

# SOUTHWEST CATALYSIS SOCIETY



## 2010 SPRING SYMPOSIUM

March 12, 2010

Duncan Hall  
McMurtry Auditorium – Martel Hall  
Rice University, Houston, TX

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The SWCS officers and I welcome you to the 2010 SWCS Spring Symposium, **March 12, 2010, Friday**, at Rice University.

We are delighted to present 7 invited speakers and 16 poster presentations for today's meeting. Meritorious posters presented by students and post-docs will be identified with **Best Poster Awards**, carrying cash prizes.

The 2010 Spring Symposium **registration fee is \$40**, which includes North American Catalysis Society and SWCS yearly membership dues and the coffee/snack breaks. To speed registration, provide your business card along with your registration fee. Do let those who cannot attend the Symposium know to mail in their membership due (\$25) to our Treasurer, Prof. George Stanley (mailing address shown at left). Unfortunately, we cannot take credit cards for payment.

The student registration fee is \$10, which includes NACS and SWCS membership. Thanks to a grant from the NACS, the SWCS will pay the registration fee for all students and postdocs again this year. Depending on the remaining funds, we may be able to announce additional reimbursement opportunities for students / postdocs (especially for those living outside Houston) at the meeting.

Enjoy!

Michael Wong  
Chair



## FINAL PROGRAM

- 8:00 AM Registration – John Novak, Director** Duncan Hall – Martel Hall
- 8:30 AM Welcoming Remarks – Michael Wong, Chair**  
Duncan Hall – McMurtry Auditorium
- 8:35 AM Prof. Kerry Dooley (LSU, Baton Rouge, LA)**  
"Perspectives on Catalytic Oxidative Desulfurization"
- 9:05 AM Prof. Ilke Arslan (UC Davis, Davis, CA)**  
"Advanced Characterization of Catalysts Using Novel Techniques in the Electron Microscope"
- 9:35 AM Coffee Break / Poster Setup** Duncan Hall – Martel Hall
- 10:00 AM A. Rider Barnum, Prof. George Stanley (LSU, Baton Rouge, LA)**  
"The Dramatic and Unexpected Effect of Water on a Bimetallic Hydroformylation Catalyst: Aldehyde-Water Shift Catalysis and Hydrocarboxylation"
- 10:30 AM Dr. David Graf (The Dow Chemical Company, Freeport, TX)**  
"A Dow Perspective on Alternative Feedstocks & Separations Needs for the Chemical Industry"
- 11:00 AM Lunch Break (on your own) / Poster Preview**  
Rice Student Center
- ~12:10 PM Re-assemble in Duncan Hall – McMurtry Auditorium**
- 12:15 PM Prof. Friederike C. Jentoft (University of Oklahoma, Norman, OK)**  
"Stabilization of Catalytic Alkane Isomerization"
- 12:45 PM David J. DiCamillo (Criterion Catalysts, Houston, TX)**  
"Beyond ULSD: Technology Enhancements to Improve Distillate Product Quality"
- 1:15 PM Prof. Keith Stevenson (UT Austin, Austin, TX)**  
"'Templated' Nanocatalysts for Electrochemical Energy Conversion: The Challenges for Synthesis and Characterization"
- 1:45 PM Poster Session / Coffee Break**  
Duncan Hall – Martel Hall
- 3:30 PM Poster Awards and SWCS Business**  
Duncan Hall – McMurtry Auditorium
- 4:00 PM Adjourn**



## Perspectives on Catalytic Oxidative Desulfurization

Kerry Dooley\*

Dept. of Chemical Engineering, Louisiana State University, Baton Rouge, LA

\*dooley@lsu.edu

Increasingly strict regulations on sulfur content in transportation fuels, and the myriad potential uses of H<sub>2</sub>, has prompted research on alternatives to catalytic hydrotreating for the past two decades. Alternatives include selective sulfur adsorption, selective sulfur oxidation (oxidative desulfurization, ODS) and biodesulfurization. This talk will review the field of ODS, including some recent work at LSU, and offer possibilities for future directions.

ODS has potential advantages over HDS, apart from non-usage of H<sub>2</sub>. The ODS reactions can be conducted at relatively mild conditions – often below 100°C. The sulfoxide / sulfone products (especially the sulfones) are polar enough that they can be separated from the remaining fuel by selective adsorption, or by extraction with polar solvents. Finally, the most refractory sulfur-containing heterocycles, such as alkylated dibenzothiophenes, are more easily converted to their sulfones than is thiophene, in contrast to HDS. Many studies on both oxidants and catalysts have been published (although there has been minimal mechanistic work), and some catalysts show significant activity for oxidation of the typical sulfur heterocycles. Based on the oxidant, these ODS systems can be broadly classified as O<sub>2</sub>-based, or peroxide-based ODS.

For peroxide-based ODS, the insolubility of aqueous H<sub>2</sub>O<sub>2</sub> presents an obstacle that has been attacked by using either a solvent to extract organosulfur compounds into the aqueous phase, a phase transfer catalyst, or a peroxide with high solubility in fuels, such as t-butyl hydroperoxide. In some cases peroxide initiators are combined with O<sub>2</sub>. Catalysts run the full range from low-temperature, peroxide-binding catalysts (e.g., heteropolyacids) to more typical oxidation catalysts normally associated with nucleophilic oxygen (e.g., V<sub>2</sub>O<sub>5</sub>/TiO<sub>2</sub>). Some key considerations that are often overlooked include the peroxide efficiency (how much oxidation takes place per peroxide molecule decomposed) and the reaction selectivity.

Recently there has been a flurry of papers dealing with O<sub>2</sub> as oxidant, or with a combination of O<sub>2</sub> and sacrificial oxidant such as isobutyraldehyde. These oxidations are typically slower and less selective (for sulfones), but the limited studies to date suggest there is promise. Again, a wide range of catalysts have been tested, mainly on artificial feeds or with limited analytical or mechanistic goals. Recent work at LSU has compared a wide range of catalytic materials for ODS with O<sub>2</sub> on a semi-realistic feed (a synthetic #2 diesel), with detailed results on sulfur oxidation selectivity. These will be reviewed and compared to recent literature.

*Kerry Dooley is the BASF Professor of Chemical Engineering at Louisiana State University. He has worked in the fields of heterogeneous catalysis, reactor design and high-pressure materials processing for over 30 years and in that time has authored over 75 publications and 4 patents, while supervising over 30 graduate students and postdocs. He has also consulted or performed contract research for several firms in the CPI. He is the Associate Editor of the RSC "Catalysis" series, and he chaired the 2007 North American Catalysis Society meeting.*

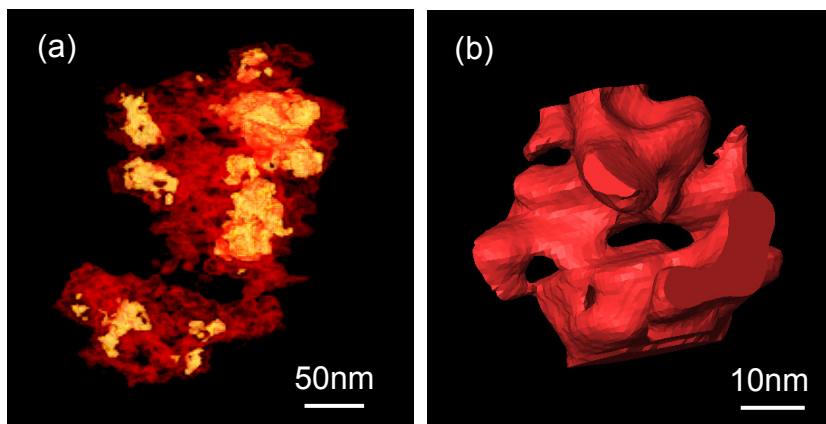
## Advanced Characterization of Catalysts Using Novel Techniques in the Electron Microscope

Ilke Arslan (iarслан@ucdavis.edu)

Chemical Engineering and Materials Science, University of California at Davis

The complex processes taking place during catalysis are largely determined by the intricate three-dimensional (3-D) nanoscale architectures of both the support and the catalyst, the atomistic interactions at the interfaces between the two, and the harsh, non-equilibrium conditions under which successful reactions can take place. In order to nano-engineer the next generation of efficient catalysts, a fundamental understanding of the materials is necessary on the atomic- and 3-D nano-scales, and in an in-situ gas environment.

In this talk I will review the state-of-the-art in electron microscopy characterization for catalysis, highlighting the research in this area currently being performed at UC Davis. The majority of the presentation will focus on 3-D methods to quantify Fischer-Tropsch catalysts using scanning transmission electron microscope (STEM) tomography, through which we have been able to understand the nanoscale size, distribution, architecture, pore sizes, porosities, etc. of the catalyst and its support. An electron tomogram showing (a) the large scale distribution of catalyst on support, and (b) porosity of one catalyst cluster can be seen below. I will conclude the talk by discussing the development of new stages to perform these measurements in gaseous and liquid environments, and show first results from our newly commissioned liquid stage.

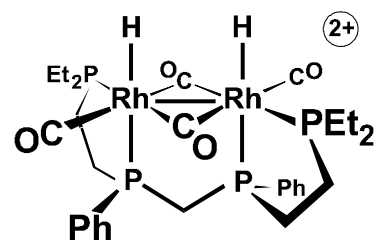


*Ilke Arslan is an Assistant Professor in the Chemical Engineering and Materials Science Department at the University of California at Davis. She received her B.S. and M.S. in Physics from the University of Illinois at Chicago, transferring to finish her Ph.D. in Physics in 2004 at UC Davis. Before moving back to Davis, she held fellowships from the NSF and the Royal Society to perform postdoctoral work at the University of Cambridge, and a Truman Fellowship to perform independent research for 3 years at Sandia National Laboratories.*

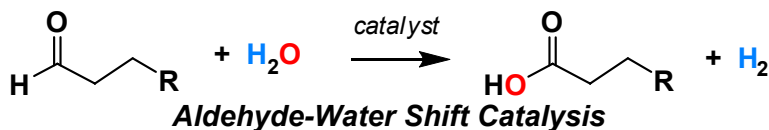
## The Dramatic and Unexpected Effect of Water on a Bimetallic Hydroformylation Catalyst: Aldehyde-Water Shift Catalysis and Hydrocarboxylation

A. Rider Barnum, Novella Bridges, David Aubry, Bobby Barker, & George G. Stanley\*  
 Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803-1804.  
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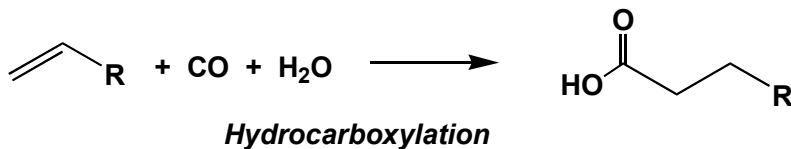
We have shown that a homobimetallic rhodium complex using the binucleating tetra-phosphine ligand *racemic*-(Et<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>)(Ph)PCH<sub>2</sub>P(Ph)(CH<sub>2</sub>CH<sub>2</sub>PEt<sub>2</sub>), et,ph-P4, is a highly active and selective hydroformylation catalysts for a variety of 1-alkenes (Cf. *Science* **1993**, 260, 1784). We have investigated the exact nature of the bimetallic cooperativity in this novel catalyst via *in situ* FT-IR, NMR, kinetic, isotopic labeling experiments, DFT calculations and molecular modeling studies. The FT-IR and NMR studies clearly indicate that the key catalyst species is an unusual dicationic M-M bonded Rh(+2) oxidation state bimetallic complex, *rac*-Rh<sub>2</sub>H<sub>2</sub>(μ-CO)<sub>2</sub>(CO)<sub>2</sub>(et,ph-P4)<sup>2+</sup> (*Angew. Chem. Int. Ed. Engl.* **1996**, 35, 2253).



A remarkable new catalytic reaction can occur under the proper conditions when water is added to the acetone solvent. Under mild hydrogen deficient conditions the reaction of aldehyde and water can occur to produce carboxylic acid and H<sub>2</sub>. This reaction is inhibited by H<sub>2</sub>, which has, so far limited the number of turnovers performed.



The net stoichiometry of hydroformylation combined with this unusual aldehyde-water shift catalysis is that of hydrocarboxylation, an extremely difficult reaction to perform selectively or under mild conditions.



DFT calculations and experimental studies point to [Rh<sub>2</sub>(μ-CO)<sub>2</sub>(CO)<sub>2</sub>(et,ph-P4)]<sup>2+</sup> as the likely active catalyst for the aldehyde-water shift catalysis. We believe that bimetallic cooperativity plays an important role in this catalysis as it does in hydroformylation.

*Mr. Rider Barnum, originally from Natchitoches, Louisiana, received a B.S. in Chemistry from Loyola University New Orleans (2007), while performing research into organometallic catalysts with anti-viral properties. He is currently third-year student at Louisiana State University and a PhD Candidate working under Professor George Stanley. His research focus builds on the Stanley research on bimetallic rhodium hydroformylation catalysts.*





## **A Dow Perspective on Alternative Feedstocks & Separations Needs for the Chemical Industry**

David D. Graf, The Dow Chemical Company, Freeport, TX (DDGraf@dow.com)

Alternative feedstocks are a critical issue to the chemical industry. Most industrial chemicals are derived from crude oil or natural gas and thus the price and availability is strongly dependent on the fuels market. Over the last 5 years, the large rise in energy prices and corresponding feedstock prices have continued to erode the profitability of American based chemical companies. One response to this cost has been to move operations overseas to tap into lower cost feedstocks (e.g. the MiddleEast). In another move, many chemical companies are looking at alternative feedstocks that are not derived from crude-oil and natural gas. In this talk, we will outline the underlying issues behind these alternative feedstocks needed for chemical manufacturing. We will also highlight key separation issues that need to be solved before some alternatives can become economically competitive with traditional feedstocks.

*Dr. David Graf received a BS in Chemistry from Michigan State University (1992) and a Ph.D. in Chemistry from University of Minnesota (1996). After a postdoc in the Chemistry Department at MIT (1996-1998), he joined Dow in Midland, MI, working in polyolefins and alkane activation research. He is currently Senior Technical Leader in Hydrocarbons and Energy R&D.*



## Stabilization of Catalytic Alkane Isomerization

Friederike C. Jentoft<sup>a</sup>, Matthew J. Wulfers<sup>a</sup>, Genka Tzolova-Müller<sup>b</sup>, Carine Chan Thaw<sup>b</sup>, José Ignacio Villegas<sup>c</sup>, Dmitry Yu. Murzin<sup>c</sup> (fcjentoft@ou.edu)

<sup>a</sup>Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK 73019

<sup>b</sup>Department of Inorganic Chemistry, Fritz Haber Institute, Max Planck Society, 14195 Berlin, Germany

<sup>c</sup>Laboratory of Industrial Chemistry, Åbo Akademi University, 20540 Turku, Finland

Alkane isomerization catalysts such as chlorided alumina, H-mordenite and anion-modified zirconia require platinum doping and addition of H<sub>2</sub> to the feed to stabilize performance<sup>1,2</sup>. The role of the H<sub>2</sub>/Pt combination is discussed controversially, proposed are (i) coke prevention by hydrogenation of unsaturated species<sup>1</sup>, (ii) facilitation of dehydrogenation, isomerization via alkenes and re-hydrogenation<sup>2</sup>, and (iii) formation of additional acid sites<sup>3</sup>. We have investigated the formation of surface deposits on sulfated zirconia and H-mordenite catalysts during n-butane isomerization using in situ ultraviolet-visible and infrared spectroscopy.

On sulfated zirconia in the absence of platinum and H<sub>2</sub>, water is initially formed and retained (at 373 K), while unsaturated species of allylic type slowly accumulate with time. These unsaturated species may contribute to the deactivation, but are not the sole cause because they are not always found, for example not on manganese-promoted sulfated zirconia. On H-mordenite in the absence of H<sub>2</sub>, allylic species similar to those on sulfated zirconia are formed, although the reaction temperature is much higher (573–673 K vs. 373 K). One of the species can be partially removed by hydrogenation if the catalyst contains platinum; however, the catalytic activity is not recovered, suggesting that the remaining surface deposits poison the catalyst. Detailed investigations into the stability of Pt/H-mordenite catalysts as a function of H<sub>2</sub> partial pressure show that the desired reaction, the isomerization to butane, and undesired side reactions that yield propane, are both suppressed by H<sub>2</sub>. Catalyst deactivation and formation of surface deposits start concomitantly when the H<sub>2</sub> level becomes too low; the exact level depends on the reaction conditions.

In conclusion, well-defined surface species, which can be detected with high sensitivity by UV-vis spectroscopy, are characteristic of the reaction pathways during alkane conversion. The same species seem to lead to catalyst deactivation on sulfated zirconia and on H-mordenite although the reaction temperatures differ significantly. Some of these species are spectators, whereas others poison the active sites. This knowledge can be used to direct future catalyst or process improvements.

1. R.A. Asuquo, G. Eder-Mirth, K. Seshan, J.A.Z. Pieterse, J.A. Lercher, *J. Catal.* 168, 292 (1997).
2. H. Liu, G.D. Lei, V. Adeeva, W.M.H. Sachtler, *J. Molec. Catal.* 100, 35 (1995).
3. H. Hattori, T. Shishido, *Catal. Surv. Japan* 1, 2005 (1997).

*Friederike C. Jentoft (née Lange) is Associate Professor of Chemical Engineering at the University of Oklahoma in Norman. She received her doctoral degree in 1994 at the University of Munich and then became a postdoctoral researcher at UC Davis. In 1996, she was appointed as a research group leader at the Fritz Haber Institute of the Max Planck Society in Berlin. Since October 2008, she conducts her research in the areas of petro- and biofuels at OU, with focus on the preparation of new acid and base catalysts and the investigation of catalyst-reactant interactions by spectroscopy and calorimetry. Jentoft is a member of the editorial board of Applied Catalysis A: General and serves as an associate editor of Advances in Catalysis.*





## **Beyond ULSD: Technology Enhancements to Improve Distillate Product Quality**

David J. DiCamillo, Lawrence Kraus, Criterion Catalysts and Technologies, Houston, TX  
(Dave.DiCamillo@CRI-Criterion.com)

With the initial wave of ULSD production well established in many areas of the world, attention has turned toward maximizing the use of these new assets as well as looking forward to anticipate future requirements. ULSD is an ideal platform for providing opportunities to further upgrade diesel quality, since the chemistry/catalysis for cetane improvement, aromatics reduction, cold flow improvement, density reduction, biodiesel processing, and conversion can be achieved by applying the right catalyst and process system. This paper discusses a range of commercially proven options for achieving one or more of these additional diesel-upgrading objectives. These solutions can significantly improve overall refinery economics by leveraging this critical ULSD asset, providing flexibility to upgrade heavier feeds to make more diesel, maximize LCO into the on-road diesel pool, and provide capability to process more difficult crudes.

*David J. (Dave) DiCamillo is Team Lead - Americas Hydroprocessing Technical Support at Criterion Catalysts and Technologies L.P. with 36 years experience in catalyst R&D and refinery catalyst applications including 16 years with the former American Cyanamid Company Catalyst Research Department and 20 years with Criterion. Dave's major area of expertise is distillate processing. He has a B.S. in Chemical Engineering from the University of Connecticut and a B.A. in Engineering from Fairfield University. He was an NPRA Q&A panelist in 1996.*



## **“Templated” Nanocatalysts for Electrochemical Energy Conversion: The Challenges for Synthesis and Characterization**

Keith J. Stevenson, Cori Atkinson, Anthony Dylla, Sankaran Murugesan  
*Department of Chemistry and Biochemistry*  
The University of Texas at Austin (stevenson@cm.utexas.edu)

This presentation will introduce strategies for synthesizing and characterizing the performance of nano-catalysts for electrochemical energy conversion; and will also highlight the development of new analytical tools for studying catalytic activity. Correlating the structure and reaction kinetic properties of catalysts as functions of size, shape, morphology and composition is a major challenge in homogeneous and heterogeneous catalysis. Yet obtaining information of this kind would facilitate the discovery and mechanistic understanding of new catalysts. Template-based syntheses using structure-directing agents such as dendrimers and polyol surfactants have facilitated our ability to more precisely control structural and compositional characteristics. In particular, we will highlight polyol-mediated approaches for preparing monometallic catalysts, multimetallic alloys and core@shell morphologies. Unfortunately, when evaluated in energy conversion processes, these new catalyst architectures are difficult to characterize by ensemble-averaging, bulk experimental methods. In this regard, we will describe the development of a new electroanalytical method for assessing the catalytic activity of water-soluble, colloidal catalysts of different size and shape.

*Stevenson is a well-established electrochemist with over 85 refereed publications, three patents, and two book chapters in this field. He is a recipient of a NSF CAREER award (2002), the Conference of Southern Graduate Schools New Scholar Award (2004), Jack S. Josey Fellowship in Energy Studies (2004-2006), and the Society of Electroanalytical Chemistry (SEAC) Young Investigator Award (2006). He is also a member of the Center for Nano- and Molecular Science and Technology (CNM), Texas Materials Institute (TMI), and an executive member of the Center for Electrochemistry (CEC). His research interests are aimed at elucidating and controlling chemistry at solid/liquid interfaces vital to many emerging technologies. To this end, his group is pursuing a multi-tiered approach of developing new materials synthesis methods for creation of advanced functional electrode materials, as well as, new high-resolution surface analytical tools for their characterization. A fundamental understanding of the intricate relationships between interfacial structure, surface reactivity, and mass transport is critical to advancing an array of important electrochemical materials applications including chemical sensing, energy conversion and storage, electrochromics, and electrocatalysis.*



## POSTER ABSTRACTS

### 1. Oxygen Exchange in the Selective Oxidation of 2-butanol on Oxygen Pre-covered Au(111).

Authors: **Ting Yan, Jinlong Gong, and C. Buddie Mullins**

Departments of Chemical Engineering and Chemistry, University of Texas at Austin, University Station C0400, Austin, Texas, 78712-0231, U.S.A.

Direct evidence for C-O bond cleavage in the partial oxidation of 2-butanol on oxygen pre-covered Au(111) is provided using temperature programmed desorption (TPD) and molecular beam reactive scattering (MBRS) under ultra-high vacuum (UHV) conditions. Oxygen pre-covered Au(111) surface can promote the partial oxidation of 2-butanol into 2-butanone with near 100% selectivity at low oxygen coverages, while 2-butanol adsorbs and desorbs molecularly on the clean Au(111) surface. Both  $C_2H_5C^{16}OCH_3$  and  $C_2H_5C^{18}OCH_3$  are observed in TPD after 2-butanol ( $C_2H_5C^{16}OHCH_3$ ) was dosed onto Au(111) pre-covered with  $^{18}O_a$ . This oxygen exchange phenomenon serves as a strong evidence for the C-O bond cleavage in 2-butanol partial oxidation to 2-butanone. Two surface intermediates are proposed for the selective oxidation of 2-butanol: 2-butoxide and  $\eta^2$ -aldehyde. As oxygen coverage increases, full oxidation is activated in addition to selective partial oxidation.

### 2. Methanol Steam Reforming in Pd-Ag Membrane Reactor: Experiments and Modeling.

Authors: **Sameer H. Israni and Michael P. Harold**

Department of Chemical Engineering, University of Houston, 4800 Calhoun Road, Houston, TX 77204.

Pd membrane based reactors have the potential to generate high purity H<sub>2</sub> in a single unit for stationary and mobile applications spanning power stations, soldier-power, and vehicles. Previous studies [1,2] from our group have analyzed in some detail the use of methanol reforming in membrane reactors as a way of intensifying the reaction and separation/purification into a single unit. In the current study methanol steam reforming was carried out in both a regular packed bed reactor (PBR) and a number of packed



bed membrane reactor (PBMR). Pd-Ag membranes (3.1 micron thickness nanopore membrane) were used in the PBMR to separate the hydrogen from the reaction mixture. The catalyst used in this study was Cu/ZnO/Al<sub>2</sub>O<sub>3</sub>. Since our previous studies [3,4] have highlighted that slow radial diffusion of hydrogen is one of the major factors limiting productivity & utilization in the membrane reactor, the reactor diameters of the PBMRs were varied to further study this effect. The methanol conversion, hydrogen productivity, hydrogen utilization and outlet CO/CO<sub>2</sub> ratio for the PBR and the PBMRs were compared at different pressures and temperatures. Separate studies were carried out to investigate the effect of the reactants and products (methanol, water, CO, CO<sub>2</sub>) on the H<sub>2</sub> flux through the Pd-Ag membrane. A 2-dimensional model was also developed to simulate the results and to elucidate the rate limiting processes. The results of these experiments and simulations were then used to develop a 3-dimensional model for multi-fiber PBMR in which various aspects of the design were explored, including spacing between the membranes.

#### References

1. Harold, M.P., B. Nair, and G. Kolios, "Hydrogen Generation in a Pd Membrane Fuel Processor: Assessment of Methanol-Based Reaction Systems," *Chemical Engineering Science*, 58, 2551-2571 (2003).
2. Lattner, J.R., and M.P. Harold, "Comparison of Methanol Based Fuel Processors for PEM Fuel Cell Systems," *Appl. Catalysis B. Environmental*, 56, 149-169 (2005).
3. Nair, B., and M.P. Harold, "Experiments and Modeling of Transport in Composite Pd and Pd/Ag Coated Alumina Hollow Fibers," *J. Membrane Sci.*, 311, 53-67 (2008).
4. Israni, S.H., B. Nair and M. P. Harold, "Hydrogen Generation and Purification in a Composite Pd Hollow Fiber Membrane Reactor: Experiments and Modeling," *Catalysis Today*, 139, 299-311 (2008).

### 3. Mixed Rare-Earth Oxides for Hot Gas Desulfurization and Tar Cracking.

Authors: **Rui Li, Sumana Adusumilli and Kerry Dooley\***

Dept. of Chemical Engineering, Louisiana State University, Baton Rouge, LA.

Gasification of biomass or coal/biomass at >900 K reduces formation of tars and leads to higher conversions to desired CO and H<sub>2</sub>. Economically, it is desirable to remove residual H<sub>2</sub>S and tars at conditions near those of the gasifier. To this end, we are studying sorbents/catalysts for simultaneous removal, based on the rare-earth oxides (REOs), in some cases with added transition metals. For example, CeO<sub>2</sub> shows good capacity for H<sub>2</sub>S, but its capacity and stability (retention of surface area, multiple adsorption/regeneration cycles) can be improved greatly by adding La<sub>2</sub>O<sub>3</sub>, Tb<sub>2</sub>O<sub>3</sub>, Gd<sub>2</sub>O<sub>3</sub>, MnO, FeO, or combinations of these, and by supporting these oxides on Al<sub>2</sub>O<sub>3</sub> or ZrO<sub>2</sub>. We have determined that mixed Ce/La/Mn oxides show improved capacity at 903 K, compared to mixed Ce/La oxides. Such oxides also simultaneously adsorb and



reform tar compounds such as naphthalene, although the naphthalene capacities roughly double if H<sub>2</sub>S is not present. Adsorption, TPD, and reaction studies will be presented, along with some materials characterizations of surface area, DSC, and XRD. Current work includes using other group VII-VIII metals with REOs, alternative preparation methods to increase mesoporosity, better characterization of superior materials by XAS and XPS, and tests of regeneration using CO and CO<sub>2</sub> instead of air.

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#### 4. Catalytic Oxidative Desulfurization of Model Diesel

Authors: **Dongxing Liu, Janetta Yakshimuradova and Kerry Dooley\***

Dept. of Chemical Engineering, Louisiana State University, Baton Rouge, LA.

An analysis of heterogeneous oxidation catalysts was performed to determine the activities and optimal operating conditions for the multiphase oxidative desulfurization (ODS) reactions, using a model diesel. Catalysts studied included well-characterized Pd on Al<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub> and activated carbon supports, and carbon-supported Mo<sub>2</sub>C and W<sub>2</sub>C, which were prepared by temperature programmed reaction. Several other typical oxidation catalysts were also examined.

The model diesel consisted of ~1 wt% sulfur compounds (thiophene and dibenzothiophene) with appropriate amounts of aliphatic, alkylaromatic and N-heterocyclic compounds to simulate a raw number 2 diesel. With oxygen as the oxidant in ODS reactions (70-90°C, 0.8-1.8 MPa, feed vol/wt cat. =100 mL/g) of this model diesel, Pd/C and Mo<sub>2</sub>C/C showed the best selectivity for oxidizing the N- and S-heterocycles vs. the alkylaromatics. Increasing the pressure increased the reaction rates of the N- and S-heterocycles. Except for thiophene, there was only a small dependence of observed rates on temperature, which suggests the reactions were partially diffusion (of O<sub>2</sub>) controlled.

Current work includes further investigations of the better catalysts, full characterization of the products by GC-MS, and kinetics measurements using catalyst monoliths in a piston-oscillating reactor, which can eliminate the diffusion limitations and provide a uniform hydrodynamic environment.

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## 5. Selective Catalytic Reduction of NO on Fe based Zeolite Monolith Catalysts.

Authors: **Pranit S. Metkar, Nelson Salazar, Michael P. Harold and Rachel Muncrief**  
Department of Chemical & Biomolecular Engineering, University of Houston, Houston, TX, United States.

$\text{NO}_x$ , emitted from diesel vehicles is a major cause of ground-level ozone and hence its emission needs to be controlled. Thus selective catalytic reduction (SCR) of  $\text{NO}_x$  in presence of ammonia is gaining a lot of attention. In this study we carried out SCR of NO with  $\text{NH}_3$  as a reductant over iron based zeolite catalyst. Fe-ZSM-5 catalyst was prepared for this study and was deposited on a monolith support. SCR studies were performed on this catalyst and compared with a commercial sample. The kinetics of standard SCR reaction was studied in the temperature range of  $200^\circ\text{C}$  -  $325^\circ\text{C}$ . We found that the reaction is first order in NO, half order in  $\text{O}_2$  and -0.3 order w.r.t.  $\text{NH}_3$ . Apparent activation energy of this reaction is found to be 41kJ/mol. Kinetics of NO oxidation and  $\text{NH}_3$  oxidation were also studied in this temperature range from which we conclude that NO oxidation, which forms  $\text{NO}_2$  as an intermediate product, is a likely rate determining step in this standard SCR chemistry. Mechanisms and rate expressions will be presented that are consistent with the experimental data.

## 6. Selective Decomposition of Formic Acid on Molybdenum Carbide: A New Reaction Pathway.

Authors: **David W. Flaherty, Sean P. Berglund, C. Buddie Mullins\***  
Department of Chemical Engineering, Center for Nano- and Molecular Science and Technology, The University of Texas at Austin, 1 University Station, CO400 University of Texas at Austin, Austin, Texas, 78712. [\\*mullins@che.utexas.edu](mailto:mullins@che.utexas.edu)

Selective decomposition of formic acid is important as a prototype to study selective bond cleavage of oxygenates. We demonstrate that carbon-modified Mo(110), C-Mo(110), is up to 15 times more selective for the dehydrogenation of formic acid than Mo(110). Reflection absorption infrared spectroscopy (RAIRS) indicates that carbidic carbon blocks active sites for C-O bond cleavage, decreasing the rate of dehydration. Steady-state reactive molecular beam scattering (RMBS) shows that dehydration is the dominant reaction pathway on clean Mo(110), while C-Mo(110) selectively promotes





dehydrogenation. Kinetic analysis of RMBS data reveals that formic acid dehydrogenation on Mo(110) has an activation energy of  $34.4 \pm 3.3 \text{ kJ}\cdot\text{mol}^{-1}$  while the C-Mo(110) surface promotes distinct pathways for dehydrogenation with an activation energy of only  $12.8 \pm 1.0 \text{ kJ}\cdot\text{mol}^{-1}$ . RAIRS spectra suggest the new pathways include the formation of monodentate formate and at temperatures of 500 K and greater direct activation of the C-H bond to form carboxyl, both of which decompose *via* a  $\text{CO}_2^{\delta-}$  intermediate to evolve  $\text{CO}_2$  and  $\text{H}_2$ .

## 7. Estimation of Effective Diffusivity of Stored NOX in the Barium Phase of Pt/BaO/Al<sub>2</sub>O<sub>3</sub> Catalysts using TAP.

Authors: **Ashok Kumar, Michael P. Harold, and Vemuri Balakotaiah**

Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX 77204 – 4404, United States.

A systematic study over Pt/BaO/Al<sub>2</sub>O<sub>3</sub> powder catalyst is carried out using Temporal Analysis of Products (TAP) to estimate the effective diffusivity of stored NOX in the barium phase. The prenitration of Pt/BaO/Al<sub>2</sub>O<sub>3</sub> using sequential pulses of NO followed by reduction with H<sub>2</sub> results in the evolution of N<sub>2</sub> and NH<sub>3</sub>. The reduction is carried out in the NOX transport limited regime in which diffusion of the stored NOX from BaO storage phase to Pt/BaO interface was determined to be the rate controlling process. The effluent profiles of N containing species (2N<sub>2</sub>+NH<sub>3</sub>) were used to estimate stored NOX diffusivity in barium phase and the apparent activation energy. The activation energy (76 kJ/mol) is in good agreement with the estimated value of 75 kJ/mol from a recent NOX trap modeling study.



## 8. Interaction of Water with oxygen and CO dissociation enhanced by water and oxygen on Ir(111).

Authors: **Ming Pan, Son Hoang, Jinlong Gong, C. Buddie Mullins**

Departments of Chemical Engineering and Chemistry, Center for Nano and Molecular Science and Technology, Texas Materials Institute, and Center for Electrochemistry, University of Texas at Austin, Austin, TX 78712-0231, USA.

Adsorption and reaction of water on the clean and oxygen-modified Ir(111) surface is studied using temperature programmed desorption (TPD) and molecular beam reactive scattering (MBRS) techniques under ultra high vacuum (UHV) conditions. We found water dissociate on clean Ir(111) with a small dissociation probability ( $< \sim 0.016 \pm 0.0015$ ) at various water coverages (0.34-2.59 monolayer). To scatter water molecular beam on Ir(111) resulted in water probabilities ranging from  $\sim 0.0005$  to 0.012 with increasing surface temperatures from 300 to 900K, indicative of a thermally activated process. The apparent activation energy of water dissociation has been estimated to be  $170 \pm 5$  kJ/mol. However, we speculated that water dissociation on clean (111) occurs on defective sites. Employing isotopically labeled reactants, a strong interaction of H<sub>2</sub>O and oxygen has been observed on Ir(111) and hydroxyl group (OH) is formed as intermediates, suggested by scrambling water and oxygen as well as a new water desorption feature at a high temperature (235K). CO dissociation is also investigated on Ir(111) under UHV conditions. Although CO does not dissociate on the clean Ir(111) surface, atomic oxygen induces CO dissociation at low temperatures ( $< 400$  K). The similar phenomenon has been observed on Ir(111) modified by water and oxygen.

## 9. Overall mass transfer coefficients and controlling regimes in catalytic monoliths.

Authors: **Saurabh Y. Joshi, Michael P. Harold, Vemuri Balakotaiah**

Department of Chemical and Biomolecular Engineering, University of Houston, 4800 Calhoun Road, Houston TX, 77204.

It is well known that the performance of a catalytic monolith is bounded by two limits: the kinetic regime at low temperatures (or before ignition for the case of exothermic reactions) and the external mass transfer controlled regime at sufficiently high temperatures (or after the ignition). The washcoat diffusional resistance can also be



significant over an intermediate range of temperatures. The transition temperatures at which the controlling regime changes from kinetic to washcoat diffusion to external mass transfer depend on the various geometric properties of the monolith, flow properties, the catalyst loading and washcoat properties. We present analytical criteria for determining these transition temperatures. These are derived using the recently developed low-dimensional model and the concepts of internal and external mass transfer coefficients. The criteria are more general than those in the literature and are useful in analyzing the experimental data. Further, we present an explicit expression for the experimentally measurable dimensionless apparent mass transfer coefficient ( $Sh_{app}$ ) in terms of individual transfer coefficients in each phase. It is shown that  $Sh_{app}$  can be lowered by orders of magnitude compared to the theoretical upper bound obtained in the limit of external mass transfer control. Low values of  $Sh_{app}$  are obtained due to a small value of effective diffusivity in the washcoat, low catalyst loading or a reaction with low activation energy. The analytical criteria may be used for the design of monolith properties and experimental conditions so that the performance of the monolith approaches the upper limit defined by the external mass transfer controlled limit.

Keywords: Catalytic converter, light-off, kinetic regime, washcoat diffusion, LNT, SCR, effectiveness factor .

## 10. Preparation and Characterization of Co-Rh Bimetallic Model catalysts: from Thin Films to Dispersed Clusters.

Authors: **Zhoujun Wang, Fan Yang, Stephanus Axnanda, D. Wayne Goodman**  
Department of Chemistry, Texas A&M University, College Station, TX 77843.

Co-Rh bimetallic model catalysts were prepared as thin films on a Mo(100) substrate and as dispersed clusters on a SiO<sub>2</sub> support under ultrahigh vacuum conditions. The surface composition and electronic structure of the Co-Rh thin films on Mo(100) substrate were characterized with low energy ion scattering spectroscopy (LEIS) and X-ray photoelectron spectroscopy (XPS). Co-Rh thin films formed a stable alloy between 700 and 1000 K with substantial enrichment in Co compared to the bulk composition. Annealing a 1:1 Co-Rh thin film at 700 K for 30 min synthesized an alloy with 78% (atomic concentration) of Co at the outmost surface layer. The surface composition and morphology of the Co-Rh dispersive clusters on SiO<sub>2</sub> support were determined by LEIS, XPS and transmission electron microscopy (TEM) with energy dispersive X-ray spectroscopy (EDX). The Co and Rh atoms were mixed and the bimetallic clusters



formed between 700 and 800 K with Co segregated to the cluster surface. Annealing a 1:1 Co-Rh mixture on  $\text{SiO}_2$  at 700 K for 10 mins yielded bimetallic clusters with a Co surface composition of 78%. TEM images showed the bimetallic Co-Rh clusters were well dispersed and the average particle size of the bimetallic clusters increased monotonically with the Co bulk composition. Further studies of the structure-reactivity correlation over the Co-Rh/ $\text{SiO}_2$  model catalyst are currently in progress.

## 11. Deposition of metal clusters on single-layer graphene/Ru(0001): factors that govern cluster growth.

Authors: **Zihao Zhou, Feng Gao, and D. Wayne Goodman\***

Department of Chemistry, Texas A&M University, P.O. Box 30012, College Station, TX 77842-3012.

Fabrication of nanoclusters on a substrate is of great interest in studies of model catalysts. The key factors that govern the growth and distribution of metal on graphene have been studied by scanning tunneling microscopy (STM) based on different behaviors of five transition metals, namely Pt, Rh, Pd, Co, and Au supported on the template of a graphene moiré pattern formed on Ru(0001). Our experimental findings show that Pt and Rh form finely dispersed small clusters located at fcc sites on graphene while Pd and Co form large clusters at similar coverages. These results, coupled with previous findings that Ir forms the best finely dispersed clusters, suggest that both metal-carbon (M-C) bond strength and metal cohesive energies play significant roles in the cluster formation process and that the M-C bond strength is the most important factor that affects the morphology of clusters at the initial stages of growth. Furthermore, experimental results show Au behaves differently and forms a single-layer film on graphene, indicating other factors such as the effect of substrate metals and lattice match should also be considered. In addition, the effect of annealing Rh on graphene has been studied and its high thermal stability is rationalized in terms of a strong interaction between Rh and graphene as well as sintering via Ostwald ripening.



## 12. Pulsed-Field Gradient NMR Investigations of the Organocation Role in the First Stages of Silicalite-1 Synthesis.

Authors: **Alejandra Rivas-Cardona and Daniel F. Shantz\***

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, Texas 77843-3122.

Pulsed-field gradient nuclear magnetic resonance (PFG-NMR) spectroscopy has been used to study the first stages of the silicalite-1 synthesis in optically transparent mixtures of organocation, tetraethyl orthosilicate (TEOS) and water. Two organocations, methyltripropylammonium (MTPA) and ethyltripropylammonium (ETPA), have been used as structure directing agents (SDAs) to study the influence of the cation identity in the nucleation and growth of silicalite-1. The PFG-NMR experiments show the selfdiffusion coefficient of MTPA is larger than that of ETPA cation in aqueous solutions. Moreover, the decrease of the diffusion coefficients of both cations with the addition of silica (TEOS) is observed due to a reduction in cation mobility while interacting with the silica nanoparticles. The diffusion data is analyzed with a two-site model in order to calculate the fractions of free and silica-bound cations. The bound fractions are fitted to a Lineweaver-Burk model from which the energetic of the system is obtained. In addition, pH and conductivity measurements show the presence of a critical aggregation concentration (CAC), which has been previously reported. The results of our investigations suggest that the organocation-silica interactions play an important role in zeolite formation and depend on the solution conditions such as the concentration of the species as well as on the organocation identity.

## 13. Kinetic and Spectroscopic Investigations of C<sub>2</sub>H<sub>4</sub> Hydroformylation on Planar Oxide Supported Rh Nanoparticles at Near Atmospheric Pressures.

Authors: **Sean M. McClure, M. Lundwall, Z. Zhou, D. W. Goodman**

Goodman Research Group, Department of Chemistry, Texas A&M University  
P.O. Box 30012, College Station, TX 77842-3012.

Model catalyst surfaces, consisting of metal nanoparticles supported on a planar oxide support, hold the potential to bridge the material gap between single crystal and technical catalyst studies. When coupled with near atmospheric pressure kinetic and spectroscopic techniques, these well-defined model catalyst surfaces represent a useful



approach to provide insights into the structure-activity relationships of industrially relevant reactions. Here, we present recent results of our investigations into the structure sensitivity of the  $C_2H_4$  hydroformylation reaction ( $C_2H_4+CO+H_2$ ) at near atmospheric pressures on Rh/SiO<sub>2</sub> model catalyst surfaces. Experiments are conducted in a contiguous UHV/high pressure reactor cell system, enabling elevated pressure kinetic and PM-IRAS measurements on Rh/SiO<sub>2</sub> surfaces which have been characterized by a variety of surface analytical techniques (e.g. STM, TPD, etc) and probe reactions. As will be presented in detail, kinetic and spectroscopic measurements (PM-IRAS) can provide insights into particle morphology, surface adsorbates and the observed structure-sensitivity (activity and selectivity) during  $C_2H_4$  hydroformylation at near atmospheric pressures.

#### 14. Li Promotion of CuCo/SiO<sub>2</sub> Catalysts for Ethanol Production from Syngas.

Authors: **Miranda Smith and James Spivey**

Cain Department of Chemical Engineering, Louisiana State University,  
Baton Rouge, LA.

CuCo/SiO<sub>2</sub> catalysts, one unpromoted and one promoted by lithium, were synthesized by incipient wetness impregnation and calcined. These catalysts are candidates for CO hydrogenation to ethanol and other C<sub>2+</sub> oxygenates. Tests performed on each catalyst included temperature programmed reduction (TPR), temperature programmed desorption of CO (CO-TPD), and temperature programmed surface reaction (TPSR). TPR results indicated that Li increased the reduction temperature of the active metals. CO-TPD suggested that Li promotion enabled CO dissociation at slightly lower temperature than did the unpromoted catalyst. Mass spectrometry data (m/z = 31 and m/z = 16) from TPSR showed that Li was able to suppress methane formation at high temperatures (above 375°C) but had no obvious effect on the temperature at which alcohols were formed.





## 15. Bromide Poisoning Study for CO Oxidation over Titania Supported Gold Nanoparticles.

Authors: **Shane M. Kendell, Christopher J. Pursell, Bert D. Chandler**  
Chemistry Department, Trinity University, San Antonio

The effects of Br<sup>-</sup> poisoning on Au/TiO<sub>2</sub> catalysts were investigated. A commercial 1%Au/TiO<sub>2</sub> catalyst was obtained from the World Gold Council (WGC). A total of eight different bromide poisoned WGC catalysts were prepared, with Br<sup>-</sup> to Au molar ratios ranging from 1% to 12%. The bromide was added by incipient wetness impregnation using solutions of NaBr in methanol. A linear relationship between catalyst activity and bromide content was found. This plot indicates that there is a fixed number of equivalent active sites on the WGC catalyst, rather than a distribution of sites with differing activities. The O<sub>2</sub> reaction order ( $0.25 \pm 0.03$ ), CO reaction order ( $\sim 0$ ) and apparent activation energy ( $29 \pm 3 \text{ kJ mol}^{-1}$ ) are not significantly affected by bromide poisoning. This indicates that bromide functions primarily as a site-blocking agent, preventing access of oxygen to the active sites, but does not substantially impact the reaction mechanism. Applying some reasonable assumptions regarding the distribution of Br<sup>-</sup> across the catalyst allows for an estimation of the number of active sites on the Au/TiO<sub>2</sub> catalyst.

## 16. Bimetallic Palladium-on-Gold Nanoparticle Catalysts for Groundwater Remediation

Authors:

**Yu-Lun Fang<sup>1</sup>, Pedro J. J. Alvarez<sup>2, 4</sup>, Jeffery T. Miller<sup>5</sup>, and Michael S. Wong<sup>1, 3, 4</sup>**

<sup>1</sup> Department of Chemical and Biomolecular Engineering, Rice University

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<sup>3</sup> Department of Chemistry, Rice University

<sup>4</sup> Center of Biological and Environmental Nanotechnology, Rice University

<sup>5</sup> Argonne National Laboratory

Palladium-on-Gold nanoparticles (Pd/Au NPs) were investigated as a catalyst for hydrodechlorination (HDC) reaction of trichloroethene (TCE). TCE is one of the most common hazardous organic contaminants found in groundwater. This chlorinated solvent has been widely used in various fields; thus, lots of TCE has entered the environment through leakage, disposal and other pathways. Compared to conventional physical displacement methods such as air-stripping and carbon adsorption,



remediation through the catalytic reductive dechlorination of TCE molecules is a more effective and desirable approach. Colloidal Pd/Au NPs have been shown to catalyze TCE HDC reaction in water, at room temperature, and in the presence of hydrogen, with the most active Pd/Au NPs (rate constant  $k = 1900 \text{ L/g}_{\text{Pd}}/\text{min}$ ) found to be >70 times more active than conventional mono-metallic Pd supported on alumina ( $k = 26 \text{ L/g}_{\text{Pd}}/\text{min}$ ) on a per-Pd atom basis. Of note, Pd/Au NPs exhibited a volcano-like catalytic activity profile with different Pd surface coverage.

In the poster presentation, recent progress of Pd/Au NP catalysts for TCE HDC reaction in different aspects will be addressed. A kinetic analysis of Pd-based catalysts for TCE HDC was established and a reaction mechanism was proposed. Nanostructures of Pd/Au NPs were characterized by X-ray absorption fine structure (XAFS) spectroscopy. Reaction activity profile was correlated with nanostructures for understanding of Au promotion effect. Immobilized and supported NP catalysts were developed for long-term application. Lab-scale flow reactor was tested to show stability; pilot-scale flow reactor is in development.



## A Brief History of the Southwest Catalysis Society

As recounted by Joe W. Hightower, Professor Emeritus, Rice University (April 2009)  
B.S. '59 - Harding University; M.S. '61 and Ph.D. '63 - The Johns Hopkins University

I came to Rice University from the Mellon Institute in Pittsburgh during the summer of 1967 and immediately set out to meet catalyst people in the area. We announced an organizational meeting to be held at Rice, **Fall 1967**. There were 63 people as charter members of what was to become the Southwest Catalysis Club. Jim Richardson (Esso Research and Engineering, now University of Houston) drafted the Bylaws and was elected Vice President, Jack Lunsford (Texas A&M University) was Secretary, Paul Conn (Shell Oil) was the Treasurer, and I served as the first elected President. The officers held the first all-day Spring Symposium in May 1968 in the Grand Hall at Rice, and the SWCS was off and running (42 years and counting!). [As a note, I did my PhD thesis research with **Professor Paul Emmett** at Johns Hopkins, which involved isotopic tracer studies of secondary reactions that occur during catalytic cracking of petroleum products.]

At the time we started, there were about half a dozen "Catalysis Clubs" scattered around the country: Chicago, Pittsburgh, New York, Philadelphia, California, and perhaps one more. I knew people in all these "Clubs" though groups like the Gordon Research Conferences on Catalysis, and they all encouraged us to start a club in the SW. **Why 5 states?** Texas was obvious. Arkansas was included because of Sam Siegel (Chemist at UArk); Louisiana, because of several researchers at Esso in Baton Rouge; Oklahoma, because of several Phillips researchers in Bartlesville; and New Mexico, because of people at University of New Mexico and at Sandia National Labs in Albuquerque. In spite of the long distances, people from all these places attended some of the early meetings held twice a year, which sometimes had attendance near 200. Most of the early meetings were held at Rice or in the Auditorium at the Shell-Westhollow labs. In later years, the meeting was held in nearby places like Austin, College Station, and New Orleans.

What was going on that made the late 60s an optimal time to establish the SWCS? I think the biggest factor was Shell downsizing its labs in Emeryville, CA and moving most its catalysis people to a new research facility at Westhollow. At the same time, Esso was increasing its applied catalysis work both in Baytown 30 miles east of the city and in Baton Rouge. For several years, Phillips Petroleum had been accumulating an amazing number of patents in catalysis at their laboratories in Bartlesville. Bob Eischens came from New York and was applying his pioneering infrared studies at Texaco in Port Arthur. Celanese had several catalysis people doing research near Corpus Christi. Many of you may recall that Texas City was devastated by the largest US chemical plant explosion of an ammonium nitrate ship in the mid-40s. After the explosion, Monsanto rebuilt its facilities there, where workers were doing research on improving catalytic processes for styrene and acrylonitrile manufacture. Petrotex Chemical in



Pasadena, another suburb on Houston's ship channel, was optimizing its butadiene and C<sub>4</sub> olefins production through catalytic processes.

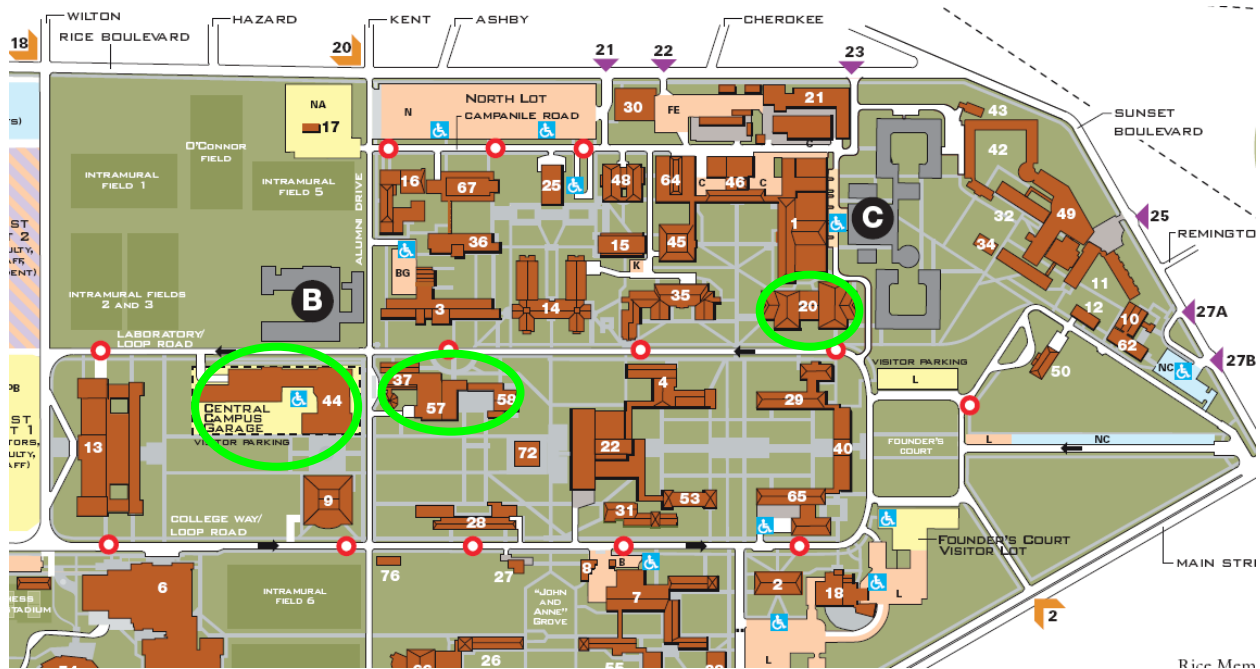
In addition, catalysis groups were springing up at several universities, including surface science by the late John Mike White at the University of Texas, Jack Lunsford's and Wayne Goodman's highly productive groups at Texas A&M, Richard Gonzales at Tulane, Jim Richardson at U of H, Kerry Dooley at LSU, Tom Leland and me at Rice, and groups at other universities in the 5-state area. What was lacking? There was no formal mechanism for these diverse groups to exchange information or get advice in the southwest. The time was ripe for an organization where catalysis could be openly discussed. Although much catalysis research is proprietary, enough was sufficiently open to create a stimulating environment for sharing mutual interests, many focusing on new ultra-high vacuum analytical equipment that was being rapidly developed.

The first thing we did was to organize an NSF-supported workshop at Rice which (not surprisingly) concluded that more funding was needed for research on catalysts for fuels, environmental protection (cat converters), chemicals, etc. At that time, demand was also great for new employees with catalysis training, but the supply was quite limited. This provided an occasion for the development of short courses to train industrial employees in heterogeneous catalysis. Several courses were started around the country. One of the most successful was started at Rice and has continued for more than 30 years through the University of Houston. It can be said, then, that **SWCS was instrumental in starting these heterogeneous catalysis short courses.**

The "Club" was soon invited to join the other half dozen Clubs as a part of the growing North American Catalysis Society. Being the new kid on the block, our Club was asked to host its first biennial North American Meeting (NAM-2) in February 1971, which was held at the Astrodome Hotel in Houston. Jim Richardson and I were Associate and General Chair of the meeting, while Paul Venuto (Mobil Research/Development and a colleague of the late Heinz Heinemann) was in charge of the Program. At that meeting the late Dr. R. J. Kokes (one of my professors at Johns Hopkins) and Dr. H. S. Bloch (Universal Oil Products) were recipients, respectively, of the first Paul H. Emmett and Eugene J. Houdry Awards in fundamental and applied catalysis.

In 1985, the Southwest Catalysis Society was again called on to host a five-day 9th North American Meeting (NAM-9) at Houston's Adam's Mark Hotel. This time, Jack Lunsford and Lynn Slaugh were General and Vice Chair; I was Technical Program Chair. Most recently, the SWCS members organized the spectacular North American Meeting at Houston's downtown Hilton Americas Hotel in 2007, attended by over 1000 delegates from all over the world, "Celebrating Catalysis Texas Style." Kudos again to SWCS officers Kerry Dooley, Brendan Murray, Scott Mitchell, Michael Reynolds, Yun-Feng Chang, Michael Wong, and many, many others! **All told, the SWCS has hosted 3 national events now: 1971 (NAM-2), 1985 (NAM-9) and 2007 (NAM-20).**

## Rice University Campus Map



### Building numbers

**20: Duncan Hall (meeting site)**

**57: Rice Memorial Center (student center)**

**44: Central Campus Garage**



## UPCOMING CATALYSIS EVENTS

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### ACS Spring Meeting

March 21-25, 2010 San Francisco, CA

Several symposia organized by Catalysis Science and Technology Division (CATL)

<http://catl.sites.acs.org/>

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### Short Course on Applications of Heterogeneous Catalysis

May 10-14, 2010 University of Houston

Course directors: Profs. Jim Richardson ([jtr@uh.edu](mailto:jtr@uh.edu)) and Dan Luss ([dluss@uh.edu](mailto:dluss@uh.edu))

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### 2010 Gordon Research Conference on Catalysis

June 27 - July 2, 2010 Colby-Sawyer College, New London, NH

<http://www.grc.org/>

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### Celebration Symposium in Honor of Jack Lunsford

October 15, 2010 College Station, TX

**Sponsors: TAMU Department of Chemistry and Southwest Catalysis Society**

This one-day symposium will celebrate Dr. Lunsford's service to the Chemistry Department and his achievements in catalysis.

Meeting organizer: Prof. D. Wayne Goodman (TAMU)

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### Southwest Catalysis Society 2011 Spring Meeting

April 2011

For your planning purposes, the next meeting will likely be held in April next year.

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### 22<sup>nd</sup> North American Meeting – North American Catalysis Society

June 5-11, 2011 Detroit, MI

<http://www.22nam.org/>

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