CHMENG 186/286 Fundamental Electrochemistry Summer Session A 2025 (6 weeks)

Transcript Title: Fund Electrochem

I. Course Identity, Teaching Staff, and Logistics

Instructor: Prof. Shannon Boettcher, email: boettcher@berkeley.edu, Office: 212 Gilman

This is a new lecture course that would be taught/co-taught by Prof. Boettcher, Prof. Bryan McCloskey, Prof. Niel Razdan, Prof. Nitash Balsara, PhD level Lawrence Berkeley scientists, or a new electrochemistry instructor / program director (PhD level, TBD).

Graduate Student Instructor (GSI): Student Name will serve as a GSI for this course. They are available at <u>GSIemail@berkeley.edu</u> and will schedule weekly tutorial office hour sessions to assist in learning the material.

Office hour: There will be three office hours per week, held in Gilman 212. The times will be determined on the first day of lecture based on student availability.

Format: The course will be offered in person. The course will make use of pre-recorded lecture content a blend of lecture and active learning in particular through think-pair-share activities during the in person in class.

Students in CHMENG 286 will have required projects that are not required for undergraduate CHMENG 186 students.

Credits: 3

Location: Lectures will be held in Building, Room# four days per week (M, Tu, W, Th). Each class will be 1.5 h in duration and generally held in the mid morning.

Required course materials:

Bard, Faulkner, and White. *Electrochemical Methods: Fundamentals and Applications 3rd Edition* Wiley 2022.

Supplementary course materials:

Fuller and Harb. *Electrochemical Engineering*. Wiley 2018. (this text will be used extensively in the following Electrochemical Engineering course, if you plan to take that course, you should purchase this book now)

Schmickler and Santos, Interfacial Electrochemistry, 2nd ed. 2010 Springer

Course website: Lecture notes, videos, homework solutions, and grades will be posted on the course site website. Daily discussion will generally not be recorded.

Prerequisites:

Undergraduates in CHMENG 186 are generally expected to have completed junior-level courses in their major.

- Chemistry students must have taken at least one semester of physical chemistry, CHEM 120A or 120B.
- CBE majors must have taken at least one semester of upper division coursework including one of CHMENG 142, CHMENG 150B, or CHEM 120A.
- Materials Science and Engineering Majors should have taken at least one semester of MSE 103, MSE 111, or MSE 112, in addition to completing required PHYS 7A-C and ENG 40.
- Mechanical Engineering Majors should have taken required PHYS 7A-B and CHEM 1A, in addition to taking MEC ENG 40 (Thermodynamics) and MEC ENG 106 (Fluid Mechanics).
- Physics majors should have taken CHEM 1A or have AP-level high school chemistry, have completed lower division coursework in physics, and taken at least one semester of upper division physics coursework such as Physics 111A or 110A.

Graduate students in Chemistry, Engineering or Physics disciplines should be suitably prepared to enroll in CHMENG 286 but are recommended to review preparatory materials posted on the Center for Electrochemical Science, Engineering, and Technology website: https://electrochemistry.berkeley.edu/education

II. Course Catalog Description

Electrochemistry is a field of science that describes the interrelation of chemical and electrical effects. Much of the field deals with describing how chemical changes are caused by the passage of electrical current or how the production of electrical current can be caused by chemical reactions. Electrochemists rely on a foundational understanding of chemical thermodynamics and electrostatics, chemical and electron-transfer kinetics, and mass-transport phenomena – each of which are treated and developed in this course in the context of electrochemical phenomena. Additional topics include electrochemical instrumentation, practical electrochemistry, and electrochemical impedance spectroscopy.

Projects

Students enrolled in CHMENG 286 will be able to gain deeper experience in two projects selected from the topics made available by the instructors. Example areas include special topics presentations (such as scanning electrochemical methods, absorption isotherms in electrochemistry, semiconductor photoelectrochemistry, modern electrocatalysis), experimental data collection, practical electrochemical data analysis, and computer-simulating

electrochemical data. Example experimental projects may include (1) the fabrication and testing of reference electrodes, setting up a basic electrochemical cell, and performing basic electrochemistry measurements, (2) measuring/analyzing electrocatalytic properties and electrode kinetics, (3) collecting and analyzing cyclic voltammetry data. Students will be responsible for scheduling time using available equipment to complete the projects for those that require experimental facilities.

Please discuss this with the instructors before you select your project topics. **Please see the attached project addendum.**

III. Expected Learning Outcomes

- Learn and critically apply foundational concepts in chemical thermodynamics, kinetics, and mass transport to analyze electrochemical data and predict the response of electrochemical systems.
- Understanding and employ models of the electrical double layer to predict reactions and rates in electrochemical devices.
- Understand and apply concepts of electrochemical impedance analysis to model electrochemical systems.

IV. Estimated Student Workload

Course participants will attend lecture, perform assigned reading and watch/study assigned pre-class lectures, work assigned problem sets, and demonstrate the knowledge learned on exams. The table below shows the estimated workload.

Activity	Estimated hours per term	Comments	
Lectures	36	6 h / wk * 6 weeks	
Assigned Reading and Video Content	36	From Fuller and Harb	
Problem Sets	54	Assigned Weekly	
Projects (CHEMENG 286 students only)	(16)	8 h /project	
Exam Preparation	10	4 h for midterm, 6 h for final	
Total hours:	136 (or 152)	Consistent with 3 credit workload	

V. How Grades Will Be Determined

The grades will be determined based on the following percentage breakdown of the final total score:

Graduate Students

Problem Sets and in-class work - 20% Exam - 40%	Projects - 20%	Midterm Exam - 20%	Final
Undergraduate Students			
Problem Sets and in-class work - 35%	Midterm Exam - 25%	Final Exam - 40%	

Problem sets will be graded for completion, students who complete each problem set and turn them in by the deadline will receive full credit. Each problem must be fully worked, with clear logical explanation of the approach to receive credit.

Projects will be graded based on the quality of the project report. Reports are expected to be concise formal documents with professional quality graphs and analysis and insightful discussion (5 pages of concise, single spaced, scientific writing for each). Each project assignment is accompanied by a document outlining project expectations (see attached rubric). These projects will include work-up of provided real-word data, simulation, and analysis of large data sets.

A = Clearly written, concise document, with high-quality figures. All required pieces of data are shown and discussed without major errors in the interpretation.

B = One or more issues with the items above.

C = Multiple issues with quality of the written document and interpretation/discussion.

D = Multiple issues and incomplete.

The midterm and final exams will be based largely on the content in the assigned problem sets, content emphasized in class discussion, and that emphasized in the projects. Letter grades will not be assigned on these exams, students will receive a percentage score for the exam.

Students earning >90% in the course will earn at least and A, > 80% at least a B, >70% at least a C, and >60% at least a D. The instructor may curve the course to increase the letter grades for a given percentage score to account for variations in difficulty of the exam questions from year-to-year. Students with a given percentage score will not, however, earn a grade lower than that indicated above.

VI. Course Schedule and Assignments

Assigned reading and pre-class lecture videos: Sections from Bard and Faulkner given parenthetically after each topic. You will also be assigned pre-class videos to watch to prepare for in-class discussion and work.

<u>Week 1</u>

Lecture 1: What is electrochemistry? Overview of fundamentals: thermodynamics, kinetics, and transport

Lecture 2: Introduction to electrochemical methods, cells, and instrumentation. Faradaic versus non-Faradaic processes. Introduction to stirred voltammetry for Nernstian systems and the effects of mass transport.

Reading: Introduction to Electrochemistry (1.1-1.6, pg 1-51; section 1.9 will be of interest if you are taking the concurrent laboratory course)

Problem set 1: Selected problems from Chapter 1.

Lecture 3: Finish stirred voltammetry for Nernstian systems and the effects of mass transport.

Lecture 4: Reversibility, Free Energy, half-reactions and reduction potentials.

Reading: Potentials and Thermodynamics of Cells (2.1 - 2.3.3, pg 61-96)

Problem set 2: Selected problems from Chapter 2 and instructor supplement.

Project 1: Select project topic from options provided by instructor.

Week 2

Topics Class 5-6

Lecture 1: Formal potentials. Reference electrodes

Lecture 2: The electrochemical potential, its uses, and its relation to the Fermi Level in a solid. **Reading:** Electrochemical Potential Primer:

https://pubs.acs.org/doi/10.1021/acsenergylett.0c02443

Problem set 2: Selected problems from Bard and Faulkner Chapter 2 and instructor supplement.

Topics Class 6-7

Lecture 3. Finish electrochemical thermodynamics fundamentals. Introduction to Pourbaix diagrams.

Lecture 4: Construction and use of E-pH (Pourbaix) diagrams.

Reading: Handout from: The Aqueous Chemistry of the Elements, *Scheitzer and Pesterfield*, 2010. Pg 3-32.; also re-read 2.1.9.

Problem set 3: Constructing a Pourbaix diagram problems.

Week 3

Lecture 1: The structure of the double layer and its effect on electrode kinetics
Lecture 2 Derivation and use of the Butler-Volmer and Tafel equations
Reading: Electrode Kinetics (Ch. 3.1-3.4, pg 121-142)
Project 1 due.
Problem set 4: Selected problems from Chapter 3 and instructor supplement.
Lecture 3: Continued; theories of electrode kinetics
Lecture 4: Multistep mechanisms. Marcus Theory

Reading: (3.5, pg 142-168) Midterm (take-home, details TBD)

Week 4

Topics:

Lecture 1: Mass transfer via diffusion and migration. The Nernst-Planck Equation **Lecture 2:** Potential Step Experiments and the Cottrell Equation.

Reading: (4.1-4.5, pg. 183-204, 5.1, pg. 207-214) (see Fuller and Harb as an additional resource that is perhaps simpler to read than Bard and Faulkner on this topic).

Project 2: Select project topic from options provided by instructor.

Problem Set 5: Work handout on diffusion and migration, selected problems from Bard and Faulkner.

Lecture 3: Potential step and sweep methods

Lecture 4: Discussion of electrochemical simulations of voltammetry

Reading: (6.1 pages 261-275 and Dempsey J. Chem. Ed. A Practical Beginner's Guide to Cyclic Voltammetry <u>https://pubs.acs.org/doi/10.1021/acs.jchemed.7b00361</u>, and (12.1, pg. 471-476), **Problem Set 6: Voltammetry**

Week 5

Lecture 1: Multi step reactions (CE, EC, ECE, etc.)

Lecture 2: Simulations and analytical expressions for multistep reaction kinetics and analysis **Reading:** Bard and Faulkner multistep reactions 13.1 pages 539-545, impedance 11.1-11.4 pages 443-469

Lecture 3: Impedance Introduction (AC circuits, complex numbers, etc)

Lecture 4: Equivalent circuit fitting and analysis

Problem Set 6: Electrochemical Impedance

<u>Week 6</u>

Lecture 1: in class project presentations, questions, structured feedback

Lecture 2: in class project presentations, questions, structured feedback

Lecture 3: Review for final exam

Lecture 4: Final Exam

VII. Course Policies

- Late or missed work will not generally be accepted without prior approval.
- For students in the graduate level course: Project reports must be your own work. You may share data across the class if it strengthens the quality of the report but the analysis and discussion of the data in the report must be your own work.
- There will be a zero-tolerance policy for plagiarism and or cheating on exams.
- Homework solutions must be your own work. You must clearly show your own work and the reasoning used to obtain the answer to get credit.

Academic Misconduct: The University Student Conduct Code (available at <u>https://conduct.berkeley.edu/code-of-conduct/</u>) defines academic misconduct. Students are prohibited from committing or attempting to commit any act that constitutes academic misconduct. By way of example, students should not give or receive (or attempt to give or receive) unauthorized help on assignments or examinations without express permission from the instructor. Students should properly acknowledge and document all sources of information (e.g. quotations, paraphrases, ideas) and use only the sources and resources authorized by the instructor. If there is any question about whether an act constitutes academic misconduct, it is the students' obligation to clarify the question with the instructor before committing or attempting to commit the act.

Use of Artificial Intelligence, ChatGPT, and other related technologies:

Al is a powerful tool to help you learn and improve your communication. You are welcome to make use of Al tools in this class. However, directly copying from Al sources is considered plagiarism. Al written text is also poor and use of Al without applying your own critical thinking and editing skills will likely result in a poor grade. Al may also be helpful in performing calculations. However, each student is responsible for understanding the calculations and analysis as well as the language used in their writing. Any student may be asked to explain concepts and repeat calculations in person if there is suspected plagiarism from Al work or from other humans.

Statement on Classroom Climate:

We are all responsible for creating a learning environment that is welcoming, inclusive, equitable, and respectful. The expectation in this class is that we all live up to this responsibility, even during vigorous debate or disagreement, and that we will intervene if exclusionary or harassing behavior occurs. If you feel that these expectations are not being met, you can consult your instructors or seek assistance from campus resources.

Academic Accommodations and Accessibility:

The purpose of academic accommodations is to ensure that all students have a fair chance at academic success. If you have Letters of Accommodations from the Disabled Students' Program or another authorized office, please share them with me as soon as possible, and we will work out the necessary arrangements. While individual circumstances can vary, requests for accommodations often fall into the categories listed on the <u>Academic Calendar</u> <u>and Accommodations website</u>. The campus has well-developed processes in place for students to request accommodations, and you are encouraged to contact the relevant campus offices listed on the <u>Academic Accommodations Hub</u>. These offices, some of which are confidential, can offer support, answer questions about your eligibility and rights, and request accommodations on your behalf, while maintaining your privacy.

CHMENG 286 Electrochemistry Fundamentals Project Assignments

As part of this graduate level course, each student must complete **two independent projects**. Project 1 will be due in Week 4, after the midterm exam. Project 2 will be due by the end of the 6 week course.

The independent projects can take one of three forms. *Students are welcome to choose the format that best accommodates their interests and personal situation. Generally students complete the experimental project.*

Format 1: Laboratory projects.

Student will apply a set of techniques related to the content learned in the course using the equipment in the shared electrochemical device laboratory. The established experimental project for the first portion of the course covers reference electrode fabrication, mass transfer limited voltammetry, and electrochemical kinetics through Tafel analysis. The established experimental project for the second portion of the course covers cyclic voltammetry with analysis using simple CV simulation software in EC lab. The students will use safe aqueous electrolytes and low voltage power sources for these studies.

Format 2: Literature research and presentation

Students will select a topic from the electrochemical literature or industry and conduct rigorous literature research to understand the fundamental principles (thermodynamics, kinetics, and transport) governing the behavior of the system(s) and the current research and/or development challenges and approaches. Students will write a concise 5-page fully referenced report (typically 20-30 references) and lead a 25 min lecture/discussion in class on the topic. **The topics must be pre-approved by the instructor.** Students are encouraged to discuss their understanding of the topics with the instructors as they prepare their materials for submission/presentation.

Format 3: Computational project

Students will use COMSOL (class license available to all students) to create an electrochemical simulation. Several pre-defined projects are available including simulating a double layer in an inert electrolyte and cyclic voltammetry. Students enrolled concurrently in the electrochemical simulations course should simulate a different system. Some possibilities include voltammetry at 3d nanoelectrodes, transport through ionomer membranes for fuel cells or electrolyzers, or other topics to be discussed and approved in advance with/by the instructor. The student will prepare a high-quality 5-page written report on their results following provided guidelines.

	4 - Good	3 – Barely/nearly acceptable	2 - Needs improvement	1 - Not acceptable	0 – Bad	SCORE
Introduction	A cohesive, but concise, well-written summary (including all relevant chemistry, physics, and engineering concepts) of the background material pertinent to the experiment with appropriate references. Places the purpose of the experiment in context.	Is nearly complete but does not provide context for minor points. Contains relevant information but fails to provide background for one aspect of the project or certain information is not cohesive. Certain major introductory points are missing (ex: background, theory, context, etc.) or explanations are unclear and confusing. References are used properly.	Certain major introductory points are missing (ex: background, theory, chemistry, context, etc.) or explanations are unclear and confusing. References are used properly but are not complete.	Very little background information is provided and/or information is incorrect. Poor use of references.	None or unrelated	
Experimental	Contains details on how the experiment/simulation was performed and the procedures followed. The experimental setup must be described, detailing the instrumentation/software used and what purpose each piece of equipment serves in the overall experiment. This information should be presented in a brief and concise manner. Written grammatically correctly and omits information that can be assumed by peers (electrochemists)	Narrative includes most important experimental detail but is missing one or more relevant pieces of information.	Missing several experimental details or some incorrect statements.	Several important experimental details are missing. Narrative is incorrect, illogical, or copied directly from other sources. Written in the incorrect tense.	None or unrelated	
Results Including experimental data, provided project data, or data from numerical simulation	All figures, graphs, and tables are numbered with appropriate captions and of professional quality. All units are provided for data. All tables, figures, etc. are explicitly mentioned in the text. Relevant experimental data are presented which are used in the discussion.	All figures, graphs, and tables are correctly drawn, but some have minor problems that could be still be improved. Units are used consistently. Figures quality is good, but could be improved. All data and associated figures, etc. are mentioned in the text. Most relevant data present.	Most figures, graphs, and tables are included, but some important or required features are missing. Certain data reported are not mentioned in the text or are missing. Captions are not descriptive or incomplete.	Figures, graphs, and tables are poorly constructed; have missing titles, captions or numbers. Certain data reported are not mentioned in the text. Important data missing.	None or unrelated	× 2

Electrochemistry Science, Engineering, and Technology Course Sequence Project and Laboratory Report Grading Rubric

Discussion/ Conclusions	Demonstrates a logical, coherent working knowledge and understanding of important concepts, forms appropriate conclusions based on interpretations of results, includes references, data and analysis, refers to the literature when appropriate, and demonstrates accountability by providing justification for any errors. Key equations are justified and their application appropriately discussed. All equations are appropriately typeset. Address all specific points or questions posed in the project/laboratory guidelines/manual.	Demonstrates an understanding of the majority of important concepts, forms conclusions based on results and/or analysis but either lacks complete interpretation, refers to the literature insufficiently, or lacks complete justification of error and or use of models and theoretical equations. Address most of the specific points or questions posed in the project/laboratory guidelines/manual.	While some of the results have been correctly interpreted and discussed, partial but incomplete understanding of results is evident. Student fails to make one or two connections to underlying theory. Address only some of the specific points or questions posed in the project/laboratory guidelines/manual.	Does not demonstrate an understanding of the important experimental concepts, forms inaccurate conclusions, suggests refers to the literature insufficiently, and lacks overall justification of error and/or use of models and theoretical equations. Address none of the specific points or questions posed in the project/laboratory guidelines/manual.	None or unrelated	× 2
References	All sources (information and graphics) are accurately documented in ACS or AIP format.	All sources are accurately documented, but formatting is not consistent or always correct.	Some sources are not accurately documented. Formatting is not consistent or correct.	Sources are not accurately documented. Formatting is not consistent or correct.	None or unrelated	× 0.5
Overall Style, Organization, and Writing Quality	Appropriate as a piece of scientific or engineering writing, words were chosen carefully and appropriately. Figures of professional quality. Sentence structure was clear and as concise. Includes no excess or unnecessary text. Evidence the report was edited by the author to improve clarity and readability. From a technical standpoint, the paper is free of spelling, punctuation, and grammatical errors	Minimal awkward phrasing or word choices. Report is easy to read and constructed properly. Some excess unneeded text. Evidence of editing. Acceptable quality figures. Few grammar and spelling errors.	Many passages are phrased poorly, contained awkward word choices, or many long sentences. Narrative is disorganized in many places. Substantial excess text that should be eliminated by editing .Tense not appropriate or not in agreement in several places. Multiple grammatical and/or spelling errors.	Poorly organized narrative with frequent awkward phrases and poor word choices. Setences are too long or short. Lacks cohesion, style and fluidity. Many instances of verb tenses not agreeing. No evidence of editing. Frequent spelling and grammar errors. Focus on technical writing improvement critical	Poor style, format, and organization. Extreme writing errors. Report very difficult to read. Focus on technical writing improvement critical	
					SUM	/30

 $\begin{array}{ll} Grading: A-range = 26 \text{ to } 30 & D-range = 13 \text{ to } 17 \\ B-range = 21 \text{ to } 26 & below 17 = F \\ C-range = 17 \text{ to } 21 \end{array}$