
7	Other selected topics. Non-ambient condition structural analysis. Introduction to popular software, databases, web resources. Further readings.

Resources:

1) Course website: http://owl.uwo.ca/ (requires login with UWO email account).

2) Textbook: None. Some recommended reference books will be available from library or online.

3) Lecture notes and handouts will be provided via Owl.

4) Laptop PC with Windows OS is recommended.

Lectures / seminars:

Day/s: Thursdays

Time/s: 2:30 – 4:30 PM

Mode of instruction: In person

Evaluation

Problem sets (3 assignments)	60%
Comprehensive project	40%

Course attendance and missed/late assignments

If you are unable to meet a course requirement due to illness or other serious circumstances, you must provide valid medical or other supporting documentation to your instructor immediately. It is the student's responsibility to make alternative arrangements with their instructor once the accommodation has been approved and the instructor has been informed.

Notes on Academic Honesty

Scholastic offences are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following Web site:

www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_grad.pdf

All required papers may be subject to submission for textual similarity review to the commercial plagiarism detection software under license to the University for detection of plagiarism. All papers submitted for such checking will be included as source documents in the reference database for the purpose of detecting plagiarism of papers subsequently submitted to the system. Use of the service is subject to the licensing agreement, currently between The University of Western Ontario and Turnitin.com (http://www.turnitin.com).

Health and Wellness

As part of a successful graduate student experience at Western, we encourage students to make their health and wellness a priority. Western provides several on campus health-related services to help you achieve optimum health and engage in healthy living while pursuing your graduate degree. For example, to support physical activity, all students, as part of their registration, receive membership in Western's Campus Recreation Centre.

Numerous cultural events are offered throughout the year. For example, please check out the Faculty of Music web page http://www.music.uwo.ca/, and our own McIntosh Gallery http://www.mcintoshgallery.ca/. Information regarding health- and wellness-related services available to students may be found at http://www.health.uwo.ca/. Students seeking help regarding mental health concerns are advised to speak to someone they feel comfortable confiding in, such as their faculty supervisor, their program director (graduate chair), or other relevant administrators in their unit. Campus mental health resources may be found at http://www.health.uwo.ca/mental_health/resources.html.

Use of Generative Artificial Intelligence (AI)

The use of generative artificial intelligence (AI) tools/software/apps is acceptable, and permitted in the course as long as such use is appropriately disclosed with sufficient details provided. For more information about the AI policy, please visit SGPS Provisional Guidance for the use of Generative AI in Graduate Studies at:

https://grad.uwo.ca/about us/policies procedures regulations/ai.html