

# University of Notre Dame Spring 2001

## Chemistry 618A: Special Topics in Surface Chemistry

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Schedule: Monday, Wednesday, and Friday

This is a three-credit graduate course in surface chemistry. The first six weeks will be spent studying the catalytic hydrogenation of nitrogen. This reaction serves as an introduction to metal surface structure, chemi- and physisorption of small molecules, UHV systems, high-vacuum characterization techniques, and how metals act to catalyze reactions. The second topic, lasting about 4 weeks, will be an introduction to self-assembled organic thin films, or "wet" surface chemistry. The final topic will cover recent developments in the field of molecular electronics. By the end of the course, you will be able to:

- Describe current scientific understanding of these areas of chemistry and the evidence on which it is based.
- Use experimental results to evaluate alternate scientific models, drawing appropriate conclusions and suggesting additional experiments to clear up unresolved points.
- Read primary literature critically.
- Present a critical analysis of experimental results, both orally and in writing.

Texts: The main text for the class is *Introduction to Surface Chemistry and Catalysis*, G. A. Somorjai (Wiley, 1994). This text contains a good introduction to surface and overlayer structure and reactivity, focusing almost exclusively on UHV applications. Also recommended is the ICE Solid State Model Kit; two copies of this kit will be available from ML. *The Oxford Primer in Surface Chemistry*, and *Building Scientific Apparatus, 2<sup>nd</sup> edition*, Moore, Davis, and Coplan (Addison-Wesley 1989) describe surface analytical techniques and the experimental methods and instruments necessary for the study of clean surfaces in UHV (the latter book will be very useful as a handbook for anyone doing any UHV work). "Formation and structure of self-assembled monolayers," A. Ulman, Chem Rev. (1996) 96 1533-1554 gives up-to-date lead references for forming and studying monolayers in ambient conditions. The molecular electronics section will rely on the primary literature since there is no suitable textbook.

Assignments: 2 problem sets on experimental methods/data interpretation @15%	30%
3 critical analysis papers (4 pages each) @5%	15%
3 presentations @ 5, 10, & 15%	30%
Final exam	25%

Work load: Expect to spend 8 hr per week outside of class, averaged over the semester. If the coursework is taking significantly more time than this, talk to the instructor.

Grading scale:

A-level performance: Student has a strong understanding of the principles of surface chemistry, can evaluate data and interpretations independently, and can connect new material with old knowledge about chemistry. Student is prepared for class and contributes to class discussions. Papers show evidence of original thought and are well-researched and well-written. Oral presentations are engaging and convey a creative "take" on the material.

B-level performance: Student has a good understanding of fundamental principles of surface chemistry and can understand and evaluate experimental data. Student can follow arguments in the literature, detects some errors in data interpretation, and can sometimes connect new material with old knowledge. Student is prepared for almost every class and participates in class discussions. Papers are well-researched and clear, but have fewer original insights. Oral presentations are clear and relevant to the topic, but may miss important content, interpretations of data, or significant results. Student may give poor presentations at first, but shows good improvement over time.

C-level performance: Understanding of principles is weak, student often cannot apply them to a new situation or integrate them with old knowledge of chemistry. Student is prepared for most classes. Student can follow arguments in a paper but usually accepts them uncritically. Papers are full of typos, or poorly researched, or poorly put together, and show a lack of critical thinking. Presentations are unclear, disorganized, or painful to watch, with little improvement over time.

## Unit 1--Heterogeneous Catalysis & the Haber Process

Week	Topics	Class
1	Introduction	(ML out of town 1/16) Class intro, expectations Ammonia synthesis: history and state of the art.
2	Solid-state packing	Solid state packing of metals and semiconductors
	Miller indices	Miller indices
	UHV work, adsorbate overlayers, BET coverage, TDS.	Experimental methods Surface mesh structures. Physisorption/chemisorption. Adsorption isotherms.
3	UHV methods 1: XRD, LEED	Surface structures by diffraction—laser model
	UHV methods 2: XPS, AES	Analysis of XPS data
	Read Strongin & Somorjai paper	Discuss S&S paper
4	Read Paffett, Campbell, & Taylor paper on LEED/XPS & write conclusions section	discuss experimental data & conclusions
	Reaction thermodynamics, considerations for catalysis	Ammonia synthesis costs PS #1 due (UHV experimental methods)
	N <sub>2</sub> and NH <sub>3</sub> on clean metal	discuss papers
5	Promoters	discuss papers Draft of paper DUE
	Mechanistic proposals--read Science paper!!	discuss mechanisms Discuss your draft with ML
6		Critical analysis paper + presentation

## Unit 2      Self-Assembly at Surfaces and Interfaces: Organic Thin Films

7	Amphiphiles, films, biomembranes, and micelles	
8	Langmuir-Blodgett films: $\pi$ -A isotherms, transfer, IR spectroscopy	
9	SAMs: Formation, film structure determination	PS #2 due (ambient experimental methods)

10		Spring Break
11		Critical analysis paper + presentation

Unit 3      Recent Progress in Molecular Electronics

12	Conventional electronics, photolithography, and the silicon roadmap	
13-14	Paradigms in molecular electronics: Cross-bar architecture, DNA computing, QCA, quantum computing.	(easter holiday weeks 12/13)
14-15	Discussion of important papers in molecular electronics.	
16-17		Work on hypertext assignment
18		Final exam