

The University of Western Ontario  
Chemistry 9702R, Fall 2023 (Oct 26 – Dec 7)  
**Materials under Extreme Conditions**

**Instructor:**

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**Description:**

Materials under extreme conditions can exhibit exotic phenomena and behave drastically differently than at ambient conditions. The course addresses structures and properties of materials and their potential applications under extreme conditions especially at high pressures. Topics include principles of high-pressure materials science and technology, history and development in generation of extreme conditions, in situ structure and property characterization methods including spectroscopy and synchrotron techniques, as well as computational methods for high-pressure materials research. Examples of recent advances will be given to illustrate the application of these techniques in this highly interdisciplinary area involving high-pressure chemistry, physics and materials science.

**Topics:**

| <b>Week</b> | <b>Topic</b>   |
|-------------|--|
| 1           | Overview of extreme conditions. Physical principles of high pressure. Structure and properties of materials under high pressure. Pressure induced structural transformations. Chemical reactions at high pressures.  |
| 2           | High pressure techniques. Extreme condition generation. Pressure calibration. Overview of structural characterization tools.   |
| 3           | X-ray probes for in situ characterization. Introduction of x-ray diffraction (single crystal and powder). Microdiffraction for diamond anvil cells. Instrumentation, pattern acquisition and processing. Phase transitions and data analysis.                              |
| 4           | Spectroscopic probes for in situ characterization. Basic principles of Raman and IR spectroscopy and microscopy. Synchrotron IR source and characteristics. In situ Raman and IR micro-spectroscopy and spectral analysis for materials under high pressures.              |
| 5           | Theoretical and computational methods in high pressure materials research. Basics of quantum mechanics and density functional theory. Prevailing computational methods for structural prediction, optimization and calculation of material properties in condensed matter. |
| 6           | Recent advances of high-pressure materials science. Selected topics.   |
| 7           | Essays and presentations.  |

## **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.

## **Lectures / seminars:**

Day/s:           Thursdays

Time/s:          2:30 – 4:30 PM

Mode of instruction: In person

## **Evaluation**

Problem sets (2 assignments)      50%

Short essay                              25%

Short presentation on essay        25%

## **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](http://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](http://www.health.uwo.ca/mental_health/resources.html).