MSE 597RB

Introduction to the Modeling of Rechargeable Batteries

Instructors

Prof. Edwin García and Dr. David Ely

Course description

Electrochemical materials and its application to energy storage and conversion devices, such as batteries and fuel cells are a rapidly growing field, particularly for portable technologies and electric and hybrid vehicles. This course will deliver an introduction to the modeling and simulation of rechargeable batteries by starting from basic electrochemistry principles. Applications to currently existing and emerging rechargeable batteries (lithium-ion batteries in particular) will be reviewed. Theoretical and practical aspects of battery operation will be conveyed, while placing an emphasis on the integration of electrochemical principles and materials science for rechargeable battery technology. An introduction of the simulation methods being used by the battery industry will be presented. Current trends and directions of the field of battery technology will also be outlined.

Grading Policy

Homework	20%
Project Report #1	40%
Project Report #2	40%

Two projects will be assigned during the course where students will exercise the concepts and techniques learned to address short problems. There will be NO final exam. In addition, several homework assignments will be assigned during the semester.

References

We will primarily use seminal and review papers on the field, which will be readily provided to students as electronic handouts. Class notes and example Python scripts simulating the electrochemical kinetics of porous rechargeable batteries will complete the to-be transferred teaching material.

Supplementary References

J. Newman, K. E. Thomas-Alyea *"Electrochemical Systems."* Wiley Interscience, third edition, 2004.
R. Huggins *"Advanced Batteries. Materials Science Aspects."* Springer, first edition, 2009.
C. A. Vincent, B. Scrosati *"Modern Batteries. An Introduction to Electrochemical Power Sources."* Butterworth-Heinemann, second edition, 2003.

Topics

A. Basic Principles and Introductory Material
    a. Chemical and Electrochemical Reactions
    b. Concepts of Charge, Energy, and Power Density
    c. Ragone plot, Capacity Curve, and other graphical means to compare batteries
    d. Battery Architectures
    e. Modeling Macroscopic Equilibrium Battery Parameters

B. Electrode Kinetics and Other Interfacial Phenomena
    a. The Structure of the Double Layer
    b. The Overpotential Approximation
    c. Interfacial Kinetics: The Butler-Volmer Equation and other Approximations
    d. Irreversible Reactions
    e. The Surface Electrolyte Interface
    f. Dendrite Formation
    g. Battery Fading
    h. Modeling Interfacial Kinetics in Rechargeable Lithium-Ion Batteries

C. Transport Processes in Electrochemical Cells
    a. Introduction to Irreversible Thermodynamics
    b. Multicomponent Diffusion of Charged Species
    c. Mobilities and Diffusion Coefficients (The Transference Number)
    d. The Diluted Limits
    e. Concentrated Solutions
    f. Extension to Thermal Transport
        i. Transport in the Bulk
        ii. Transport in the Interface
    g. Modeling Mass and Charge Transport in Electrochemical Systems

D. Theory of Porous Electrodes
    a. Macroscopic Approximation and Averaging of Microstructures
    b. Material Balance of Solutes
    c. Electroneutrality and Charge Conservation
    d. Interfacial Effects
    e. Newman Approach to Battery Modeling

E. Thermodynamics of Electrochemical Cells
    a. Chemical Potential and Electrochemical Potential
    b. Equilibrium Cell Voltage and Cell Capacity
    c. Temperature Dependence on Cell Voltage
    d. The Gibbs Phase Rule and the Open Circuit Voltage (OCV)
    e. OCV and its relation to the Binary Phase Diagram of an Electrode Material
    f. Ternary Systems: Examples
    g. Chemical Expansion/Contraction in Rechargeable Batteries
    h. Modeling Thermodynamic Potentials of Rechargeable Lithium-Ion Batteries

F. Cathode Materials
    a. Lithium Manganese Oxide
    b. Lithium Cobalt Oxide
    c. Lithium Iron Phosphate and Associated Compounds
G. Anode Materials
    a. Graphite
    b. Lithium as an Anode Material
    c. Other Anode Materials
H. Electrolytes
I. Battery Design

General Administrative Matters

I. Campus Emergency Policy

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances. Any such changes will be posted to the course website on *the nanoHUB*. If you are unable to use the nanoHUB from home please let us know early in the semester so we can make other arrangements for your special needs.

Use of cell phones and similar devices, including texting, is strongly discouraged during class. However, please make sure that such devices are set to silent or vibrate mode in order to be informed in case of a campus emergency. If you receive a message indicating an emergency, please communicate Purdue's announcement to the class.

II. General Statement on Academic Dishonesty

Purdue University Regulations, Part 5, Section III-B-2-a describes the formal policies governing academic dishonesty. Purdue prohibits "dishonesty in connection with any University activity. Cheating, plagiarism, or knowingly furnishing false information to the University are examples of dishonesty." A guide providing specific examples, tips, and consequences is available from the Office of the Dean of Students at:

http://www.purdue.edu/odos/osrr/academicintegritybrochure.php .

As discussed in this brochure on *Academic Integrity*, there are many dishonest ways to gain an advantage over another student in an assignment. The goal is not to list these here, but these rules cover <u>any</u> assignment for which the instructor will assign a grade (homework, quizzes, exams, laboratory reports, term paper, etc.). Rather, students should ask themselves this question when working on all class assignments: *"If I use this information, will the completed assignment represent only my efforts?"* If the answer is no, then don't do it. The test is simple. For example, turning in a term paper obtained from a website does not represent your efforts. Turning in copied homework from another student or solutions manual does not represent your efforts either.

III. Specific Statement on Academic Dishonesty For MSE 597RB

Homework in MSE 597RB: The homework solutions are worth only 20% of the final grade. The benefits of learning from mistakes made in thinking for yourself on the homework far outweigh the risks of cheating. Discussion between students regarding the concepts and general approach used for a homework problem is allowed (and strongly encouraged). However, the solutions you turn in for grading must be your own original work. *Ask me if you are confused about this policy*.

Term Papers in MSE 597RB: When you are using information that has previously been published (article, book, etc.) it is required that you reference it. If you are using exactly or nearly exactly a paragraph from a published work it must be put in quotations. MSE is now using a variety of software to check your work against prior lab reports and other published works for plagiarism.

IV. Consequences of Academic Dishonesty in MSE

The teaching staff for this course will diligently monitor academic dishonesty in all assignments. Students found to engage in academic dishonesty are subject to discipline to potentially include: a grade of zero for the assignment, a grade of F for the course, a permanent letter added to your file, and reporting the incident to the Dean of Students for further action. Two letters in your file will result in an automatic forwarding of the case to the Dean of Students.

Please note that students who share their prior assignments with students currently enrolled in the course can also be disciplined.