MSE 597: Introduction to the Materials Science of Rechargeable Batteries

Monday, Wednesday, and Friday, from 10:30 to 11:30 AM in ARMS 1103

Instructor
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Course description
MSE 597 is aimed at junior/senior undergraduate and graduate students interested on developing an understanding on the Materials Science of Rechargeable Batteries. The focus is on electrochemical materials, its non-idealities (e.g., transport limitations, failure mechanisms), and its application to energy storage devices, such as batteries and fuel cells, particularly for portable electronics and hybrid/electric vehicles. This course will deliver an introduction to basic electrochemistry, principles of electrochemical devices, and electroactive materials as used in such systems. Current trends and directions in the field of battery technology will be outlined.

Grading Policy
Homework 20%
Exam #1 40%
Exam #2 40%

Two exams will be issued 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. These assignments will be graded as either complete or incomplete. A one-week grace period to submit the homework will be issued.

References
We will primarily use seminal and review papers on the field, which will be readily provided to students as electronic handouts.

Supplementary References

Topics
A. Basic Principles and Introductory Material (one week)
   a. Chemical and Electrochemical Reactions
c. Ragone plot, Capacity Curve, and other graphical means to compare batteries

HW1
B. Thermodynamics of Electrochemical Cells (two weeks)
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

HW2
C. Electrode Kinetics and Other Interfacial Phenomena (two weeks)
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

HW3
D. Transport Processes in Electrochemical Cells (one week)
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

HW4
E. Theory of Porous Electrodes (one week)
a. Macroscopic Approximation and Averaging of Microstructures
b. Material Balance of Solutes
c. Electroneutrality and Charge Conservation
d. Interfacial Effects
e. Introduction to Battery Modeling

F. The Lithium-Ion Battery (three to four weeks)
a. Cathode Chemistries
b. Anode Chemistries
c. Electrolyte Chemistries

HW5+6
G. Other Battery Chemistries (one or two weeks)
a. The Li-Air Battery
b. The Na/NiCl₂ Battery
c. The Lead-Acid Battery
d. The Ni-MH Battery
e. The Ni-Cd Battery

H. Battery Architectures (one lecture)
   a. Cylindrical
   b. Prismatic
   c. 3D Batteries

HW7
   I. Chemico-Mechanical Stresses in Li-ion Batteries (if time permits)
   J. Battery Benchmarking and Characterization (if time permits)

HW8 (if time permits)
   K. Principles of Battery Design (one week, if time permits)

HW9 (if time permits)

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 me know early in the semester so I can make other arrangements to meet 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 any 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 597

Homework in MSE 597: The homework solutions are worth only 20% (each HW is 2.5%) of the final grade. The benefits of learning from mistakes made in thinking for yourself 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.

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.