DALHOUSIE UNIVERSITY

Faculty of Science Course Syllabus (Section A)
Department of Physics and Atmospheric Science/Department of Chemistry

CHEM 5312

Advances in Battery, Fuel Cell and Supercapacitor Materials

Winter 2023

Dalhousie University is located in Mi'kma'ki, the ancestral and unceded territory of the Mi'kmaq. We are all Treaty people.

Instructor: *Michael Metzger, Chongyin Yang, Penghao Xiao*

(E-Mails: michael.metzger@dal.ca, c.yang@dal.ca, penghao.xiao@dal.ca)

Lectures: *Monday, Wednesday, Friday 10:35-11:25 (credit hours: 3)*

Office hours: *Monday, Wednesday, Friday 11:30-12:30*

Dunn building, Rooms 329 (MM), 224 (CY), 230 (PHX)

Course delivery: *In-person, Studly Campus, LSC-Common Area, Room C234*

Course Description

This course will present the cutting-edge advances in the materials used in energy storage systems, such as batteries (particularly Li-ion batteries), fuel cells and supercapacitors. Discussions will include component materials (electrodes, electrolytes, separator) and full devices.

Course Prerequisites

CHEM 4311.03 / CHEM 5311.03, or permission of the instructor.

Course Exclusion

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Learning Objectives

Students should develop an in-depth understanding of battery technology at the graduate level. We discuss the latest developments in the field with an emphasis on advanced batteries. This course is meant to prepare students for graduate work in batteries and/or a career in the battery industry.

Course Materials and Delivery

- Recommended textbook: K. W. Beard and T. B. Reddy. "Linden's Handbook of Batteries", 5th edition (2019).

DALHOUSIE UNIVERSITY

- Other textbooks: K. Xu. "Electrolytes, Interfaces and Interphases, 1st Edition", RSC (2023); T. F. Fuller and John N. Harb. "Electrochemical Engineering, 1st Edition", Wiley (2018); R. A. Dunlap. "Sustainable Energy, 2nd Edition", Cengage (2017).
- Other resources: We will provide theses and research papers that cover important topics.
- Brightspace page: **CHEM 5312 – Advances in Battery, Fuel Cell and Supercapacitor Materials (Sec 1) - 2023 Winter**.
- Slides: We will use slide decks for each chapter (see below) to discuss the relevant contents. PDFs of all slides shown in the course will be made available on the Brightspace page.
- Examples: During the course, examples may be given by the instructor using a document camera. It is expected that the students write down these examples in their notebooks for later reference.
- Assignments: There will be problem sets provided as homework assignments on the Brightspace page. Students will need access to a computer to upload their solutions to the Brightspace page.

Course Assessment

Assessment	Weight (% of final grade)	Date
Assignments		
#1	*10*	*Start: January 23, 2023 / Due: January 30, 2023*
#2	*10*	*Start: January 30, 2023 / Due: February 06, 2023*
#3	*10*	*Start: February 06, 2023 / Due: February 13, 2023*
#4	*10*	*Start: February 13, 2023 / Due: February 27, 2023*
#5	*10*	*Start: February 27, 2023 / Due: March 06, 2023*
#6	*10*	*Start: March 06, 2023 / Due: March 13, 2023*
#7	*10*	*Start: March 13, 2023 / Due: March 20, 2023*
#8	*10*	*Start: March 20, 2023 / Due: March 27, 2023*
#9	*10*	*Start: March 27, 2023 / Due: April 03, 2023*
#10	*10*	*Start: April 03, 2023 / Due: April 10, 2023*
Final exam		
There will be no final exam.		

Other course requirements

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Conversion of numerical grades to Final Letter Grades follows the Dalhousie Common Grade Scale

A+ (90-100)	**B+** (77-79)	**C+** (65-69)	**D** (50-54)
A (85-89)	**B** (73-76)	**C** (60-64)	**F** (<50)
A- (80-84)	**B-** (70-72)	**C-** (55-59)	

DALHOUSIE UNIVERSITY

Course Policies on Missed or Late Academic Requirements

- Students are expected to use the Student Declaration of Absence form for late or missed assignments. The form may be used 2 times in this course.
- If problem solutions to assignments are handed in up to 1 week late, they will count half (5% of final grade).
- If no problem solutions to assignments are handed in more than 1 week after due date, they will count zero.

Course Policies related to Academic Integrity

It is expected that students discuss assignment problems as a group. However, it is an academic offense to copy the solution of someone else. Allegations will be submitted to an Academic Integrity Officer of the Faculty of Science for evaluation and possible sanction. The minimum sanction is zero on the assignment.

Course Content

During the term, we will attempt to cover the course material grouped in the below chapters. Grey/cursive text applies to bonus topics that might be skipped in the interest of time. The chapters will be delivered by Michael Metzger (MM), Chongyin Yang (CY), and Penghao Xiao (PX) as indicated in the list below. If appropriate and available, experts from academia or industry will be invited to give guest lectures.

Tentative schedule
January 9, 2023 – April 11, 2023
Holidays/Break: Munro Day (February 3, 2023), Heritage Day (February 20, 2023), Winter Study Break (February 20-24, 2023), Good Friday (April 7, 2023)
Total sessions: 35

Chapter 1: Battery Fundamentals -- [Sessions 1-3, MM]

1.1. Battery History

1.1.1. Battery Pioneers

1.1.2. Canadian Contributions

1.2. Battery Types

1.2.1. Primary Batteries

1.2.2. Lithium-ion Batteries

1.2.3. Other Secondary Batteries

1.3. Battery Characteristics

1.3.1. Capacity and State-of-Charge

1.3.2. Cell Performance

1.3.3. Ragone Plots

1.3.4. Heat Generation

1.3.5. Efficiency of Secondary Cells

1.3.6. Charge Retention and Self-Discharge

1.3.7. Capacity Fade in Secondary Cells

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Chapter 2: Battery Active Materials -- [Sessions 4-17, PX+CY]

- **2.1. Battery Active Materials Structures**
  - 2.1.1. Positive Electrode Materials
    - a) Layered Structures
    - b) Spinel and Rock Salt Structures
    - c) Olivine and Other Structures
  - 2.1.2. Negative Electrode Material Structures
    - a) Graphite
    - b) Hard and Soft Carbons
    - c) Oxides
    - d) Alloy Materials
- **2.2. Battery Materials Theory**
  - 2.2.1. Lattice Gas Model of Intercalation
  - 2.2.2. Mean Field Theory
  - 2.2.3. Staging in Layered Compounds
  - 2.2.4. Ab-initio Methods
- **2.3. Materials Characterization Techniques**
  - 2.3.1. Diffraction
    - a) X-ray Diffraction
    - b) Neutron Scattering
  - 2.3.2. Microscopy
    - a) Secondary Electron Microscopy
    - b) Transmission Electron Microscopy
    - c) Electron Energy Loss Spectroscopy
    - d) Energy Dispersive X-ray Spectroscopy
  - 2.3.3. Spectroscopy
    - a) X-ray Fluorescence Spectroscopy
    - b) X-ray Absorption Spectroscopy
    - c) X-ray Photoelectron Spectroscopy

Chapter 3: State-of-the-Art Batteries -- [Sessions 18-23, CY+MM]

- **3.1. Battery Electrolytes and Interphases**
  - 3.1.1. Electrolyte Components
  - 3.1.2. Importance of Interphases
  - 3.1.3. Diffusivity and Transference Number
  - 3.1.4. Ion Mobility Migration
  - 3.1.5. Advanced Electrolyte Model
- **3.2. Battery Cell and Pack Design**
  - 3.2.1. Cell Fabrication
  - 3.2.2. Cell Spreadsheet Model
  - 3.2.3. Pack Design
  - 3.2.4. Battery Management Systems

DALHOUSIE UNIVERSITY

- **3.3. Battery Cost and Sustainability**
  - 3.3.1. Bill-of-Materials
  - 3.3.2. Lithium Resources
  - 3.3.3. Critical Metals

Chapter 4: Battery Analytics -- [Sessions 24-29, MM]

- **4.1. Battery Aging Diagnostics**
  - 4.1.1. Ultra-high Precision Coulometry
  - 4.1.2. Differential Voltage Analysis
  - 4.1.3. Electrochemical Impedance Spectroscopy
  - 4.1.4. Battery Gas Analysis
- **4.2. Battery Safety Testing**
  - 4.2.1. Battery Accidents
  - 4.2.2. Thermal Runaway
  - 4.2.3. Safety Testing
  - 4.2.4. Accelerating Rate Calorimetry
  - 4.2.5. Cell Thermal Model

Chapter 5: Beyond Lithium-ion Batteries -- [Sessions 30-31, CY]

- **5.1. (Aqueous) Monovalent Batteries**
  - 5.1.1. Sodium-ion Batteries
  - 5.1.2. Potassium-ion Batteries
- **5.2. (Aqueous) Multivalent Batteries**
  - 5.2.1. Zinc-ion Batteries
  - 5.2.2. Magnesium-ion Batteries
  - 5.2.3. Calcium-ion Batteries
  - 5.2.4. Aluminum-ion Batteries
- **5.3. Solid-State Batteries**
  - 5.3.1. Oxide-based SSBs
  - 5.3.2. Sulfide-based SSBs
  - 5.3.3. Polymer-based SSBs
- **5.4. Conversion Batteries**
  - 5.4.1. Metal-Sulfur Batteries
  - 5.4.2. Metal-Air Batteries

Chapter 6: Fuel Cells -- [Sessions 32-33, MM]

- **6.1. Hydrogen**
  - 6.1.1. Properties of Hydrogen
  - 6.1.2. Hydrogen Production
  - 6.1.3. Hydrogen Transport and Storage

6.2. Fuel Cell Types
- 6.2.1. Proton Exchange Membrane FCs
- 6.2.2. Alkaline FCs
- 6.2.3. Phosphoric Acid FCs
- 6.2.4. Molten Carbonate FCs
- 6.2.5. Solid Oxide FCs

6.3. Fuel Cell Characteristics
- 6.3.1. Polarization Curve
- 6.3.2. Operating Conditions
- 6.3.3. Power Output
- 6.3.4. Electrode Structure

6.4. Fuel Cell Stack and System Design
- *6.4.1. System Overview and Analysis*
- *6.4.2. Basic Stack Design Concepts*
- *6.4.3. Cell Stack Configuration*
- *6.4.4. Basic Construction and Components*
- *6.4.5. Utilization of Oxidant and Fuel*
- *6.4.6. Flow-Field Design*
- *6.4.7. Water and Thermal Management*

Chapter 7: Redox-Flow Batteries -- [Session 34, CY]

7.1. Electrochemical Reactors
- 7.1.1. Design of Electrochemical Reactors
- 7.1.2. Anolytes and Catholyte Choices
- 7.1.3. Membrane Choices

7.2. Commercial Systems
- 7.2.1. Flow Battery Types
- 7.2.2. Cell Operation
- 7.2.3. Rebalancing
- 7.2.4. Thermal Management

Chapter 8: Supercapacitors -- [Session 35, CY]

8.1. Electric Double-Layer Capacitors
- 8.1.1. Porous EDLC Electrodes
- 8.1.2. Operation of EDLCs
- 8.1.3. Degradation of EDLCs
- 8.1.4. Pseudo-Capacitance

8.2. Commercial Supercaps
- 8.2.1. Power and Energy Capability
- 8.2.2. Design Considerations
- 8.2.3. Applications

DALHOUSIE UNIVERSITY

Addendum A: Thermodynamics, Kinetics and Transport

- ***A.1. Thermodynamics***
  - *A.1.1. Cell Potential*
  - *A.1.2. Standard Potentials*
  - *A.1.3. Effect of Temperature on Cell Potential*
  - *A.1.4. Simplified Activity Correction*
  - *A.1.5. Use of Cell Potential*
  - *A.1.6. Pourbaix Diagrams*
  - *A.1.7. Reference Electrodes*
  - *A.1.8. Debye-Hückel Theory*
- ***A.2. Kinetics***
  - *A.2.1. Electrical Double Layer*
  - *A.2.2. Impact of Potential on Reaction Rate*
  - *A.2.3. Butler-Volmer Kinetics*
  - *A.2.4. Reaction Kinetics in Cells*
- ***A.3. Transport***
  - *A.3.1. Fick's Law*
  - *A.3.2. Nernst-Planck Equation*
  - *A.3.3. Conservation of Material*
  - *A.3.4. Convective Mass Transfer*
  - *A.3.5. Transport in Cells*

Addendum B: Sustainable Transportation*10.1. Fundamentals*

- ***B.1. Fundamentals***
  - *B.1.1. Energy in the Transportation Sector*
  - *B.1.2. The Need for Electrification*
- ***B.2. Internal Combustion Engine (ICE)***
  - *B.2.1. Fuel Efficiency*
  - *B.2.2. Hybrid Electric Vehicles (HEVs)*
- ***B.3. Battery Electric Vehicles (BEVs)***
  - *B.3.1. Battery Requirements*
  - *B.3.2. History of BEVs*
  - *B.3.3. Modern Li-ion Cells for BEVs*
  - *B.3.4. Vehicle-to-Grid*
- ***B.4. Hydrogen Vehicles***
  - *B.4.1. Hydrogen Internal Combustion Vehicles*
  - *B.4.2. Fuel Cell Electric Vehicles (FCEVs)*
  - *B.4.3. Hydrogen Refueling Infrastructure*
- ***B.5. Efficiency of Transportation Technologies***
  - *B.5.1. Wells-to-wheels Efficiency*
  - *B.5.2. Carbon Footprint Analysis*

DALHOUSIE UNIVERSITY

Faculty of Science Course Syllabus (Section B)

PHYC/ENVS 2310

Advances in Battery, Fuel Cell and Supercapacitor Materials

Winter 2023

University Policies and Statements

This course is governed by the academic rules and regulations set forth in the University Calendar and by Senate

Academic Integrity

At Dalhousie University, we are guided in all of our work by the values of academic integrity: honesty, trust, fairness, responsibility and respect (The Center for Academic Integrity, Duke University, 1999). As a student, you are required to demonstrate these values in all of the work you do. The University provides policies and procedures that every member of the university community is required to follow to ensure academic integrity.

Information: https://www.dal.ca/dept/university_secretariat/academic-integrity.html

Accessibility

The Advising and Access Services Centre is Dalhousie's centre of expertise for student accessibility and accommodation. The advising team works with students who request accommodation as a result of a disability, religious obligation, or any barrier related to any other characteristic protected under Human Rights legislation (Canada and Nova Scotia).

Information: https://www.dal.ca/campus_life/academic-support/accessibility.html

Student Code of Conduct

Everyone at Dalhousie is expected to treat others with dignity and respect. The Code of Student Conduct allows Dalhousie to take disciplinary action if students don't follow this community expectation. When appropriate, violations of the code can be resolved in a reasonable and informal manner—perhaps through a restorative justice process. If an informal resolution can't be reached, or would be inappropriate, procedures exist for formal dispute resolution.

Code: https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html

Diversity and Inclusion – Culture of Respect

Every person at Dalhousie has a right to be respected and safe. We believe inclusiveness is fundamental to education. We stand for equality. Dalhousie is strengthened in our diversity. We are a respectful and inclusive community. We are committed to being a place where everyone feels welcome and supported, which is why our Strategic Direction prioritizes fostering a culture of diversity and inclusiveness

Statement: http://www.dal.ca/cultureofrespect.html

Recognition of Mi'kmaq Territory

Dalhousie University would like to acknowledge that the University is on Traditional Mi'kmaq Territory. The Elders in Residence program provides students with access to First Nations elders for guidance, counsel and support. Visit or e-mail the Indigenous Student Centre (1321 Edward St) (elders@dal.ca).

Information: https://www.dal.ca/campus_life/communities/indigenous.html

Important Dates in the Academic Year (including add/drop dates)
https://academiccalendar.dal.ca/Catalog/ViewCatalog.aspx?pageid=viewcatalog&catalogid=117&chapterid=-1&topicgroupid=31821&loaduseredits=False

University Grading Practices

https://www.dal.ca/dept/university_secretariat/policies/academic/grading-practices-policy.html

DALHOUSIE UNIVERSITY

Faculty of Science Course Syllabus (Section C)
PHYC/ENVS 2310
Advances in Battery, Fuel Cell and Supercapacitor Materials
Winter 2023

Student Resources and Support

Advising

General Advising https://www.dal.ca/campus_life/academic-support/advising.html

Science Program Advisors: https://www.dal.ca/faculty/science/current-students/undergrad-students/degree-planning.html

Indigenous Student Centre: https://www.dal.ca/campus_life/communities/indigenous.html

Black Students Advising Centre: https://www.dal.ca/campus_life/communities/black-student-advising.html

International Centre: https://www.dal.ca/campus_life/international-centre/current-students.html

Academic supports

Library: https://libraries.dal.ca/

Writing Centre: https://www.dal.ca/campus_life/academic-support/writing-and-study-skills.html

Studying for Success: https://www.dal.ca/campus_life/academic-support/study-skills-and-tutoring.html

Copyright Office: https://libraries.dal.ca/services/copyright-office.html

Fair Dealing Guidelines https://libraries.dal.ca/services/copyright-office/fair-dealing.html

Other supports and services

Student Health & Wellness Centre: https://www.dal.ca/campus_life/health-and-wellness.html

Student Advocacy: https://dsu.ca/dsas

Ombudsperson: https://www.dal.ca/campus_life/safety-respect/student-rights-and-responsibilities/where-to-get-help/ombudsperson.html

Safety

Biosafety: https://www.dal.ca/dept/safety/programs-services/biosafety.html

Chemical Safety: https://www.dal.ca/dept/safety/programs-services/chemical-safety.html

Radiation Safety: https://www.dal.ca/dept/safety/programs-services/radiation-safety.html

Scent-Free Program: https://www.dal.ca/dept/safety/programs-services/occupational-safety/scent-free.html

Dalhousie COVID-19 information and updates: https://www.dal.ca/covid-19-information-and-updates.html