Chemistry 579/488: Special Topics in Chemistry
Grand Challenges in Catalysis Across Disciplines

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Location (SEC 208)
Tuesday & Friday 10:20 am-11:40 am

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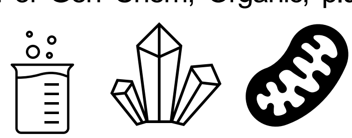
COURSE DESCRIPTION:

This course will give an overview of the fundamentals of catalysis and their application through studies of the grand challenges in catalysis across scientific disciplines. It will begin with an overview of fundamental concepts in catalysis (X-Catalysis 101) covering, biological, molecular (organometallic), heterogeneous and electrocatalysis. These four units will be taught using traditional pedagogical reading assignments. The pedagogical structure will then shift to apply these concepts to past and present grand challenges in catalysis that scientists have solved using the logic of chemistry (or are still trying to solve). Case studies of four grand challenges in catalysis will be presented taken from the disciplines of *biology, geology and chemistry* performed by enzymes/metabolic pathways, minerals/heterogenous catalysts and molecular catalysts, respectively. This comparison will juxtapose how the three disciplines devise catalytic solutions for the same reaction under different environmental constraints. These grand challenges have a historical importance and a large impact on the global scale. I will end with a historical grand challenge from WWII, the Manhattan Project on catalysis.

LEARNING OBJECTIVES:

The aim of this course is to introduce the fundamentals of catalysis through the lens of grand challenges. A second objective is to apply these concepts across the branches of chemical science that overlap with biology and geology. A third objective is to illustrate the use of the Scientific Method to assess literature (as Sagan says, detect baloney), construct a hypothesis (not merely an unformulated idea), design quantitative tests of it, and defend it in public. By the end of the course, students will have gained a theoretical foundation in catalysis, its functional occurrence in industry and nature, and be effective in applying the Scientific Method. This knowledge is essential for aspiring scientists and innovators who aim to use catalysis concepts to examine problems in biology, chemistry and geology. Learning will be guided by lectures, literature readings, instructor Q&A, student poster, student Q&A.

PREREQUISITES: 1 or more semester each of Gen Chem, Organic, plus either Inorganic Chem, Biochem, Geochem or instructor's permission.



ASSIGNMENT AND GRADING (based on 1.5 credits mini-course, one meeting per week):

1. Attendance & Engagement: *150 pts (15*10)*
2. Three Quizzes *300 pts*
3. Poster graphics *50 pts*
4. Poster oral presentation *50 pts*
5. Poster questions submitted to instructor *50 pts*
6. Poster answers evaluated by instructor *100 pts*
7. **Total:** *700 pts*

#	Date	Topics	Assignments
1	Jan 20	Course overview & objectives Review of the Scientific Method	Daily Q&A
2	Jan 27	Molecular/ Homogeneous Catalysis 101	
3	Feb 3	Heterogeneous Catalysis 101	
4	Feb 10	Sabatier Principle	
5	Feb 17	Electrocatalysis 101 H_2 evolution	Quiz 1 (#1- #4) in class
6	Feb 24	Theoretical Surface Science & Catalysis	
		Comparative Case Studies: Molecular/Heterogeneous/Biological	
7	Mar 3	Water Oxidation/O_2 reduction	
8	Mar 10	Water Oxidation/O_2 reduction	
9	Mar 24	Activation of N_2 & CO	Quiz 2 (#5- #8) in class
10	Mar 31	N_2 Reduction to Ammonia	
11	Apr 7	Catalytic Metabolic Networks 101 Biological CO_2 Reduction & Conversion	
12	Apr 14	Carboxylation: Electrocatalytic CO_2 Reduction & Conversion	
13	Apr 21	History of hydrocarbon reforming to high octane fuels: WWII Manhattan II Project	Quiz 3 (# 9-#12) in class
14	Apr 28	Student Posters (#2 to #13)	Poster + Oral + Q + A

READING ASSIGNMENTS:

1. **The Scientific Method:**
The Demon-Haunted World. "The Fine Art of Baloney Detection" Carl Sagan and Ann Druyan. Condensation is available online here: https://getpocket.com/explore/item/the-baloney-detection-kit-carl-sagan-s-rules-for-bullshit-busting-and-critical-thinking

2. & 3. **Catalysis 101:**
Concepts of Modern Catalysis and Kinetics, 2nd Ed. Ib Chorkendorff and Hans Niemantsverdriet, ISBN: 978-3-527-31672-4. Online at: Heterogeneous catalysis: the fundamentals, J W (Hans) Niemantsverdriet; https://www.catalysiscourse.com/aboutcatalysis.html

(a) Ch 2. Catalysts break bonds
(b) Ch 3. Kinetics

4. **The Sabatier principle**
(a) Ooka, H., et al. (2021). "The Sabatier Principle in Electrocatalysis: Basics, Limitations, and Extensions." **Frontiers in Energy Research**, Volume 9 - 2021.

5. **Electrocatalysis 101 and HER:**
(a) Electrocatalysis 101, T.Jaramillo; selected sections TBD. https://jaramillogroup.stanford.edu/pdfs/Electrocatalysis101.pdf
(b) Seh, Z. W., et al. (2017). "Combining theory and experiment in electrocatalysis: Insights into materials design." **Science 355**(6321): eaad4998. HER Reaction Only
(c) Ďurovič, M., et al. (2021). "Electrocatalysts for the hydrogen evolution reaction in alkaline and neutral media. A comparative review." **Journal of Power Sources 493**: 229708. Selected pages TBD.

6. **Theoretical surface science and catalysis**
Theoretical surface science and catalysis - calculations and concepts. Hammer, B., & Nørskov, J. K. (2000). ***Advances in Catalysis***, *45*, 71. Selected pages TBD.

7. & 8. **Catalysis of water oxidation/O_2 reduction:**
(a) *"Water Oxidation by the [Co4O4(OAc)4(py)4]+ Cubium is Initiated by OH– Addition." Smith, et al. (2015).* ***JACS 137****(49): 15460–15468.*
(b) Song, Y.-T., et al. (2023). "Is There a Different Mechanism for Water Oxidation in Higher Plants?" ***The Journal of Physical Chemistry B 127****(30): 6643–6647.*
(c) A Perovskite Oxide Optimized for Oxygen Evolution Catalysis from Molecular Orbital Principles Jin Suntivich*, et al.* ***Science*** *9 December 2011: Vol. 334 no. 6061 pp. 1383-1385 ; DOI: 10.1126/science.1212858 ; read* this short Perspective: On Discovering descriptors for catalyst performance. A Vojvodic, J K Nørskov, ***Science*** 2011;334:1355-1356.
(d) see 4(b) above, Seh, Z. W., et al. (2017). OER Reaction Only

9. & 10. **Catalysis of N_2 to ammonia:**
(a) Reactions at Surfaces: From Atoms to Complexity (Nobel Lecture). Gerhard Ertl, **Angew Chemie**, 2008; DOI: 10.1002/anie.200800480. Ertl's Nobel lecture can be found here: https://mediatheque.lindau-nobel.org/recordings/34695/gerhard-ertl-catalysis-surfaces-atoms
(b) Singstock, N. R. and C. B. Musgrave (2022). "How the Bioinspired Fe2Mo6S8 Chevrel Breaks Electrocatalytic Nitrogen Reduction Scaling Relations." **Journal of the American Chemical Society 144**(28): 12800–12806
(c) Siegbahn, P. E. M. (2024). "Computational Model Study of the Experimentally Suggested Mechanism for Nitrogenase." **The Journal of Physical Chemistry B 128**(4): 985–989.

11. **Biological CO_2 reduction and conversion**
(a) Types of Metabolic Networks: https://en.wikipedia.org/wiki/Metabolic_pathway ;
(b) Rubisco Function, ~~Evolution, and Engineering~~. Savage et al. **Annu. Rev. Biochem**. 2023. 92:385–410. https://doi.org/10.1146/annurev-biochem-040320-101244. Assigned reading is p 385 to 395 (not Evolution , not Engineering)
(c) Revised mechanism of carboxylation of ribulose-1,5-biphosphate by rubisco from large scale quantum chemical calculations. Peter L. Cummins, Babu Kannappan, Jill E. Gready **J Comput Chem**, (2018) Volume: 39, Issue: 21, Pages: 1656-1665, DOI: (10.1002/jcc.25343)

12. **Electrocatalytic CO_2 reduction and conversion.**
(a) See 4(b) above, Seh, Z. W., et al. (2017). CO_2 Reduction only.
(b) TBD, instructor's choice.

BACKGROUND KNOWLEDGE

Background readings will be recommended for those who want a refresher on fundamental concepts.