

A Computational Investigation of Alcohol Degradation on Metal Surfaces

Faculty Research Grant Proposal

Faculty Development Committee

Submitted by:

Kimberly A. Lawler-Sagarin, Ph.D.

Assistant Professor

Department of Chemistry

I. Project Summary

One of my major research interests is the exploration of chemical reactions that occur with the help of a metal surface. Surface reactions are very important in industrial synthesis and many commercial processes. A metal surface may act as a catalyst which promotes or enhances a desired (or an undesired) reaction pathway. Perhaps one of the best known examples of the importance of surface catalysis is found in an automobile's emissions system. Among other things, the automobile's catalytic converter converts harmful gaseous nitric oxide (NO) to elemental nitrogen (N₂) and oxygen (O₂). From a chemical standpoint, often not much is known about surface catalysis. A surface used in such a way is often viewed as a "black box" by chemists. Our understanding of the mechanisms of most reactions that occur with the help of surfaces is rather limited. This is one of the reasons why catalysis is such a fertile area for exploration. A greater understanding of mechanisms of surface reactions can help in the design of more efficient and more selective catalysts, as well as contribute to our general understanding of chemical reactions. Quite a number of researchers are exploring industrially significant surface chemistry by experimental means. Computational work on such systems is somewhat more limited. The theoretical studies described here will compliment the experimental work and yield additional information about these processes. I am currently studying one set of reactions, the reactions of alcohols and aldehydes on group VIIIIB metal surfaces such as palladium, rhodium and platinum.

Alcohols and aldehydes are classes of oxygen containing compounds which are commercially important. There is experimental evidence that suggests that alcohols react differently on rhodium and palladium surfaces, whereas aldehydes undergo the same transformations on both metals. In preliminary work, we studied the beginning stages of these reactions and have uncovered some evidence for the origin of the different pathways. In the current proposed project, I seek to expand this research by investigating additional steps in the reaction pathways and utilizing additional computational methods. A description of how I plan incorporate undergraduate researchers into my research program is included here as well.

II. Project Narrative

II.1 Current Situation

II.1a Background

Metal surfaces are often used in the synthesis of oxygen containing compounds, such as alcohols and aldehydes. One example is the commercial production of methanol (CH₃OH) and larger alcohols (those containing two or more carbon atoms). Carbon-carbon (C-C) and carbon-oxygen (C-O) bond formation and breakage are the elementary steps in this type of process. The metal surface plays a primary role in the efficiency and selectivity of these steps.

A related process is the degradation of oxygen containing compounds on metal surfaces. Degradation reactions of oxygen containing compounds have been invoked as the reverse of their catalytic synthesis from carbon monoxide (CO) and hydrogen (H₂)[1]. Thus, studying the degradation process computationally can lead to useful information regarding the selectivity and efficiency of the metal catalysts in the synthesis of such compounds. This is the main focus of the proposed project.

II.1b Summary of the Research Problem

Experimental work by the Barteau group at the University of Delaware has raised some interesting questions about the role rhodium and palladium surfaces play in the degradation of alcohols. There is experimental evidence that alcohols undergo a different reaction pathway on rhodium surfaces than they do on palladium surfaces[2, 3, 4, 5].

In the case of ethanol ($\text{CH}_3\text{CH}_2\text{OH}$), a simple alcohol, Barteau's group has proposed the pathway shown schematically in Figure 1[2, 3].

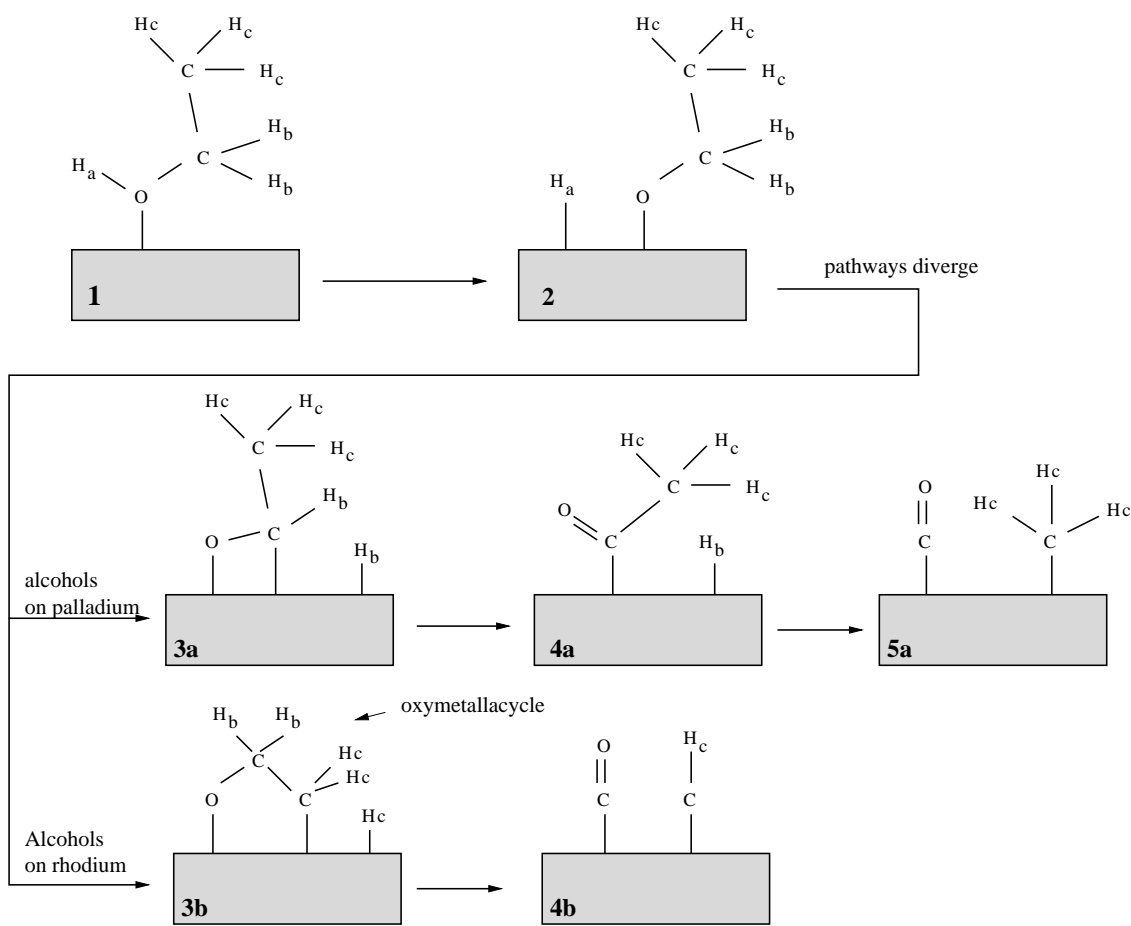


Figure 1: General reaction scheme for the degradation of ethanol (an alcohol) on the Pd(111) and Rh(111) surfaces

Ethanol is first adsorbed molecularly **1**. This is followed by abstraction of the hydrogen bound to the oxygen (H_1) to form the species shown in **2**. At this point the mechanisms on palladium and rhodium diverge. In the case of palladium, a C-H bond on the carbon adjacent to the oxygen atom is broken and the resulting species binds to the surface via the oxygen and the adjacent carbon as in **3a**. For rhodium however, the next step is believed to be the breaking of the distal C-H bond (a C-H bond on the second carbon) and the forming of an *oxymetallacycle*, shown in **3b**. This is followed by further degradation as shown in **4b** and **5b**. Interestingly, aldehydes follow the same pathway on both metal surfaces. Aldehydes on palladium or rhodium first bind to the surface via the oxygen and are rapidly converted to the configuration shown in **3a**. The remainder of the pathway is analogous to that shown for ethanol on palladium (**4a** and **5a**)[4, 5].

The observation that alcohols undergo degradation via different reaction pathways on the rhodium surface is interesting and suggests differences in the way alcohols interact with the two metal surfaces. Solid rhodium and palladium have the same geometrical structure and the interatomic (Rh-Rh and Pd-Pd) distances are almost identical for the two metals. Given these similarities, it is difficult to imagine the different pathways arising from such structural considerations. This opens up the possibility that the origin of the different behaviors is electronic in nature.

Electrons (negative particles that are components of atoms) are responsible for chemical bonding and chemical reactivity. In a sense, electrons comprise the “glue” that holds multiple atoms together, which in turn allows complex molecules to be formed. My research area is electronic structure theory, which is the

study of the role these electrons play in chemical bonding, molecular structure, and chemical and physical properties. Computational methods allow us to determine, in an average way, “where the electrons are” in a chemical system. This in turn provides information about chemical bonding and properties - information that can then be used to design new materials with desirable properties.

II.1c Previous Work

The interaction of a model alcohol (methanol, CH_3OH) and a model aldehyde (formaldehyde, CH_2O) with palladium and rhodium surfaces was explored. On a molecular level, metal surfaces are not perfectly flat, but rather may be compared to something like a filled carton of eggs, or the top of a stack of oranges at the grocery store. Thus, a molecule that is being adsorbed onto the surface of a metal has a number of possible binding sites - choices about where to lie on the surface.

We investigated the possible binding sites for methanol on rhodium and palladium surfaces, and found something very interesting. On the rhodium surface, methanol showed a strong preference for an “on-top” adsorption site - with the oxygen atom sitting directly on top of a metal atom. On palladium, no such site preference was observed. We have reason to believe that this difference results in different reaction pathways on the two metals. The “on-top” site preference shown by rhodium allows the straightforward formation of an oxymetallacycle (Figure 1, 3b).

We now believe that the origin of the on-top preference for methanol on rhodium is a result of a highly directional rhodium-oxygen bonding interaction. In the case of palladium, the palladium-oxygen interaction is not as directional. Our calculations indicate this difference arise from the different electron counts in the two metals (palladium atoms have one more electron than rhodium).

In related work, we also explored a model alcohol on nickel, platinum and cobalt surfaces. As with palladium, no significant site preferences were found for any of these metals, also in agreement with experimental results in the literature.

II.2 Project Plan

The preliminary results discussed above are promising and I would like to continue this project this summer in collaboration with 1-2 research students. The computational method I have been using in the preliminary work on this project is the Extended Hückel Tight Binding method. This method allows us to determine “where the electrons are” in a system which provides information about chemical bonding. Each step in a particular reaction can be viewed as a “snapshot”. By performing electronic structure calculations on each “snapshot”, we can develop a clear understanding of the reaction as it proceeds. In the preliminary work above, we investigated one step in the degradation reaction pathway on the two metals (step 2 in Figure 1). The current proposal seeks to expand this work to explore the remainder of the mechanism and utilize additional computational techniques.

The three primary components of the proposed study are:

1. to explore the remainder of the two different reaction pathways on both palladium and rhodium (step 3 and beyond in Figure 1) to understand the chemical bonding present and elucidate differences in the two metal surfaces.
2. to understand the formation of the oxymetallacycle intermediate species (step 3b in Figure 1). Oxymetallacycles have been suggested as intermediates and in other surface reactions and have been explored experimentally[6, 7, 8, 9, 10].
3. to determine if the site preferences found for alcohols on rhodium is replicated at a higher level of theory (using different computational techniques).

The extended Hückel Tight Binding method is capable of handling large systems efficiently and provides results which are relatively easy to interpret chemically. There are several advantages to using this method to explore surface catalysis. Because it handles large systems well, we can model the metal surface as a large slab, rather than using a simple model containing only one or two metal atoms, which is insufficient in many cases. Its efficiency allows us to perform numerous calculations in a relatively short period of time. Its ease of interpretation makes it an ideal method to be used by students. However, the extended Hückel Tight Binding method also has some limitations. For example, some calculated properties are very sensitive to interatomic distances and while relative energy calculations are qualitatively correct, they contain substantial uncertainties[11]. For these reasons it is desirable to investigate the observed site preference utilizing additional computational means. For example, I plan to perform *ab initio* calculations, where the surface is represented by a small cluster of metal atoms. *ab initio* refers to “from first principles”. Such computations don’t use empirical parameters derived from experiment to simplify the calculations, bypassing some of the problems associated with semi-empirical methods such as extended Hückel.

I believe that this study will yield fundamental information about the alcohol degradation reaction on palladium and rhodium, thus giving some insight into the role of the metal catalyst in oxygenate synthesis. We must explore the role metal surface play in these types of reactions if we are to rationally (i.e. predictively) design more efficient and more selective catalysts. The design of better catalysts is desirable from an economic standpoint as well as a scientific one. For instance, the use of palladium as a catalyst in the synthesis of alcohols produces methanol (CH₃OH). However, the synthesis of longer chain alcohols (those containing more carbon atoms) requires a different catalyst[5]. It is possible to form these longer chain alcohols using rhodium, however rhodium is about \$500 a gram whereas palladium is less than \$40 per gram. Understanding the factors which give rise to such different behavior can lead to the design of less expensive catalysts.

II.3 Faculty Expertise

My graduate research primarily consisted of electronic structure investigations. I received my Ph.D. from Cornell University in 1994, where I worked with Nobel Laureate Dr. Roald Hoffmann. As a faculty member at California State University, Fresno, I engaged in independent research in collaboration with student researchers on this project as well as a number of others. In total, I have supervised one M.S. student and eight undergraduate students. This has resulted in four student presentations at national meetings, and three at regional meetings.

I have used the Extended Hückel Tight Binding Method to explore solid state structures extensively. I have also used *ab initio* computational methods to perform calculations on small metal systems. In 1997, I spent the summer in the research group of Dr. Tom Cundari at the University of Memphis. This resulted in experience combining different computational methods for metal-based systems.

In 2000, I left Fresno State to relocate to the Chicago area, where my spouse holds a faculty position. I worked in administration at Northwestern before coming to Elmhurst College. The administrative position did not allow me to continue my chemical research, which is one of the reasons I came to Elmhurst. This grant would be instrumental in restarting my research program.

My full *curriculum vitae* is included in Appendix A.

II.4 Plans for Evaluation and Dissemination

Increasing undergraduate research activity in the Chemistry Department is particularly desirable. Students participating in this study will gain invaluable research experience as well as a familiarity with common computational methods in chemistry. Additional benefits for the students will come with publication and presentation of the work. Students working with me in the summer of 2003 would be able to present their

work at the undergraduate research symposium at the American Chemical Society National Meeting in March of 2004.

Ultimately, results of this project will be submitted to a peer-reviewed journal such as Surface Science or Journal of Catalysis. The study of heterogeneous catalysis is also a fertile area for attracting external funding. Completion and subsequent publication of this study will make external proposals for future work in this area more likely to be successful.

III. Time Line

This summer, I would work closely with one or two research students. This could be accomplished by having one student working 30 hrs/week for 8 weeks, or 2 students working a combined average of 15/hrs per week. The project is very modular and can easily be broken into smaller projects suitable for undergraduates. Once undergraduates are recruited, about two weeks will be spent working with them to orient them to the software and the theoretical background. The remainder of the summer they will spent working closely with me to perform and interpret calculations.

In the fall, the student(s) would submit the results of their summer research to the undergraduate research symposium at a regional or national meeting of the American Chemical Society.

IV. Budget

Item	Amounts	Total requested
a) Supplies and Equipment		
Software: Spartan (Wavefunction, Inc.)	1,000	
General Supplies (backup media, etc)	150	
		1,150
b) Student Assistants		
Undergraduate summer stipends (240 hrs @ \$8/hr)	1,920	1,920
c) Travel		
Conference Travel	430	430
Total Amount		3,500
Funds Requested		3,500

Budget Justification:

I am not requesting summer salary, but instead, am requesting funding for students. I believe getting students involved in this research is crucial both for my department and the college. I also already have one month of summer funding for a joint project with Anne Britt at Northern Illinois University. This funding is for materials development for the project "Improving Students' Comprehension and Construction of Arguments" (see grants, below). With careful planning, this should not impact my ability to guide students on the proposed research project over the summer, as my contributions to the outside project will also be performed at Elmhurst College.

Visualization is very helpful in my computational work and it is particularly helpful for students with little experience. Thus, I am requesting a copy of the computational chemistry program Spartan, from Wavefunction, Inc. Spartan allows students to build and manipulate molecular models on the computer screen and has a very user-friendly interface. It has a variety of capabilities (specifically the ability to perform *ab initio* and Density Functional calculations) that are not present in software currently owned by the Chemistry Department. Additional software necessary for the project is "shareware" and is free to

academic users.

V. Current and Previous Grants

I've included here a list of my three most recent grants from external funding agencies. All of these were co-written, so I have included a full list on my *curriculum vitae* in Appendix A.

- **U.S. Department of Education Office of Educational Research and Instruction**

“Improving Students’ Comprehension and Construction of Arguments” PI M.A. Britt (Department of Psychology, Northern Illinois University); Co-PI’s C. R. Wolfe (Miami University) and K. Lawler-Sagarin (Elmhurst College).

Amount: \$358,876

Awarded: 9/02

- **Andrew J. Mellon Foundation**

“Gateway Science Workshop Program at Northwestern University” G. Light (Project Director) with Co-PI’s: K. Bain, K. Lawler-Sagarin, L. Pinto, E. Lowe

Amount: \$560,000

Awarded: 8/01

- **PPG Foundation**

“Molecular Modeling and Computational Chemistry throughout the Undergraduate Chemistry Curriculum” Co-PIs: Joseph Gandler (project director), Kimberly Lawler, Jose Sy

Amount: \$10,000

Awarded: 2/00

VI. Publications and Presentations

A full list is available in my *curriculum vitae* in Appendix A.

1. Light, Gregory; Luna, Melissa; Lawler-Sagarin, Kimberly A. “Realizing the Reflective Professor: Integrating Teaching and Research” Featured presentation scheduled for the 22nd Annual Lilly Conference on College Teaching, November 2002.
2. Goto, Kim F.; Lawler, Kimberly A. “A Computational Investigation of CH₃O on Pt(111), Co(0001) and Ni(111)” Presented at the 219th National Meeting of the American Chemical Society, March 2000.
3. Goto, Kim F.; Lawler, Kimberly A. “A Computational Investigation of Methoxy on Cobalt, Nickel and Platinum Surfaces” Central California Research Symposium, Fresno, CA, April 2000.
4. White, Jason D.; Fox, Shawn M.; Walker, Gail M.; Lawler, Kimberly A. “Formaldehyde Coupling on Metal Surfaces - A Computational Investigation” Central California Research Symposium, Fresno, CA, April 2000.
5. Blanken, Hiram W.; Lawler, Kimberly A. “A Computational Investigation of Methoxy on Rhodium and Palladium Surfaces” Central California Research Symposium, Fresno, CA, April 2000.

References

- [1] Sachtler, W. M. H.; Ichikawa, M. *J. Phys. Chem.* **1986**, *90*, 4758.
- [2] Davis, J. L.; Barteau, M. A. *Surf. Sci.* **1990**, *235*, 235.
- [3] Houtman, C. J.; Barteau, M. A. *J. Catal.* **1991**, *130*, 528.
- [4] Davis, J. L.; Barteau, M. A. *J. Am. Chem. Soc.* **1989**, *111*, 1782.
- [5] Brown, N. F.; Barteau, M. A. *Langmuir* **1992**, *8*, 862.
- [6] Brown, N. F.; Barteau, M. A. *Surf. Sci.* **1993**, *298*, 6.
- [7] Xu, X.; Friend C. M. *J. Am. Chem. Soc.* **1991**, *113*, 8572.
- [8] Xu, X.; Friend C. M. *J. Am. Chem. Soc.* **1991**, *113*, 6779.
- [9] Xu, X.; Friend C. M. *J. Phys. Chem.*, **1991**, *95*, 10753.
- [10] Xu, X.; Friend C. M. *Langmuir* **1992**, *8*, 1103.
- [11] Lowe, J. P. *Quantum Chemistry*; 2nd Edition; Academic Press, San Diego. 1993.
- [12] Pérez, J. M.; Cases, F. J.; Vásquez, J. L.; Aldaz, A. *Surf. Sci.*, **1990**, *235*, 307.
- [13] Pérez, J. M.; Cases, F. J.; Puig, F. J.; Vásquez, J. L. *J. Mol. Struct.*, **1992**, *254*, 379.
- [14] Jørgensen, K. A.; Schiøtt, B. *Chem. Rev.*, **1990**, *90*, 1483.
- [15] Blyholder, G.; Lawless, M. *J. Am. Chem. Soc.*, **1989**, *111*, 1275.

Appendix A: Abbreviated CV, Kimberly A. Lawler-Sagarin

Education

Cornell University, Ithaca, New York

Doctor of Philosophy

August 1994

Master of Science

July 1992

Major Subject: Theoretical Chemistry

Minor Subject: Physical/Inorganic Chemistry

Thesis Advisor: Dr. Roald Hoffmann

Dissertation: Theoretical Studies of Chemical Bonding in Early Transition Metal Clusters, Dinuclear Complexes and an Organometallic Polymer.

Harvey Mudd College, Claremont, California

Bachelor of Science (Chemistry)

May 1989

Academic Experience

Department of Chemistry, Elmhurst College

Assistant Professor

January 2002 - present

Searle Center for Teaching Excellence, Northwestern University

Associate Director

August 2000 - January 2002

Consultant

January 2002 - present

Department of Chemistry, California State University, Fresno

Assistant Professor (tenure-track)

1994 - 1999

Assistant Professor (tenured)

1999 - 2000

Awarded Promotion to Associate Professor

June 2000

On leave

August 2000 - January 2002

Teaching Experience

Elmhurst College

January 2002-present

- Chemistry and Issues in the Environment (Nonmajors) Spring 2002, 2003
- Physical Chemistry I & II (Majors) Spring 2002, 2002-2003
- Instrumental Module: AA/UV-Vis/X-ray (Majors) Spring 2002, 2003
- Instrumental Module: Guided Project (Majors) Spring 2002, 2003
- General Chemistry (Nursing Majors) Fall 2002

California State University, Fresno

August 1994-August 2000

Taught over a dozen different courses at the non-major through graduate level. (*Course list follows.*)

- Chemistry, Its Impact on Society (Nonmajors) Each Fall 1995-98, Spring 1998

- Chemistry, Its Impact on Society Laboratory (Nonmajors) Each Fall 1995-98, Spring 1998
- Introduction to Physical Chemistry (Biochem Majors) Fall 1994, Fall 1995
- Physical Chemistry (Majors) 1996-97, 1998-99, 1999-00
- Physical Chemistry Laboratory (Majors) Each Spring 1995-2000
- Advanced Inorganic Chemistry (Majors) Fall 1998
- Advances in Inorganic Chemistry (Graduate Course) Spring 1997, 1999
- Theoretical Inorganic Chemistry (Graduate Course) Spring 1995, 1996
- Quantum Chemistry (Graduate Course) Fall 1997, 1999
- General Chemistry Laboratory (Majors) Fall 1994
- Seminar (Graduate Seminar) Fall 1997, 1998
- Introduction to the University
(This is a University Orientation course for Freshman.) Fall 1997, Spring 1998
- Atmospheric Chemistry Fall 1997
(Extended education course for Fresno Unified Middle/High School Teachers.)

Cornell University

Fall 1989 - Spring 1991

Teaching Assistant for Instrumental and Physical Chemistry Laboratory

Publications

- Lawler-Sagarin, K. A.; "Using the World Wide Web in a Chemistry and Society Course to Promote Active Learning and Student Engagement" *Under review*.
- Miller, R. L. ; Lawler, K. A.; Bennett, J. L. ; Wolczanski, P. T. "Ditungsten Siloxide Hydrides, [(silox)₂WH_n]₂ (n = 1, 2; silox = ^tBuSiO), and Related Complexes." *Inorganic Chemistry*, **1996**, *35*, 3242.
- Lawler, K. A.; Hoffmann, R.; "The Electronic Structure of [Ta₅(NH)₄Cl₁₇]⁶⁻ - A Cluster With a "Flattened" Square Pyramidal Ta₅ Core." *Inorganic Chemistry*, **1996**, *35*, 1431.
- Lawler, K. A.; Hoffmann, R.; Holl, M. Banaszak; Wolczanski, P. T.; "The Polyamidoimidonitride Clusters of Zirconium - Molecular Orbital Study." *Zeitschrift für anorganische und allgemeine Chemie*, **1996**, *622*, 392.
- Genin, H. S.; Lawler, K. A.; Hoffmann, R.; Herrmann, W. A.; Scherer, W., Fischer, R. W. "Polymeric Methyltrioxorhenium - Some Models for its Electronic Structure." *J. Am. Chem. Soc.*, **1995**, *117*, 3244.
- Lawler, K. A.; Van Hecke, G. R.; "Dilatometry of the Discotic Mesogen 2,3,6,7,10,11-hexa-*n*-octanoyloxy-triphenylene (HAT-C8): An Anomalous Discotic - Isotropic Phase Transition." *Liquid Crystals*, **1991**, *10*, 341-346.

External Grants

- **U.S. Department of Education Office of Educational Research and Instruction** "Improving Students' Comprehension and Construction of Arguments" PI M.A. Britt (Department of Psychology, Northern Illinois University); Co-PI's C. R. Wolfe and K. Lawler-Sagarin. Amount: \$358,876 Awarded: 9/02
- **Andrew J. Mellon Foundation** "Gateway Science Workshop Program at Northwestern University" G. Light (Project Director) with Co-PI's: K. Bain, K. Lawler-Sagarin, L. Pinto, E. Lowe. Amount: \$560,000 Awarded: 8/01

- **PPG Foundation** “Molecular Modeling and Computational Chemistry throughout the Undergraduate Chemistry Curriculum” Co-PIs: Joseph Gandler (project director), Kimberly Lawler, Jose Sy Amount: \$10,000. Awarded: 2/00
- **Research Corporation**
“A Computational Study of Heterogeneous Catalysis: Oxygenates on Metal Surfaces.” Amount: \$14,237 Awarded: 5/97
- **San Diego Supercomputing Center** “A project to introduce students in Chemistry 111 (Physical Chemistry Laboratory) to high-performance computing.” Supercomputer Time: 46 service units on the Cray C-90 Supercomputer. Awarded: 1/97
- **American Chemical Society - Petroleum Research Fund** “Computational Investigation of the Reductive Coupling of Carbonyls to Olefins.” Amount: \$20,000. Awarded: 5/96

Presentations at National Meetings

11. Light, Gregory; Luna, Melissa; Lawler-Sagarin, Kimberly A. “Realizing the Reflective Professor: Integrating Teaching and Research” Featured presentation scheduled for the 22nd Annual Lilly Conference on College Teaching, November 2002.
10. Goto, Kim F.; Lawler, Kimberly A. “A Computational Investigation of CH₃O on Pt(111), Co(0001) and Ni(111)” Presented at the 219th National Meeting of the American Chemical Society, March 2000.
9. Lawler, Kimberly A. “Computational Chemistry Throughout Upper Division Inorganic Chemistry” Presented at the 217th National Meeting of the American Chemical Society, March 1999.
8. Lawler, Kimberly A. “Three Years of Using the World Wide Web in a Chemistry and Society Course” Presented at the 217th National Meeting of the American Chemical Society, March 1999.
7. White, Jason D.; Fox, Shawn M.; Lawler, Kimberly A. “Carbonyl Coupling on Metal Surfaces - A Computational Investigation” Presented at the 217th National Meeting of the American Chemical Society, March 1999.
6. Silveira, William R.; Marhenke, Ronald M.; Lawler, Kimberly A. “A Computational Investigation of a Hydrocarbon with Six Five-Carbon Rings” Presented at the 217th National Meeting of the American Chemical Society, March 1999.
5. Lawler, Kimberly A. “A World Wide Web Site Created by the Students in a Chemistry and Society Course” was presented at the 213th National Meeting of the American Chemical Society, April 1997.
4. Blanken, Hiram W.; Lawler, Kimberly A. “A Computational Investigation of Alcohols and Aldehydes on Rh(111) and Pd(111)” Presented at the 213th National Meeting of the American Chemical Society, April 1997.
3. Barghouti, Samira; Lawler, Kimberly A.; Garcia, Carmelo “Spectroscopy of Catacondensed Hydrocarbons.” Presented at the 212th National Meeting of the American Chemical Society, August 1996.
2. Lawler, Kimberly A.; Hoffmann, Roald “The Electronic Structure of [Ta₅(NH)₄Cl₁₇]⁶⁻ - A Cluster With a “Flattened” Square Pyramidal Ta₅ Core.” Presented at the 209th National Meeting of the American Chemical Society, April 1995.
1. Genin, Hugh S.; Lawler, Kimberly A.; Hoffmann, Roald; Herrmann, W. A. “Polymeric Methyltrioxorhenium - Some Models for its Electronic Structure.” Presented at the 208th National Meeting of the American Chemical Society, August 1994.

Presentations at Local/Regional Meetings

8. Goto, Kim F.; Lawler, Kimberly A. “A Computational Investigation of Methoxy on Cobalt, Nickel and Platinum Surfaces” Central California Research Symposium, Fresno, CA, April 2000.

7. White, Jason D.; Fox, Shawn M.; Walker, Gail M.; Lawler, Kimberly A. "Formaldehyde Coupling on Metal Surfaces - A Computational Investigation" Central California Research Symposium, Fresno, CA, April 2000.
6. Blanken, Hiram W.; Lawler, Kimberly A. "A Computational Investigation of Methoxy on Rhodium and Palladium Surfaces" Central California Research Symposium, Fresno, CA, April 2000.
5. Lawler, Kimberly A. "Three Years of Using the Web in a Chemistry and Society Course" Excellence in Teaching and Learning Conference, California State University, Fresno, January 1999.
4. Curtis, Kathleen A.; Lawler, Kimberly A.; Fine, Lawrence J. "A Hero Lies in You: Adventure Challenge Course Experience for New University Students" Excellence in Teaching and Learning Conference, California State University, Fresno, January 1998.
3. Lawler, Kimberly A. "Web Surfing: Can We Get Students to Evaluate What They See on the Monitor?" Excellence in Teaching and Learning Conference, California State University, Fresno, January 1998.
2. Blanken, Hiram W.; Lawler, Kimberly A. "A Computational Investigation of Alcohols and Aldehydes on Rh(111) and Pd(111)" Central California Research Symposium, Fresno, CA, April 1997. ,
1. Lawler, Kimberly A.; "A World Wide Web Site Created by the Students in a Chemistry and Society Course" Conference on Excellence in Teaching and Learning, California State University, Fresno, January, 1997.

Faculty Development Workshops Presented

- Peer Facilitator Training Workshops, Science Workshop Programs (with G. Light, K. Bain) Northwestern University Fall 2000, Spring 2001, Fall 2001.
- Teaching Philosophy Statement Workshops, Preparing Future Faculty, Northwestern University. October 2000, December 2000, October 2001, December 2001.
- "Teaching in Science Courses, Developing Deeper Approaches to Learning and Problem Solving," (with G. Light) Beyond Books Program, Northwestern University, October 2000.
- Teaching Consultant Training, Small Group Analysis Service, Searle Center for Teaching Excellence, Northwestern University, Fall 2000, Fall 2001.
- "Reflections on Teaching and Learning: Developing Your Teaching Portfolio" Beyond Books Program, Northwestern University, April 2001.
- "Applying for Academic Jobs: Writing a Teaching Philosophy Statement" (with H. D. Smith) Beyond Books Program, Northwestern University, October 2001.
- Collaboration on design/presentation of over a dozen additional workshops in: the Faculty Workshop Series, the Graduate Student Workshop Series, the Searle Fellows Program, and various New Faculty Workshops (with various members of the Searle Center Staff) Northwestern University, August 2000 - January 2002
- "Fun Science Activities," IDEA Inservice Training, Fresno Unified School District, Spring 1995.

Graduate Coursework

Theoretical/Physical Chemistry:

Quantum Mechanics (2 semesters)
Statistical Mechanics
Spectroscopy

Advanced Inorganic Chemistry:

Group Theory and Main Group Chemistry
Coordination Chemistry and Organometallics
Solid State Chemistry

Additional Physics and Mathematics:

Applied Mathematics (3 semesters)
Classical Mechanics
Electromagnetism

Application to Extended Systems:

Solid State Physics
Electronic Structure of Solids