TO: The Engineering Faculty

FROM: The Faculty of the School of Materials Engineering

RE: New graduate course – MSE 57700 Materials Science of Rechargeable Batteries

The Faculty of the School of Materials Engineering has approved the following new graduate course as of Sept. 26, 2022 (see attached document for course description). This action is now submitted to the Engineering Faculty with a recommendation for approval.

FROM:

MSE 597 Materials Science of Rechargeable Batteries, Sem. 1, 2, SS, Class 3, Cr. 3.
Prerequisites: Junior standing or higher in Engineering or Science

Temporary course number. Course was taught F21, F19, F17, F15, F13. Enrollment was 39, 16, 13, 40, and 7 students, respectively.

TO:

MSE 57700 Materials Science of Rechargeable Batteries, Sem. 1, 2, SS, Class 3, Cr. 3.
Prerequisites: Junior standing or higher in Engineering or Science

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.

Reason: This course has been taught successfully as a temporary course and it is now being submitted for a permanent course number.

David Bahr
Head of MSE

Proposal for New Graduate Level Course for Academic Review
MSE 57700 – Materials Science of Rechargeable Batteries

Note: The detailed course proposal is intended for academic review by the appropriate area committee of the Graduate Council. It supplements the Form 40G that is intended for administrative review of the Graduate School and Registrar.

TO: Purdue University Graduate Council

FROM: Faculty Member: R. Edwin Garcia
Department: School of Materials Engineering
Campus: West Lafayette

DATE: March 17, 2021

SUBJECT: Proposal for New Graduate Course

MSE 57700 Materials Science of Rechargeable Batteries
SEM 1 or 2, Lecture 2, cr. 3

1. 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.

2. Justification for the Course

2.1 Justification of the need for the course

This introductory course in Rechargeable Batteries has been taught in MSE since 2010, and has been requested every year through email by students from multiple Engineering departments. The class provides an integrative approach that introduces fundamental electrochemistry and materials science principles to provide a rational basis in the design of existing and emerging rechargeable power source technology. The course incorporates elements of theory and materials modeling and enables the student to perform materials, processing, and application selection, which in turn defines a unique approach to learn the fundamentals behind battery technology.

The class standing is requested at the 500 level due to it being a historically non-traditional learning route for MSE students. The course attracts both undergraduate and graduate students. Although is a course that attracts a majority of upper division undergraduate students, it is requested at the 500 level since it is perceived as the next level towards an understanding of

Materials Science from a different perspective than the one traditionally taught in the School Curriculum.

This is the only class on Purdue's campus that provides a focus relating basic science electrochemistry and its impact on properties, processing, performance and reliability or rechargeable batteries.

3. Learning Outcomes and Methods of Assessment

3.1 Learning Outcomes

The objective of this course is on the development 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. This course will start from an introduction to basic electrochemistry, principles of electrochemical devices, and electroactive materials as used in such systems. The developed framework will be used to rationalize current and emerging performance measures, utilized language, and establish the basis for current trends and directions in the field of battery technology.

1. All Students

A. Will become familiar with lingo, language, units and quantities associated to modern battery technology.
B. Will be able to read the scientific literature on rechargeable batteries
C. Relate properties to performance (power, energy, charge, health, life, etc.)
D. Will be able communicate results of battery technology to professional audiences

2. Most Students

A. Will be able to make simple battery designs that maximize performance.
B. Will develop a basic understanding of the most widely used battery simulation software.
C. Will be able to make simple battery designs that maximize reliability.

3.2 Assessment Methods

Weekly or biweekly homework assignments will be issued during the semester as a means to practice the concepts presented in class, and as practice for the two exams. Homework can be turned in individually or as a team of 2 or more students. Two exams will be issued during the course where students will exercise the concepts and techniques learned to address short problems. Concepts are cumulative, and as the semester progresses, the concepts build on top of themselves and become more sophisticated. Exams are based on concepts covered during class, as well as reading and homework assignments that will be posted in Brightspace. The Term Project corresponds to an assigned battery architecture, chemistries, and performance and degradation goals that the students need to research by combining concepts developed in class, presented software, and existing experimental literature. Projects will be presented by each of the teams during class at the end of the semester.

3.3 Final Grading Criteria

Grading is based on a curved scale, based on the performance relative to the rest of the class.

Grading:

Assessment is achieved by:

Homework Assignments (8-10)	20%
Exam 1	20%
Exam 2	20%
Term Project	20%
Project Presentation	20%
Total	100%

Grading Scale: Historically, 85% or higher - A; 70% - B; 60% - C; 50% - D.

3.4 Methods of Instruction

Lecture – Lectures will be used to help the students to achieve the learning outcomes. These include discussions on concepts and basic principles, examples, micrographs, and analyses on experimental data.

3.5 Prerequisite(s)

Junior standing or higher in Engineering or Science.

4. Course Instructor

Edwin García, Professor MSE, member of the Graduate Faculty:

Prof. García has 20+ years of experience and training in battery theory, modeling and design. He has served as a consultant to battery companies, has submitted several patents and copyrights on battery technology and performed analyses for industrial partners during externally funded research.

5. Course Outline:

i. Basic Principles and Introductory Material (one week)
   a. Chemical and Electrochemical Reactions
   b. Concepts of Charge, Energy, and Power Density (MTSE)
   c. Ragone plot, Capacity Curve, and other graphical means to compare batteries

ii. 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

iii. 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

iv. 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

v. 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

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

vii. Other Battery Chemistries (one or two weeks)
   a. The Li-Air Battery
   b. The $Na/NiCl_2$ Battery
   c. The Lead-Acid Battery
   d. The Ni-MH Battery
   e. The Ni-Cd Battery

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

6. Reading List

-Class Notes (to be posted in Brightspace)

-Seminal and review papers on the field, which will be readily provided to students as electronic handouts (to be posted in Brightspace).

-J. Newman, K. E. Thomas-Alyea *"Electrochemical Systems."* Wiley Interscience, third edition, 2004 (optional reading; not required).

-R. Huggins *"Advanced Batteries. Materials Science Aspects."* Springer, first edition, 2009 (optional reading; not required).

- C. A. Vincent, B. Scrosati *"Modern Batteries. An Introduction to Electrochemical Power Sources."* Butterworth-Heinemann, second edition, 2003 (optional reading; not required).

G. Library Resources

Purdue University Engineering Library.

7. Past Course Syllabus

8. MSE 597: Introduction to the Materials Science of Rechargeable Batteries

8.1 Course Information

Prof. R. Edwin García:	redwing@purdue.edu		
Lectures recorded Live:	T, Th	9 to 10:15AM	ARMS 1103
Lectures Materials:	T, Th	to be posted as soon as possible	
Office Hours Physical:	W	3 to 4PM	ARMS 2325
Office Hours Virtual:	W	3 to 4PM	

8.2 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.

8.3 Learning Outcomes

Students will:

- Learn to critically read the literature on electrochemical systems, particularly Lithium-ion batteries
- Be able to perform basic materials science-based battery designs
- Learn to use industry-standard battery modeling code.

8.4 Grading Policy

Homework	20%
Exam 1	20%
Exam 1	20%
Project Report	20%
Project Presentation	20%

There will be NO final exam.

8.5 Term Project

A home examination module will be issued where students will exercise the concepts and techniques learned to address a realistic battery design problem. The module will be evaluated through a written paper that summarizes the student's calculations and/or research. The student will be expected to draw on the knowledge developed in class only.

8.6 Homework

Weekly and biweekly homework assignments will be assigned during the semester (between 7 and 10). A one-week grace period to submit the homework will be issued. **Homework will be due at the beginning of the class when it is due.**

8.7 Attendance Policy

Attendance (physical or virtual) is appreciated, but will not be recorded and will have no bearing on the final grade.

8.8 Attendance Policy During COVID-19

Students should stay home and contact the Protect Purdue Health Center (496-INFO) if they feel ill, have any symptoms associated with COVID-19, or suspect they have been exposed to the virus. In the current context of COVID-19, in-person attendance will not be a factor in the final grades, but the student still needs to inform the instructor of any conflict that can be anticipated and will affect the submission of an assignment or the ability to take an exam. Only the instructor can excuse a student from a course requirement or responsibility. When conflicts can be anticipated, such as for many University-sponsored activities and religious observations, the student should inform the instructor of the situation as far in advance as possible. For unanticipated or emergency conflict, when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email, through Brightspace, or by phone. When the student is unable to make direct contact with the instructor and is unable to leave word with the instructor's department because of circumstances beyond the student's control, and in cases of bereavement, quarantine, or isolation, the student or the student's representative should contact the Office of the Dean of Students via email or phone at 765-494-1747. Our course Brightspace includes a link on Attendance and Grief Absence policies under the University Policies menu.

8.9 Class Participation

Class participation is greatly encouraged, and questions are appreciated. The instructor will take note to resolve borderline cases at the end of the semester.

8.10 In the Case a Student is Quarantined/Isolated

If you become quarantined or isolated at any point in time during the semester, in addition to support from the Protect Purdue Health Center, you will also have access to an Academic Case Manager who can provide you academic support during this time. Your Academic Case Manager can be reached at acmq@purdue.edu and will provide you with general guidelines/resources around communicating with your instructors, be available for academic support, and offer suggestions for how to be successful when learning remotely. Importantly, if you find yourself too sick to progress in the course, notify your academic case manager and notify me via email or Brightspace. We will make arrangements based on your particular situation. The Office of the Dean of Students (odos@purdue.edu) is also available to support you should this situation occur.

8.11 Mental Health/Wellness Statement

If you find yourself beginning to feel some stress, anxiety and/or feeling slightly over-whelmed, try WellTrack (https://purdue.welltrack.com). Sign in and find information and tools at your fingertips, available to you at any time.

If you need support and information about options and resources, please contact or see the Office of the Dean of Students (https://www.purdue.edu/odos/). Call 765-494-1747. Hours of operation are M-F, 8 am- 5 pm.

If you find yourself struggling to find a healthy balance between academics, social life, stress, etc. sign up for free one-on-one virtual or in-person sessions with a Purdue Well- ness Coach at RecWell (https://www.purdue.edu/recwell/fitness-wellness/wellness/one- on-one-coaching/wellness-coaching.php). Student coaches can help you navigate through barriers and challenges toward your goals throughout the semester. Sign up is completely free and can be done on BoilerConnect. If you have any questions, please contact Purdue Wellness at evans240@purdue.edu.

If you're struggling and need mental health services: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at 765-494-6995 during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours (https://www.purdue.edu/caps/).

8.12 Accessibility Statement

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: drc@purdue.edu or by phone: 765-494-1247. More details are available on our course Brightspace under Accessibility Information.

8.13 Grading Scale

Grading will be performed relative to the average performance of the rest of the students in the class (will grade in a curve). Students within one standard deviation (above and below) the average will receive a B grade, students one standard deviation above the average will receive an A, while students below one standard deviation mark will receive a C. Students with two standard deviations below the average will receive a D, and students with 40% or less of the total number of points will receive an F. + and – grades will be assigned to distinguish borderline cases and outstanding students.

8.14 General Administrative Matters

I. Non-Discrimination Statement

Purdue University is committed to maintaining a community which recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life. More details are available on our course Brightspace table of contents, under University Policies.

II. 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. If you are unable to use the internet from home please let me know early in the semester so I 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.

Related Considerations and Guidelines

1. If you experience any symptoms of COVID-19 or suspect you may have been ex- posed to someone with COVID-19 stay home and call the Protect Purdue Health Center at 765-496-INFO.

2. Keep your cell phone on to receive a Purdue ALERT text message.

3. Log into a Purdue computer connected to the network to receive any Desktop Popup Alerts.

III. 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.

IV. 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.*

V. 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.

8.15 Class Software

https://nanohub.org/tools/dualfoil
https://nanohub.org/tools/vkmllive

8.16 References

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

8.17 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.

8.18 Topics

ix. Basic Principles and Introductory Material (one week)
   a. Chemical and Electrochemical Reactions
   b. Concepts of Charge, Energy, and Power Density (MTSE)
   c. Ragone plot, Capacity Curve, and other graphical means to compare batteries

   HW1

x. 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

xi. 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

xii. 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
(Project assignment)

xiii. 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

    HW5

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

    HW6

xv. Other Battery Chemistries (one or two weeks)
    a. The Li-Air Battery
    b. The $Na/NiCl_2$ Battery
    c. The Lead-Acid Battery
    d. The Ni-MH Battery
    e. The Ni-Cd Battery

    HW7

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

    HW8

xvii. Chemico-Mechanical Stresses and Other Degradation Mechanisms in Li-ion Batteries

    HW9

xviii. Battery Benchmarking and Characterization (if time permits)

    (Final Project Presentations)