CHBE 486/ENCH 686: Heterogeneous Catalysis for Energy Applications (3 credits) Fall 2013

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Office Hours: Friday 3-5pm, other times by appointment

Class times and location: Tuesday and Thursday, 5:00 to 6:15pm in JMP building (#083) Room 2202

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 nanomaterails characterization techniques, including adsorption/desorption isotherms, X-ray diffraction, electron microscopy, solid state nuclear magnetic resonance (NMR), 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) criticize the scientific work by other researches in materials, catalysis, and energy; (vi) for **graduate students**: come up with the approaches for literature review of their research background and apply the principles and techniques covered in the course to their own research project.

Course Pre-requisites

Prerequisite: CHBE302, CHBE424, and CHBE440; and permission of instructor. Credit only granted for: CHBE486 or ENCH686. 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 Canvas. You can log-on the elms.umd.edu using your UMD account and choose CHBE486/ENCH686.

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.** Graded problem sets will be returned in lectures on Tuesdays. 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 (date to be announced); the midterm exam will only cover the materials listed on the course calendar and will be **open book and open notes**. You may write whatever you would like on the inside of your book and 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.

Journal Article Critique
This assignment requires you to critically review a scientific journal article that involves catalysis for energy unitization. The article should be published in recent three years and in a high standard journal. Otherwise, you need to talk to Dr. Liu to provide a reasonable excuse for the article you choose that does not meet

this requirement. A written report and in-class discussion on your review comments will be required. More details on this assignment will be made available later.

Course project
A course project will be assigned during the second week of November and will be due on the last week of class. The project will require **undergraduate students** to apply principles learned in this course to an industrial chemical process. You will be expected to work on the project in groups, submit a typed report, and make an in-class presentation summarizing your group's work in the project. For **graduate students**, you will be expected to work a project that involves materials, catalysis, and energy related to your own research. More details will be provided when the project is assigned.

Class participation
The class participation score, worth 10% of the final grade, will be based on attendance and participation in the classroom and online (canvas) discussions. To secure a high class participation score, a student should ask questions and provide responses that reflect the student's advance preparation and insight into the subject material. Factors that may lead to loss of class participation points are repeated absence from class, repeated wastage of class time through questions and comments that do not reflect preparation or attention, or failure to meet "student expectations" outlined below. If a student's final course score lands the student on the border between two grades, a high class participation score will enable the student to secure the higher of the two grades.

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

	CHBE486	ENCH686
Homework:	30%	30%
Mid-term:	30%	25%
Article Critique:	10%	10%
Course Project:	20%	25%
Class participation:	10%	10%

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 2013-09-05, 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.

Important dates

Drop dates	
Last date to drop course without a "W" Last date to drop course with a "W"	University schedule; To be announced.
Exam	
Mid-term exam	2013-10-31 (Thursday)
Article crique	
Critique: Article critique (assignment) Critique: Article critique (report due and discussion)	2013-10-15 (Tuesday) 2013-11-12 (Tuesday)
Course project	
Project: topic and group assignments Project: in-class presentation Project: final report due and in-class presentation	2013-11-14 (Thursday) 2013-12-10 (Tuesday) 2013-12-12 (Thursday)

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; an alternative way is the online discussion board on Canvas. 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 Canvas. When emailing the instructor, you should begin the subject line with "CHBE486 or ENCH 686" and not use "text messaging" language. Emails that do not adhere to these guidelines cannot expect responses.

CHBE 486/ENCH 686: Course Calendar

This calendar is tentative and is subject to slight modification depending on our speed through the course. Major changes will be announced in class or Canvas. 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 (Sep. 2013-Dec. 2013)			Lecture	Reading	Topic	HW Due
Week 1	Tu	09-03	Lecture 1	HO	Introduction to fossil and renewable energy; discuss class syllabus	
	Tr	09-05	Lecture 2	1.1-1.7, Pg1-21	Introduction to catalysis	
Week 2	Tu	09-10	Lecture 3	Chapter 2	Catalysis theory: rate equation and power rate laws, reaction kinetics	
	Tr	09-12	Lecture 4	Chapter 2	Reaction thermodynamics, reaction equilibrium, and reaction mechanism.	HW 1
Week 3	Tu	09-17	Lecture 5	Chapter 3	Reaction rate theory (I)	
	Tr	09-19	Lecture 6	Chapter 3	Reaction rate theory (II)	HW 2
Week 4	Tu	09-24	Lecture 7	Chapter 4	Catalyst characterizations (I): XRD, XPS, EXAFS, TPD, TPO	
	Tr	09-26	Lecture 8	Chapter 4	Catalyst characterizations (II): SEM, TEM, AFM, NMR, BET	HW 3
Week 5	Tu	10-01	Lecture 9	Chapter 5	Solid catalysts: synthesis and textural property characterizations	
	Tr	10-03	Lecture 10	Chapter 5 & HO	Solid porous catalysts: synthesis and mechanistic characterizations	HW 4
Week 6	Tu	10-08	Lecture 11	Chapter 6	Surface reactivity of heterogeneous catalysts (I)	
	Tr	10-10	Lecture 12	Chapter 6	Surface reactivity of heterogeneous catalysts (II)	HW 5
Week 7	Tu	10-15	Lecture 13	Chapter 7	Kinetics of reactions on surface (I)	
	Tr	10-17	Lecture 14	Chapter 7	Kinetics of reactions on surface (II)	HW 6

Week 8	Tu	10-22	Lecture 15	Chapter 7	Kinetics of reactions on surface (III)	
	Tr	10-24	Lecture 16	Chapter 8	Heterogeneous catalysis in practice: Hydrogen production	HW 7
Week 9	Tu	10-29	Lecture 17	HO	Catalysis for methane utilization	
	Tr	10-31				Exam 1
Week 10	Tu	11-05	No Class. AICHE Meeting. Journal Article Critique.			
	Tr	11-07				
Week 11	Tu	11-12	Lecture 18	Chapter 9	Catalysis for oil refinery and petroleum chemistry	
	Tr	11-14	Lecture 19	Chapter 9	Catalysis for oil refinery and petroleum chemistry	Article critique
Week 12	Tu	11-19	Lecture 20	Chapter 10	Introduction to Environmental catalysis	
	Tr	11-21	Lecture 21	Chapter 10	Introduction to Environmental catalysis	HW 8
Week 13	Tu	11-26	Lecture 22	HO	Catalysis for coal and CO_2 utilization	
	Tr	11-28	No class. Thanksgiving Holiday!			
Week 14	Tu	12-03	Lecture 23	HO	Renewable energy: catalysis for biomass conversion to transportation fuels and chemicals (Generation I)	
	Tr	12-05	Lecture 24	HO	Renewable energy: catalysis for biomass conversion to transportation fuels and chemicals (Generation II)	
Week 15	Tu	12-10	Lecture 25		Project Presentation	
	Tr	12-12	Lecture 26		Project Presentation	Project report
Week 16	Tu	12-17	Final week			
	Tr	12-19				