CHBE 486/ENCH 648E: Heterogeneous Catalysis for Energy Applications (3 credits) Fall 2019

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Class times and location: Monday and Wednesday, 5:00 to 6:15pm in CHE 2110

Course Description
This course will provide a comprehensive overview of heterogeneous catalytic science and technology for energy conversion and utilization applications. Course modules will cover the preparation and mechanistic characterization of heterogeneous catalyst systems, kinetics of catalyzed reactions, adsorption and surface reactions. An introduction to heterogeneous catalysis in various energy-related applications, including renewable energy conversions such as chemicals from biomass, and fossil resource utilizations such as petroleum refining, valorization of shale gas, CO_2 utilization, etc. will be discussed. Emphasis will be placed on understanding the design and properties of hierarchical nanostructures that are utilized in advanced energy reaction engineering applications. This course will also provide the engineering students with necessary background for understanding various nanomaterials characterization techniques, including adsorption/desorption isotherms, X-ray diffraction, electron microscopy, and spectroscopic techniques. In-situ characterization of the catalytic systems will also be introduced.

Course Objectives and Expectations
At the end of the course, students should be able to (i) understand the historic perspective and future developments of catalysis and energy, (ii) be able to formulate reaction mechanisms for chemical reactions and to derive correlations between material properties and catalysis, (iii) understand various nanomaterial synthesis/characterization and in-situ catalysis characterization techniques, (iv) have a deep understanding on a variety of industrial practices for energy conversion and unitizations, especially renewable energy conversion techniques, (v) gain the knowledge of the scientific work by other researches in materials, catalysis, and energy; (vi) come up with the original idea and develop a research proposal according to the standard format of National Science Foundation (NSF) agency.

Course Pre-requisites
Prerequisite: CHBE302, CHBE424, and CHBE440; and permission of instructor. Credit only granted for: CHBE486 or ENCH648E. If you have questions about course registration, please contact Kathy Lopresti in 1109 Chemical & Nuclear Engineering Building (lopresti@umd.edu, 301-405-5888).

Textbooks
Required: Hans Niemantsverdriet & Ib Chorkendorff, *Concepts of Modern Catalysis and Kinetics (Second, Revised, and Enlarged Edition)* (Wiley-VCH, 2007). A link for this book in Wiley-VCH as well as additional resources are available at
http://www.wiley-vch.de/publish/en/books/bySubjectCH00/bySubSubjectCH40/3-527-31672-8/?sID=lk2jms7seq1arfnbi9bnkm4u04

Recommended for Additional Reading

Mark E. Davis & Robert Davis, *Fundamentals of Chemical Reaction Engineering,* McGraw-Hill, **2003**. This book is a good resource for additional practice problems and solved examples for this course.

Ertl, G., Knözinger, H., Schüth, F., & Weitkamp, J. (Eds.). *Handbook of Heterogeneous Catalysis, Second, Completely Revised and Enlarged Edition* (Wiley-VCH, **2008**). This handbook is coined as encyclopedia in catalysis field.

M. Niwa, N. Katada, K. Okumura, *Characterization and Design of Zeolite Catlaysts (Solid acidity, Shape selectivity, and loading properties)* SpringerLink, **2010.** This book will serve as good reference for characterization techniques for porous heterogeneous catalysts.

Other resources
Course website: The syllabus, course schedule, homework assignments, course material handouts and project assignments, and your grades along with the statistics for the class will be provided on elms. You can log-on the elms.umd.edu using your UMD account and choose CHBE486/ENCH648E.

UM Library research guide: http://lib.guides.umd.edu. This tutorial provides assistance with searching the scholarly literature, which you will be expected to do while doing research for the course project.

Homework
Homework will be assigned regularly and the due date will be listed on the assignment. The HW assignments will also be posted on the course website. The homework is to be turned in at the beginning of lecture on the day they are due. **Homework submitted after the instructor begins the lecture will be considered later. Late submissions carry a 50% grade penalty.** Students are encouraged to discuss the problem set with other students, but each student is required to submit and present their own solution. **Copying or paraphrasing from the web, another source, or another student's solution or permitting your own solution to be copied or paraphrased is considered cheating.** The minimum penalty for all students involved is a zero for that homework. Penalty for severe violation will be referred to the university's Code of Academic Integrity http://www.shc.umd.edu.

Examination
There will be one in-class midterm examination and one final examination (date to be announced); the exams will only cover the materials listed on the course calendar and will be **allowed to bring with exam notes**.

Calculators for the exam will be provided by the Department. No other electronic devices except a watch (without communication capability) may be used. Communication devices (cell phones, etc.) are not permitted during the examination and must remain in a sealed bag. Open possession of such items will be considered a case of cheating and the student will receive a zero grade for the exam.

No student will be permitted to take the exam before the scheduled time and no makeup exams will be given. Students who miss an exam will be given a zero grade for the exam unless personal illness or a family emergency was the reason for missing the exam. Special arrangements will be made in such circumstances provided these instances are well documented.

Re-grading of Exam and Homework
Students who wish to have their exam or homework re-graded should submit their request before lecture the day following the Discussion in which the exam or homework was returned. This request should be made in writing, indicating the possible error, and placed in Prof. Liu's mailbox in 2113 Chemical & Nuclear Engineering Building. The entire exam or homework will be reviewed by Prof. Liu for any possible oversight, and a revised grade, which may be higher or lower, will be returned to the student. ***Submitting an altered exam or homework for re-grading is a serious offense for which the student will receive an F grade in the course.***

Reading, discussion, and presentation of literature articles
Another aspect of this course is to link knowledge in textbook to research in the literature. This linkage will allow us to think of creative ideas, to troubleshoot research projects, to write compelling proposals and papers, and understand new technology market niches. Students should read all text chapters and journal articles listed in the detailed schedule in advance of lecture. There will be discussion questions to be posted to elms during the semester to guide reading of text chapters and literature articles. Additionally, teams of 2-4 students will lead discussions of primary literature assigned as class readings. Each student is expected to participate in all discussions. The teams will be randomly assigned and are posted on elms. The content covered in the class literature discussions will also be the elements in the exams.

Research proposal
Scientific writing during undergraduate and graduate education is a critical skill that you can draw on in academia, industry, and business. This semester, all students will prepare a research proposal for an original idea that that involves materials, catalysis, and energy. The idea will be written in the format of a National Scientific Foundation (NSF) Fellowship proposal. Students will submit a proposed title and a short paragraph of project summary by **Oct. 9th**. A one-page project overview (summary) will be due on **Oct. 30th**, and then the revised overview page will be due on **Nov. 11th**. Students will receive feedback and a grade on the overview draft submitted on **Oct. 30rd**. The full proposal will be due by **Nov. 27th**. Additional details are posted on elms website.

Determination of Grades
Final grades will be assigned from a histogram of the final grades based upon the following distribution:

Homework:	15%
Mid-term exam:	20%
Final exam:	20%
Literature presentation:	15%
Quiz (in-class):	10%
Research Proposal: Overview draft:	5%
Research Proposal: Full proposal:	15%

Arrangements for students with disabilities
Any students with learning disabilities will be provided the necessary accommodation(s). Students needing such assistance must see Dr. Liu before 2019-09-04, so that we can make the necessary arrangements.

Statement on Classroom Conduct
Students are expected to interact with the instructor and other students with respect and courtesy. Students should attend every class session prepared to learn and work. Participation in class is expected, which includes both speaking up and listening. Give class your full attention while here. Complete all assignments, including all reading assignments, in a timely fashion. **Turn off your cell phone for the duration of class.** Students whose behavior is disruptive either to the instructor or to the other students in the class will be asked to leave. Students whose behavior suggests the need for counseling or other assistance may be referred to counseling service. Students whose behavior violates the University Student Conduct Code will be subject to disciplinary action.

Statement on Scholastic Dishonesty
The University Student Conduct Code defines scholastic dishonesty as follows:

Scholastic Dishonesty: Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting along or in cooperation with another to falsify records or to obtain dishonestly grades, honors,

awards, or professional endorsement; altering, forging or misusing a University academic record; or falsifying data, research procedures, or data analysis.

Within this course, a student responsible for scholastic dishonesty can be assigned a penalty up to and including an 'F' or 'XF' grade for this course. If you have any questions regarding the expectations for a specific assignment or examination, please ask Dr. Liu.

Absence due to religious observation
If the observation of a religious event occurring during the semester prevents you from attending class, you may be allowed to make up for missed exams or homework. However, it is your responsibility to inform the instructor about the projected absence at least two weeks ahead on the date of the absence, whichever is earlier.

Inclement weather
In case of inclement weather, the instructor will abide by the University's policy on closures and delays, which will be posted at http://www.umd.edu. If the University closes on a class day due to inclement weather, any HW due will become due on the next lecture.

Communicating with the instructor
Email is the best way to reach the instructor. A reply to email can be expected within two business days (usually one business day). Therefore, if you have a question about an upcoming exam scheduled on a Thursday evening, your email should reach the instructor by Tuesday morning (preferably Sunday and Monday). For your own privacy, your email to the professor should originate from your umd.edu address or your University-registered email address (if different from your umd.edu address). Grades and exam or HW scores will not be given over email, and have to be accessed through elms website. When emailing the instructor, you should begin the subject line with "CHBE486 or ENCH 648E" and not use "text messaging" language. Emails that do not adhere to these guidelines cannot expect responses.

CHBE486/ENCH648E: Course Calendar

This calendar is tentative and is subject to modification depending on our speed through the course. Major changes will be announced in class or elms. Shaded rows indicate the important event in class. The numbers under the "reading" column are section numbers in the textbook that correspond to the material covered. "HO" indicates that a handout will be provided. **You are expected to prepare for class by reading the relevant material in advance.**

Date (Aug. 2019-Dec. 2019)			Lecture	Reading	Topic	HW (due)
Week 1	Mo	08-26	Lecture 1	Chapter 1	Discuss course syllabus; Introduction to catalysis, materials and energy	
	Wed	08-28	Lecture 2	Chapter 2	Thermodynamic aspects of heterogeneous catalysis	
Week 2	Mo	09-02	**Labor day (no class)**			
	Wed	09-04	Lecture 3	Chapter 2	Chemical and catalytic reaction kinetics (I)	
Week 3	Mo	09-09	Lecture 4	Chapter 2	Chemical and catalytic reaction kinetics (II)	
	Wed	09-11	Lecture 5	Chapter 2	Chemical and catalytic reaction kinetics (III)	HW 1
Week 4	Mo	09-16	Lecture 6	Chapter 5.8.2 & HO	Transport limitations of catalyzed reactions (I)	
	Wed	09-18	Lecture 7	Chapter 5.8.2 & HO	Transport limitations of catalyzed reactions (II)	HW 2
Week 5	Mo	09-23	Lecture 8	Chapter 5.8.2 & HO	Transport limitations of catalyzed reactions (III)	
	Wed	09-25	Lecture 9	Chapter 5.3.3, Chapter 6 & HO	Adsorption (I): Physisorption	HW 3
Week 6	Mo	09-30	Lecture 10	Chapter 6 & HO	Adsorption (II): Chemisorption	
	Wed	10-02	Lecture 11	Chapter 6 & HO	Adsorption (III): Chemisorption	HW 4
Week 7	Mo	10-07	Lecture 12	Chapter 6 & HO Chapter 5.1 – 5.3	Adsorption (IV): Chemisorption Structure of solid catalysts	
	Wed	10-09	Lecture 13	HO	Overview on proposal development Structure of solid catalysts	Proposal title due HW 5
Week 8	Mo	10-14	Lecture 14	Chapter 5.7 & HO	Catalyst support & Catalyst synthesis Catalyst characterizations: overview	
	Wed	10-16	Lecture 15	Chapters & HO	Heterogeneous catalysis in practice: overview	
Week 9	Mo	10-21			Exam #1	
	Wed	10-23	Lecture 16	HO	Heterogeneous catalysis in practice: H_2 economy	

Week 10	Mo	10-28	Lecture 17	HO	Catalyst characterizations (I)	Team 1 (Quiz 1)
	Wed	10-30	Lecture 18	HO	Catalyst characterizations (II) (Proposal overview page pre-due)	Team 2 (Quiz 2)
Week 11	Mo	11-04	Lecture 19	HO	Catalyst characterizations (III)	Team 3 (Quiz 3)
	Wed	11-06	Lecture 20	Chapters & HO	Catalyst characterizations (IV)	Team 4 (Quiz 4)
Week 12	Mo	11-11	No Class. AIChE Meeting. **(Revised proposal summary page due)** **Work on proposal!!!!**			
	Wed	11-13				
Week 13	Mo	11-18	Lecture 21	HO	Catalyst characterizations (V)	Team 5 (Quiz 5)
	Wed	11-20	Lecture 22	HO	Oil refinery & Petrochemistry	Team 1 (Quiz 6)
Week 14	Mo	11-25	Lecture 23	HO	Environmental catalysis	Team 2 (Quiz 7)
	Wed	11-27		No class. Thanksgiving Holiday. **DUE:** Final proposal (submit via elms by 11:59pm)		
Week 15	Mo	12-02	Lecture 24	HO	Catalysis for methane utilization	Team 3 (Quiz 8)
	Wed	12-04	Lecture 25	HO	Catalysis for CO_2 utilization	Team 4 (Quiz 9)
Week 16	Mo	12-09	Lecture 26	HO	Catalysis for biomass conversion	Team 5 (Quiz 10)
Week 17	Sat	12-14	Exam 2 (4 – 6pm)			