Topics in Physics Syllabus

Department of Physics and Atmospheric Science

PHYC 6600 Fall 2023

Dalhousie University acknowledges that we are in Mi'kma'ki, the ancestral and unceded territory of the Mi'kmaq People and pays respect to the Indigenous knowledges held by the Mi'kmaq People, and to the wisdom of their Elders past and present. The Mi'kmaq People signed Peace and Friendship Treaties with the Crown, and section 35 of the Constitution Act, 1982 recognizes and affirms Aboriginal and Treaty rights. We are all Treaty people.

Dalhousie University also acknowledges the histories, contributions, and legacies of African Nova Scotians, who have been here for over 400 years.

Course Instructor(s)

Name	Email	Office Hours
Michael Metzger	michael.metzger@dal.ca	Monday, Wednesday, Friday 14.30 – 15.00, Dunn building, Room 329

Course Description

Electrolytes are indispensable components in batteries as they determine how high the voltage of a battery is, how many times it can be charged/discharged, or how rapidly the energy stored therein can be released. The technical challenges around safety, lifetime, and cost-effectiveness of lithium-based or beyond-lithium batteries require in-depth understanding of electrolytes and interphases. This course will establish the fundamental principles for electrolyte science, before moving on to important knowledge acquired in recent years. There will be special emphasis on linking these fundamentals to real-world problems encountered in lithium-ion batteries. This course will be suitable for graduate students in physics, chemistry, materials science, and engineering, interested in electrochemical energy storage and preparing them for graduate work in batteries and/or a career in the battery industry.

Course Prerequisites

It would be useful to have taken CHEM 4311/5311 and CHEM 5312, but these are not required.

Course Exclusions

None.

Student Resources

Office hours will be held after every lecture, i.e., Monday, Wednesday, Friday 14.30 – 15.00, in the Dunn building in room 329. There will be a help page on Brightspace for questions and answers regarding course materials and assignments. Announcements related to the course will be communicated through the course website. Additionally, please use and check your Dalhousie e-mail for course related communications.

Course Structure

Course Delivery

The course will be delivered in person and not recorded. We will use slide decks for each chapter (see below) to discuss the relevant contents. PDFs of all slides will be made available on the Brightspace page prior to lectures. During the course, examples may be given by the instructor using a document camera. It is expected that the students will write down these examples in their notebooks for later reference.

Lectures

Monday, Wednesday, Friday 13.35 – 14.25, Studley LSC-BIOL&EARTH B4082

Laboratories

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Tutorials

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Course Materials

Course website: Brightspace. Included is a complete set of lecture notes, problem sets and other reference materials.

Recommended textbook: K. Xu, "Electrolytes, Interfaces and Interphases", 1st edition, RSC (2023). Fifteen copies of this book have been requested to be available at the Dal Bookstore.

Other applied textbooks: K. W. Beard and T. B. Reddy, "Linden's Handbook of Batteries", 5th edition, McGraw Hill (2019); T. F. Fuller and J. N. Harb, "Electrochemical Engineering", 1st edition, Wiley (2018).

Other fundamental textbooks: J. Newman and N. Balsara, "Electrochemical Systems", 4th edition, Wiley (2021); J. O. M. Bockris and A. K. N. Reddy, "Modern Electrochemistry", 2nd edition, Plenum Press (1998); A. J. Bard and L. R. Faulkner, "Electrochemical Methods. Fundamentals and Applications", 2nd edition, Wiley (2001).

Other resources: Selected chapters of Ph.D. theses as well as research papers will be provided.

Assessment

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. Some assignments may consist of typical quantitative problems, some of which are analytical, and some are computational. Other assignments will involve reading selected literature and presenting the key takeaways in writing. There will also be presentations and written reports (see below for details). Grades will be determined based on the weights assigned to each question, as indicated on each assignment.

Assessment	**Weight (%)**	**Date**
Assignment #1	*10*	*Start: October 3, 2023 / Due: October 16, 2023*
Assignment #2	*10*	*Start: October 16, 2023 / Due: October 30, 2023*
Assignment #3	*10*	*Start: October 30, 2023 / Due: November 10, 2023*
Assignment #4	*10*	*Start: November 10, 2023 / Due: November 27*
Presentation	*30%*	*To be scheduled towards end of term.*
Written Report	*30%*	*Due: December 6, 2023 (end of day)*

Tests/quizzes

-

Final exam

-

Other course requirements

All students will be required to meet with the instructor on a minimum of two separate occasions (each ~15 min) to discuss early drafts of their in-class presentation.

Details on presentation

Your presentation is intended to outline a *current topic* in the field of batteries. The suggested topics are meant to complement the material from the course outline. You will present your topic in person at the scheduled time and date. Other students will be in attendance and will ask questions at the conclusion of your presentation. Your slides will be made available to the class as part of their collection of course reference material.

Presentation Format

Your presentation must be between 30-35 min in length, to be followed by ~10-15 min of questions and discussion from the audience (including the instructor). The presentation must be conducted through PowerPoint (or similar format). The presentation file must be e-mailed to the instructor at least 24 hours prior to your presentation, such that the slides can be posted to the course website.

Students are required to meet with the instructor on two separate occasions. The first meeting (~15 min) is intended to go over a 'rough outline' of your presentation. You should have a sense of the material you want to discuss on a slide-by-slide basis and need to come prepared with a written draft outline. The instructor will provide suggestions to improve your presentation, and may ask that you cover additional material, or omit some. The second meeting (minimum 1 week prior to final presentation) will include a formal 'practice talk', including feedback from the instructor. The aim of these meetings is to ensure that everyone does the best possible job with their talks, and to ensure that appropriate material is presented for the benefit of the class.

Dates for meeting 1 & 2

1st meeting: minimum 3 weeks before your presentation

2nd meeting: minimum 1 week before your presentation.

The students will be responsible for scheduling these meetings with the Instructor via an MS Outlook calendar invite.

Assessment

The presentation constitutes 30 % of your total grade, with breakdown as follows:

a) 1st meeting to discuss presentation outline - *5 marks*

b) 2nd meeting with full practice talk - *5 marks*

c) Formal presentation (Level of depth of presented material, speaking style / slide quality, level of understanding of material based on audience questions) - *20 marks*

Topic Selection

A list of potential topics will be provided; however, you are free to pick any topic with an emphasis on batteries, electrolytes, and interphases. A literature search of your topic would be a good place to start. The topic can be close to your own research, but you should not be presenting data obtained through your "own" work.

Once you have selected a potential topic, you must e-mail me your topic for approval. This includes a minimum of 2 references (attach copies) and a descriptive title. It would be helpful to also provide a short abstract of what you hope to cover. Topics will be assigned on a first come, first serve basis, with a tentative presentation date determined by the instructor.

***** Deadline for *selection and approval* of your topic is October 30 (end of day) *****

Details on written report

You are asked to write a mini scientific review of the same general topic that you will present in class. The review should therefore be a direct complement to your seminar. While the research that went into your topic might be the same, the format of a written review allows you to cover the material in a different way. Your writing style should be formal, using properly formatted paragraphs (*i.e.,* do not write in point form). The material you describe must be fully cited, with references included at the end of the report, in proper scientific format. Websites may be used for some of your references, though you must include a minimum of eight peer-reviewed scientific publications amongst your reference list.

Your report will have a strict limit of **4000 words** (not including reference). The report should be prepared in Microsoft Word (single column, double spaced, 12 pt Times New Roman font). Use subheadings as appropriate to break up the main topics of your report.

Your report must also include the following:

(1) **A descriptive title**: <120 characters

(2) **Abstract**: < 150 words, summarizing the most important aspects of your review

(3) **Keywords**: 5-10

(4) **Background**: Provide immediately relevant background on your chosen topic. Note that this is a focused mini review, and so you cannot cover everything in your background. The first paragraph should very quickly funnel down from the broader field to your specific topic. Get to the point as quickly as you can, so that you have more opportunity to expand on that specific area.

(5) **Main Body**: Your literature review is presented in this section (include subheadings where appropriate). Focus on recent works (preferably in the last 5 years). Do not attempt to cover too many articles. I suggest no more than 10, but it could be as few as 3. Include relevant figures or tables (taken straight from your referenced articles) as appropriate. I expect a minimum of 2 figures or tables, but no more than 8 in total. Figure captions and table headers are included in your word count limit.

(6) **'Personal' Commentary and 5-year outlook:** This section should be brief (a paragraph or two), where you discuss the advantages and limitations of the topic, and where future research is heading.

(7) **Concluding Remarks**: This is not meant to be a summary of the review (that's what the abstract is for). Instead, this short section (~100-150 words) should provide some comments on what the reader should take away from this topic. Where does the future lie in this area? What problems remain to be overcome? How does it compare/compete against other related topics?

(8) **References**: Reference formats are specific to journals. Use the *Journal of the Electrochemical Society* format.

Deadlines

The report is due on the last day of class (December 6, end of day). A draft copy of the written report can be submitted to the instructor for feedback. The draft is not graded, but the feedback may help you in preparing the final report.

Deadline for optional submission of a draft: Nov 27, 2023

Grading:

The following breakdown will be used to assess your report. The report itself is worth 30% of your total grade.

a) Style (basic format, referencing, figure/ table layout, font styles and grammar) - *5 marks*

b) Structure (The overall 'flow' of document, paragraph structure, conveying a clear message) - *5 marks*

c) Depth (Includes sufficient depth, with material relevant to the overall objectives of this class) - *20 marks*

Conversion of numerical grades to final letter grades follows the Dalhousie Grade Scale

A+ (90-100)	B+ (77-79)	C+ (65-69)	D (50-54)
A (85-89)	B (73-76)	C (60-64)	F (0-49)
A- (80-84)	B- (70-72)	C- (55-59)	

Course Policies on Missed or Late Academic Requirements

Students are expected to use the Student Declaration of Absence form for late or missed homework assignments. If a homework assignment is handed in up to 1 week late, it will count 50%. If a homework assignment is handed in more than 1 week late, it will count 0%.

Course Policies related to Academic Integrity

It is encouraged that students discuss assignment problems as a group. However, it is an academic offense to copy the solution of someone else or to use generative AI and large language models (e.g., ChatGPT). Allegations will be submitted to an Academic Integrity Officer of the Faculty of Science for evaluation and possible sanction. The minimum sanction is zero point on the assignment.

Learning Objectives

Students will develop an in-depth understanding of battery technology with an emphasis on electrolytes and interphases. We will discuss the latest developments in the field to prepare students for graduate work in batteries and/or a career in the battery industry.

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 may have to be skipped in the interest of time. If appropriate and available, experts from academia or industry will be invited to give guest lectures.

Tentative schedule

Semester: September 5, 2023 – December 6, 2023
Holidays: Labor Day (September 4, 2023), National Day for Truth and Reconciliation (October 2, 2023), Thanksgiving Day (October 9, 2023), In lieu of Remembrance Day (November 13, 2023)
Fall Study Break: November 13-17, 2023
Total number of lectures: 35

Lecture-by-lecture description of the course contents

1 Modern Electrolytes – *Lectures 1-2*

- 1.1 What is an Electrolyte
- 1.2 Types of Electrolytes
- 1.3 In Bulk Electrolytes: Ionics
  - 1.3.1 Solvent Molecules: Dipole and Dielectric Medium
  - 1.3.2 Dielectric Constant: Capability of a Solvent to Resist an Electric Field
  - 1.3.3 Dissolution of Solutes in Solvents: Solvation Sheath
  - 1.3.4 Revisiting the Dielectric Constant: How Ions Affect It, and Its Application
- 1.4 Static Stability of Electrolytes

2 Interface vs. Interphase – *Lectures 3-4*

- 2.1 When Electrolyte Meets Electrodes: Interface
- 2.2 When Charge Transfers Across an Interface: Electrodics
- 2.3 When an Electrode Operates Beyond Electrolyte Stability Limits: Interphase
- 2.4 Electrochemical Stability Window
  - 2.4.1 Electrochemical Stability of Aqueous and Non-aqueous Electrolytes
  - 2.4.2 Expanded Electrochemical Stability Window by an Interphase
  - 2.4.3 The Function of Interphases
- 2.5 Correlation Between Electrochemical Stability Window and Interphases

3 Electrochemical Devices – *Lectures 5-6*

- 3.1 How Does an Electrochemical Energy Device Work?
  - 3.1.1 Fuel Cells
  - 3.1.2 Electrochemical Double-layer Capacitors
  - 3.1.3 Batteries
  - 3.1.4 Pseudo-capacitors
- 3.2 Comparison and Transition Between Capacitors and Batteries

4 Lithium-metal, Lithium-ion and Other Batteries – *Lectures 7-8*

- 4.1 Why Lithium?
- 4.2 The Quest for the Holy Grail: Lithium-metal Batteries
  - 4.2.1 Irreversibility
  - 4.2.2 Dangerous Morphology
- 4.3 Circumventing Irreversibility and Safety Hazards
  - 4.3.1 The Bypass via Dual Intercalation
  - 4.3.2 The Birth of Lithium-ion Chemistries
- 4.4 Emerging Chemistries and Electrolytes
  - 4.4.1 Anode
  - 4.4.2 Cathode

5 Phase Diagrams of Liquid Electrolytes – *Lectures 9-10*

- 5.1 Phase Diagram of a Pseudo-binary Non-aqueous Electrolyte
- 5.2 Experimental Mapping of Pseudo-binary Phase Diagrams
- 5.3 Thermodynamic Calculation of Higher Order Phase Diagrams

6 Ion Solvation – *Lectures 11-15*

- 6.1 Bernal–Fowler Three-layer Model
- 6.2 The Four Basic Questions
  - 6.2.1 Solvating Site
  - 6.2.2 Solvation Number
  - 6.2.3 Preferential Solvation
  - 6.2.4 Ion Solvation in the Concentrated Regime
- 6.3 Solvation Sheaths, Solvation Cages and Solvation Sites
- 6.4 Anion Solvation

7 Ion Transport – *Lectures 16-20*

- 7.1 Phenomenological Understanding: Ion Conductivity
  - 7.1.1 Why AC (Alternating Current) Techniques?
  - 7.1.2 Ion Conductivity for Practical Battery Electrolytes
  - 7.1.3 Electrolyte Engineering for Battery Applications
  - 7.1.4 Ionicity
- 7.2 Mechanistic Understanding: Speciation
  - 7.2.1 Ideality of Electrolytes: Revisiting the Einstein Equations
  - 7.2.2 The Real Meaning of Ion Transport Number
  - 7.2.3 In Practical Electrolytes: Transport Number versus Transference Number
  - 7.2.4 A Few Classical Approaches to Transference Numbers
  - 7.2.5 Reference Frame for Ionic Transference
- 7.3 Newman’s Ion Transport Theory: A Brief Introduction
  - 7.3.1 Concentrated Solution Theory
  - 7.3.2 Limitations of Newman’s Concentrated Solution Theory

8 Interfaces – *Lectures 21-23*

- 8.1 Defining an Interface
  - 8.1.1 Ionic Fluxes in Bulk and Across an Interface
  - 8.1.2 Concentration Profiles in the Bulk Region
  - 8.1.3 Concentration Profiles in the Interfacial Region

9 Interphases – *Lectures 24-29*

- 9.1 Defining an Interphase
- 9.2 Interphase is Created by Electrode-Electrolyte Mismatch in Electron Energy Levels

9.3 What Is a Good Interphase?
9.4 Charge Transfer in the Presence of 2D Interfaces and 3D Interphases
9.5 Two Distinct Manners of Forming Interphases
9.5.1 Proto-interphase and Interphase in an “Anode-free” Lithium-metal Cell
9.5.2 Rationale Behind Electrolyte Additives
9.6 Chemistry of Interphases
9.6.1 In Lithium-ion Batteries
9.6.2 In Lithium-metal Batteries
9.6.3 Interphasial Chemistries Brought by Additives
9.6.4 In “Beyond Lithium-ion” Chemistries
9.6.5 Stability of Interphasial Ingredients
9.6.6 Interphasial Components Under Debate
9.6.7 How Working Ions Travel Across Interphases

10 New Concepts and Tools – *Lectures 30-34*
10.1 Super-concentrating: Unusual Properties
10.1.1 Ethers Could Be Anodically Stable
10.1.2 Esters Could Be Cathodically Stable
10.1.3 Exotic Solvents Could Be Electrochemically Stable
10.1.4 Water Could Have a Wide Electrochemical Stability Window
10.1.5 Locally Concentrated Electrolytes, Aqueous–Non-aqueous Hybrid Electrolytes
10.2 Beyond Liquid Phases: Liquefied Gas and Frozen Ice
10.3 Solidifying Electrolytes
10.3.1 Polymer Electrolytes
10.3.2 Liquid–Inorganic Interfacing
10.3.3 True Solid Electrolytes and Their Interfaces/Interphases
10.4 Nano-confining Electrolytes
10.5 Artificial Interphases
10.6 Dynamic Interphases
10.7 New Characterization Techniques
10.8 Computer Simulations
10.8.1 Molecular Simulations
10.8.2 Prediction of Properties and Performances
10.8.3 Computational Design of Materials

11 Outlook – *Lecture 35*

University Policies and Statements

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 at 1321 Edward St or elders@dal.ca. Additional information regarding the Indigenous Student Centre can be found at: https://www.dal.ca/campus_life/communities/indigenous.html

Internationalization

At Dalhousie, ‘thinking and acting globally’ enhances the quality and impact of education, supporting learning that is “interdisciplinary, cross-cultural, global in reach, and orientated toward solving problems that extend across national borders.” Additional internationalization information can be found at: https://www.dal.ca/about-dal/internationalization.html

Academic Integrity

At Dalhousie University, we are guided in all our work by the values of academic integrity: honesty, trust, fairness, responsibility, and respect. As a student, you are required to demonstrate these values in all 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. Additional academic integrity information can be found at: https://www.dal.ca/dept/university_secretariat/academic-integrity.html

Accessibility

The Student Accessibility Centre is Dalhousie's centre of expertise for matters related to student accessibility and accommodation. If there are aspects of the design, instruction, and/or experiences within this course (online or in-person) that result in barriers to your inclusion, please contact the Student Accessibility Centre (https://www.dal.ca/campus_life/academic-support/accessibility.html) for all courses offered by Dalhousie with the exception of Truro. For courses offered by the Faculty of Agriculture, please contact the Student Success Centre in Truro (https://www.dal.ca/about-dal/agricultural-campus/student-success-centre.html)

Conduct in the Classroom – Culture of Respect

Substantial and constructive dialogue on challenging issues is an important part of academic inquiry and exchange. It requires willingness to listen and tolerance of opposing points of view. Consideration of individual differences and alternative viewpoints is required of all class members, towards each other, towards instructors, and towards guest speakers. While expressions of differing perspectives are welcome and encouraged, the words and language used should remain within acceptable bounds of civility and respect.

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 (Strategic Priority 5.2). Additional diversity and inclusion information can be found at: http://www.dal.ca/cultureofrespect.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. The full Code of Student Conduct can be found at: https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html

Fair Dealing Policy

The Dalhousie University Fair Dealing Policy provides guidance for the limited use of copyright protected material without the risk of infringement and without having to seek the permission of copyright owners. It is intended to provide a balance between the rights of creators and the rights of users at Dalhousie. Additional information regarding the Fair Dealing Policy can be found at: https://www.dal.ca/dept/university_secretariat/policies/academic/fair-dealing-policy-.html

Originality Checking Software

The course instructor may use Dalhousie's approved originality checking software and Google to check the originality of any work submitted for credit, in accordance with the Student Submission of Assignments and Use of Originality Checking Software Policy. Students are free, without penalty of grade, to choose an alternative method of attesting to the authenticity of their work and must inform the instructor no later than the last day to add/drop classes of their intent to choose an alternate method. Additional information regarding Originality Checking Software can be found at: https://www.dal.ca/dept/university_secretariat/policies/academic/student-submission-of-assignments-and-use-of-originality-checking-software-policy-.html

Student Use of Course Materials

Course materials are designed for use as part of this course at Dalhousie University and are the property of the instructor unless otherwise stated. Third party copyrighted materials (such as books, journal articles, music, videos, etc.) have either been licensed for use in this course or fall under an exception or limitation in Canadian Copyright law. Copying this course material for distribution (e.g. uploading to a commercial third-party website) may lead to a violation of Copyright law.