

Molecular Understanding of Catalysis

ECH 6537

Class Periods: Tues, Period 8 (3:00 – 3:50 PM)

Thurs, Periods 7–8 (1:55 – 3:50 PM)

Location: PSY 0130 (Tue)

WEIM 1094 (Thurs)

Academic Term: Spring 2024

Instructor:

David Hibbitts

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Office Hours: By appointment.

Teaching Assistant/Peer Mentor/Supervised Teaching Student:

- None

Course Description

Catalysts are key to the development of renewable energy, fuel, and chemicals, as well as in cleaning pollutants from waste streams. This course teaches topics relevant to modern catalysis, with an emphasis on heterogeneous catalysis, including techniques of catalyst synthesis, characterization, and kinetic testing. Students are introduced to computational tools that assist in understanding catalysis at the molecular level. Case studies of catalyzed reactions are presented.

Course Objectives

This course will teach about topics relevant to modern catalysis, with an emphasis on heterogeneous catalysis, and will introduce students to computational tools (density functional theory (DFT), molecular dynamics (MD), kinetic Monte Carlo (KMC) simulations) that can give insights into reaction behavior at catalyst interfaces. By the end of this course, students will be able to:

- Develop kinetic rate expressions for surface reactions and understand how heat and mass transport can impact observed rates.
- Understand basics related to catalyst synthesis and characterization.
- Understand how kinetic and isotopic studies can give insights into reaction mechanisms and catalyst behavior.
- Perform molecular simulations (e.g., DFT, MD, KMC) to directly predict reaction rates and mechanism at catalyst surfaces.

Required Textbooks and Software

No required textbook. Select research articles will be distributed.

Recommended Materials

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>

Available:

- 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, Spectroscopy in Catalysis: An Introduction, Wiley, 2000;
- Thomas and Thomas, Principles and Practice of Heterogeneous Catalysis, Wiley, 1996;
- Masel, Chemical Kinetics and Catalysis, Wiley, 2001;

Course Schedule

- Week 1: Class introduction, ideal reactors, and simple kinetics
- Week 2: Materials and crystal structures
- Week 3: Theory of density functional theory (DFT)
- Week 4: Practice of DFT
- Week 5: Catalyst synthesis and characterization
- Week 6: Kinetics of adsorption-desorption and chemisorption techniques
- Week 7: Kinetics of surface reactions
- Week 8: Transition state theory
- Week 9: Temperature programmed reduction, desorption, and surface reactions. (TPR, TPD, TPSR)
- Week 10: Heat and mass transport effects
- Week 11: Molecular Dynamics
- Week 12: Electrocatalysis
- Week 13: Current Topics in Catalysis: C1 chemistry: methane, methanol, and CO₂.
- Week 14: Current Topics in Catalysis: Hydrogenolysis of alkanes and plastics upcycling
- Week 15: Current Topics in Catalysis: Automotive exhaust and aqueous-phase biomass conversion

Attendance Policy, Class Expectations, and Make-Up Policy

Excused absences must be in compliance with university policies in the Graduate Catalog (<http://gradcatalog.ufl.edu/content.php?catoid=10&navoid=2020#attendance>) and require appropriate documentation.

Evaluation of Grades

Grades will be based on a semester-long research project which will involve students performing molecular simulations. The project grade will depend on an extended abstract about an existing literature paper (33%), and the presentation of students research through a written report (33%) and an oral presentation (34%).

Assignment	Percentage of Final Grade
Extended Abstracts	33%
Written Research Reports	33%
Oral Research Presentations	34%

Research Projects:

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.

Extended Abstracts:

Based on the topic chosen above, each student will select a “recent” paper from literature and prepare a three-page extended abstract (single-spaced, including Figures, Tables, and references; 12 font). This will be graded (primarily) on your ability to digest and critique published science.

Written Reports:

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.

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.

Grading Policy

Percent	Grade	Grade points
90.0 - 100	A	4.00
87.0 – 89.9	A-	3.67
84.0 - 86.9	B+	3.33
81.0 - 83.9	B	3.00
78.0 - 80.9	B-	2.67
75.0 - 77.9	C+	2.33
72.0 - 74.9	C	2.00
69.0 - 71.9	C-	1.67
66.0 - 68.9	D+	1.33
63.0 - 65.9	D	1.00
60.0 - 62.9	D-	0.67
0 - 59.9	E	0.00

More information on UF grading policy may be found at:

[UF Graduate Catalog](#)
[Grades and Grading Policies](#)

Students Requiring Accommodations

Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center by visiting <https://disability.ufl.edu/students/get-started/>. It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.

Course Evaluation

Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at <https://gatorevals.aa.ufl.edu/studentsj>. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via <https://ufl.bluera.com/uflj>. Summaries of course evaluation results are available to students at <https://gatorevals.aa.ufl.edu/public-results/>.

In-Class Recording

Students are allowed to record video or audio of class lectures. However, the purposes for which these recordings may be used are strictly controlled. The only allowable purposes are (1) for personal educational use, (2) in connection with a complaint to the university, or (3) as evidence in, or in preparation for, a criminal or civil proceeding. All other purposes are prohibited. Specifically, students may not publish recorded lectures without the written consent of the instructor.

A "class lecture" is an educational presentation intended to inform or teach enrolled students about a particular subject, including any instructor-led discussions that form part of the presentation, and delivered by any instructor hired or appointed by the University, or by a guest instructor, as part of a University of Florida course. A class lecture does not include lab sessions, student presentations, clinical presentations such as patient history, academic exercises involving solely student participation, assessments (quizzes, tests, exams), field trips, private conversations between students in the class or between a student and the faculty or lecturer during a class session.

Publication without permission of the instructor is prohibited. To "publish" means to share, transmit, circulate, distribute, or provide access to a recording, regardless of format or medium, to another person (or persons), including but not limited to another student within the same class section. Additionally, a recording, or transcript of a recording, is considered published if it is posted on or uploaded to, in whole or in part, any media platform, including but not limited to social media, book, magazine, newspaper, leaflet, or third party note/tutoring services. A student who publishes a recording without written consent may be subject to a civil cause of action instituted by a person injured by the publication and/or discipline under UF Regulation 4.040 Student Honor Code and Student Conduct Code.

University Honesty Policy

UF students are bound by The Honor Pledge which states, "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." The Honor Code (<https://sccr.dso.ufl.edu/process/student-conduct-code/>) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.

Commitment to a Safe and Inclusive Learning Environment

The Herbert Wertheim College of Engineering values varied perspectives and lived experiences within our community and is committed to supporting the University's core values, including the elimination of discrimination. It is expected that every person in this class will treat one another with dignity and respect regardless of race, creed, color, religion, age, disability, sex, sexual orientation, gender identity and expression, marital status, national origin, political opinions or affiliations, genetic information, and veteran status.

If you feel like your performance in class is being impacted by discrimination or harassment of any kind, please contact your instructor or any of the following:

- Your academic advisor or Graduate Program Coordinator
- HWCOE Human Resources, 352-392-0904, student-support-hr@eng.ufl.edu
- Curtis Taylor, Associate Dean of Student Affairs, 352-392-2177, taylor@eng.ufl.edu
- Toshikazu Nishida, Associate Dean of Academic Affairs, 352-392-0943, nishida@eng.ufl.edu

Software Use

All faculty, staff, and students of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

Student Privacy

There are federal laws protecting your privacy with regards to grades earned in courses and on individual assignments. For more information, please see: <https://registrar.ufl.edu/ferpa.html>

Campus Resources:

Health and Wellness

U Matter, We Care:

Your well-being is important to the University of Florida. The U Matter, We Care initiative is committed to creating a culture of care on our campus by encouraging members of our community to look out for one another and to reach out for help if a member of our community is in need. If you or a friend is in distress, please contact umatter@ufl.edu so that the U Matter, We Care Team can reach out to the student in distress. A nighttime and weekend crisis counselor is available by phone at 352-392-1575. The U Matter, We Care Team can help connect students to the many other helping resources available including, but not limited to, Victim Advocates, Housing staff, and the Counseling and Wellness Center. Please remember that asking for help is a sign of strength. In case of emergency, call 9-1-1.

Counseling and Wellness Center: <https://counseling.ufl.edu>, and 392-1575; and the University Police Department: 392-1111 or 9-1-1 for emergencies.

Sexual Discrimination, Harassment, Assault, or Violence

If you or a friend has been subjected to sexual discrimination, sexual harassment, sexual assault, or violence contact the **Office of Title IX Compliance**, located at Yon Hall Room 427, 1908 Stadium Road, (352) 273-1094, title-ix@ufl.edu

Sexual Assault Recovery Services (SARS)

Student Health Care Center, 392-1161.

University Police Department at 392-1111 (or 9-1-1 for emergencies), or <http://www.police.ufl.edu/>.

Academic Resources

E-learning technical support, 352-392-4357 (select option 2) or e-mail to Learning-support@ufl.edu.
<https://lss.at.ufl.edu/help.shtml>.

Career Connections Center, Reitz Union, 392-1601. Career assistance and counseling; <https://career.ufl.edu>.

Library Support, <http://cms.uflib.ufl.edu/ask>. Various ways to receive assistance with respect to using the libraries or finding resources.

Teaching Center, Broward Hall, 392-2010 or 392-6420. General study skills and tutoring.
<https://teachingcenter.ufl.edu/>.

Writing Studio, 302 Tigert Hall, 846-1138. Help brainstorming, formatting, and writing papers.
<https://writing.ufl.edu/writing-studio/>.

Student Complaints Campus: <https://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code> / <https://care.dso.ufl.edu>.

On-Line Students Complaints: <https://distance.ujl.edu/getting-help/>; <https://distance.ujl.edu/state-authorization-status/#student-complaint>.
