Chemical Engineering 6937, 4905
Molecular Understanding of Catalysis
Spring Semester 2019

Instructor: David Hibbitts (221 Chemical Engineering Hall, dhibbitts@che.ufl.edu)
Office Hours: By Appointment

Teaching Assistant: None

Class Hours: Monday 11:45-12:35pm CHE 316
Wednesday 10:40-12:35pm MAEB 328
**classes will occasionally meet for the full scheduled 2 hours.*

Useful Texts: No textbook required. Original papers will be occasionally distributed. The following are useful texts:

Boudart and Djega-Mariadassou, Kinetics of Heterogeneous Catalytic Reactions, Princeton University Press, 1986;

Chorkendorff and Niemantsverdriet, Concepts of Modern Catalysis and Kinetics, Wiley, 2003;

Niemantsverdriet, Spectrosocopy in Catalysis: An Introduction, Wiley, 2000;

Thomas and Thomas, Principles and Practice of Heterogeneous Catalysis, Wiley, 1996;

Masel, Chemical Kinetics and Catalysis, Wiley, 2001;

Freely Available:

Davis and Davis, Fundamentals of Reaction Engineering, McGraw Hill, 2003,
authors.library.caltech.edu/25070/1/FundChemReaxEng.pdf

Dumesic, Huber, Boudart, Principles of Heterogeneous Catalysis (Chapter), Wiley, 2008,
onlinelibrary.wiley.com/doi/10.1002/9783527610044.hetcat0001/abstract

Sholl and Steckel, Density Functional Theory: A Practical Guide, Wiley
https://books.google.com/books?id=_f994dmAdv0C&lpg=PT7&ots=haAGanmvrd&dq=density%20functional%20theory%20a%20practical%20introduction&lr&pg=PT7#v=onepage&q=density%20functional%20theory%20a%20practical%20introduction&f=false

Course Grade: The course grade will be determined as follows:

Research Project	50%
Oral Presentations	50%

Homework/Quizzes: Homework and in-class quizzes will be infrequent and primarily meant to provide me feedback of your understanding of the course material. They will not be graded (see "times are hard" above); but I will collect them to see areas of deficiency. I am happy to discuss them in class or office hours (when prompted).

Research Project: Each student will choose a topic of current interest in heterogeneous catalysis (or their own research with prior approval) and perform density functional theory calculations (significantly limited in scope due to time and resource constraints) which seek to discover something new (or confirm old proposals) about that topic. The student will submit their results in Figures and Tables with no more than two pages of description and discussion (single-spaced, excluding Figures and Tables). This will be graded (primarily) on your ability to present and discuss scientific data – the quality of the calculations will have little outcome on the grade. Their descriptions will also be graded based on the exact course being taken (e.g., ECH 4905 compared to ECH 6937).

Oral Presentations: The topic chosen and results obtained will be summarized by each student in 15-minute presentations with 5 minutes for discussions. These presentations will take place at the end of the semester. This will be graded (primarily) on your ability to 'orally' present and discuss scientific data – the quality of the calculations will have little outcome on the grade.

Chem. Eng. 6937 Topics Spring 2019

Topics (In rough chronological order)

Introduction (Rev. of Reaction Engr.)

Crystal Structures of Metals

Crystal Structures of Oxides

Crystal Structures of Zeolites and Other Microporous Solids

Brief Overview of Characterization Techniques

Video-Lecture on Catalyst Synthesis

Density Functional Theory

Practical DFT

Kinetics of Adsorption-Desorption and Chemisorption Techniques

Kinetics of Surface Reactions; Activated Complexes and Transition State Theory

Kinetic Monte Carlo

Temperature-Programmed Desorption and Reaction Methods; Related Transient Methods

Mass Transport Effects (Internal and External)

Molecular Dynamics

Electrocatalysis

Kinetic Isotope Effects

Methane Conversion and Other C_1 Chemistries

Isotopic, Kinetic, and Theoretical Studies of Fischer-Tropsch Synthesis

Presenting Data and Automotive Exhaust Catalysis

Acid Catalysis: Effects of Acid Strength and Confinement in Heterogeneous Catalysis

Aqueous Phase Biomass Conversions (Catal. & Electrocatalysis)

Oral Presentations (5 of them, meet for full two hours)

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Oral Presentations (5 of them, location/time TBD)