

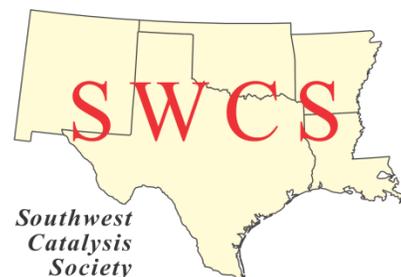
SOUTHWEST CATALYSIS SOCIETY

2012 SPRING SYMPOSIUM

April 20, 2012

Duncan Hall - McMurtry Auditorium

Rice University, Houston, TX



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The SWCS officers and I welcome you to the 2012 SWCS Spring Symposium, **Friday, April 20, 2012**, at Rice University in Duncan Hall (McMurtry Auditorium).

We are delighted to present 7 invited speakers and 26 poster presentations for this year's meeting. Meritorious posters presented by students and post-docs will be identified with **Best Poster Awards**, carrying cash prizes.

The 2012 Spring Symposium **registration fee is \$50**, which includes North American Catalysis Society and SWCS yearly membership dues, along with coffee/snack breaks. To speed registration, provide your business card along with your registration fee.

This year for the first time we will be able to accept credit cards (Visa, MasterCard, Discover, and American Express). Credit card receipts will be sent via e-mail, so please be prepared to input your e-mail address into our system when you pay. But note, that checks are faster (especially if you have them ready to go).

Do let those who cannot attend the Symposium know to mail in their membership due (\$40) to our Treasurer, John Novak (mailing address shown at left).

Checks should be made out to SWCS.

The student registration fee is \$10, which includes NACS and SWCS membership.

PARKING: The best place to park is in the central campus garage marked on the map (last page). You will need a credit card to enter. We will have parking coupons available for drivers of cars to exit the garage for free. You will input the coupon upon exiting, then run your credit card, which will not be charged.

Enjoy!

George G. Stanley
LSU Chemistry
Chair

2012 PROGRAM

- 7:30 AM Registration – John Novak, Treasurer** Duncan Hall
- All talks will be held in McMurtry Auditorium of Duncan Hall**
- 8:25 AM Welcoming Remarks – George Stanley, Chair**
Duncan Hall – McMurtry Auditorium
- 8:30 AM David Artrip (Catalytic Consultants)**
"A Conversation About Entrepreneurship in Catalysis"
- 9:00 AM C. Buddie Mullins (University of Texas – Austin, Chemistry & Chemical Engineering)**
"Surface Chemistry on H-Precovered Au(111)"
- 9:30 AM Coffee Break / Poster Setup** Duncan Hall
- 10:00 AM Mahdi Abu-Omar (Purdue University, Chemistry)**
"Kinetics of Olefin Polymerization Using Multi-Response Data
Which Includes Fitting of Molecular Weight Distributions (MWDs)"
- 10:30 AM Carl Mesters (Shell Chemical, Houston)**
"Catalysis to Meet the Energy Challenge"
- 11:00 AM Southwest Catalysis Society Excellence in Applied Catalysis Award**
**Lynn Slaugh & Richard Mullineaux (Shell Chemical, retired) for the Development of the
Shell Phosphine-Modified Cobalt Hydroformylation Process**
George Stanley & Michael Reynolds presenting
- 11:15 AM Lunch Break (on your own) / Poster Setup**
Rice Student Center
- 12:30 PM Jiming Bao (University of Houston, Electrical & Computer Engineering)**
"Nanocrystalline CoO as an Efficient Photocatalyst for Total Water Splitting Driven by
Visible Light"
- 1:00 PM Raghu Menon (Albemarle Corp., Houston, TX)**
"Oxychlorination – Investigation of a Mature Catalyst System"
- 1:30 PM Max Tirtowidjojo (Dow Chemical, Houston, TX)**
"Efficient Production of High Purity Phenolic Glycol Ethers"
- 2:00 PM Poster Session / Coffee Break**
Duncan Hall – Martel Hall
- 3:30 PM Poster Awards and SWCS Business Meeting**
Duncan Hall – McMurtry Auditorium
- 4:00 PM Adjourn**

A Conversation about Entrepreneurship in Catalysis

David J. Artrip

President, Research Catalysts, Inc.,
PO Box 8276, The Woodlands, TX 77387
E-mail: dave@catalyticconsultants.com



Following a career in the chemical industry - capped by 23 years with BASF Catalysts - Dave Artrip finally became the entrepreneur he always wanted to be, and is now in the business of supplying, testing and consulting on catalysts, for both industry and academia. In the SWCS meeting he will tell us a bit about his business and where he plans to go with it, and ask for our ideas to help him get there.

Surface Chemistry on H-Precovered Au(111)

C. Buddie Mullins

Departments of Chemical Engineering and Chemistry,
University of Texas at Austin
E-mail: mullins@che.utexas.edu



Gold-based high surface area catalysts have been investigated for hydrogenation reactions but fundamental studies on model catalysts are lacking. We present experimental measurements of the reaction of hydrogen adatoms and other adsorbed species on the Au(111) surface employing temperature programmed desorption. We show that chemisorbed hydrogen adatoms bind weakly with desorption peaks at ~110 K indicating an activation energy for recombinative desorption of ~28 kJ/mol. We further demonstrate that (i) acetaldehyde (CH_3CHO) can be hydrogenated to ethanol ($\text{CH}_3\text{CH}_2\text{OH}$) and that (ii) NO_2 can be reduced to NO on the H atom pre-covered Au(111) surface at cryogenic temperatures. Isotopic experiments employing D atoms indicate a lower reactivity.

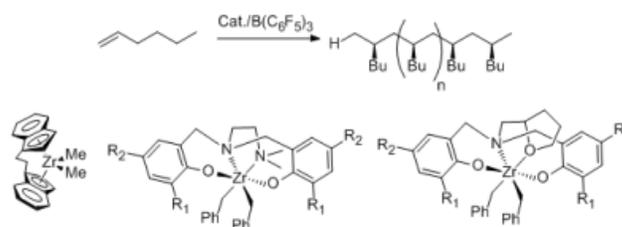
Kinetics of Olefin Polymerization Using Multi-Response Data which Includes Fitting of Molecular Weight Distributions (MWDs)

Mahdi Abu-Omar

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In order to develop a thorough understanding of single-site olefin polymerization catalysis, we have developed a quantitative kinetic modeling framework. This allows us to determine microkinetic mechanisms and associated rate constants from experimental data such as monomer consumption, molecular weight distributions (MWDs), polymer end group analyses, and active-site counting. This methodology was applied to the batch polymerization of 1-hexene by *rac*- $\text{C}_2\text{H}_4(1\text{-Ind})_2\text{ZrMe}_2$ activated with $\text{B}(\text{C}_6\text{F}_5)_3$, one of the most studied single-site systems to date, and led to the discovery that only ca. 60% of the catalyst is active. The methodology has now been applied to other single-site systems, particularly those non-Cp Zr catalysts with tetradentate salan-type ancillary ligands. These ligands provide a wide variation in chemical and structural diversity. Studies of 1-hexene polymerization revealed two key features: the presence of mis-inserted monomers, which render a significant portion of the



catalyst dormant; and how small perturbation in the ligand can impact the rate of chain transfer by orders of magnitude. It is noteworthy that these findings would not have been possible had it not been for a data set that included the MWDs at different percent monomer conversion.

Catalysis to Meet the Energy Challenge

Carl Mesters

Chief Scientist for Chemistry and Catalysis
Shell Chemical, Westhollow Technology Center, Houston, TX
E-mail: carl.mesters@shell.com



Most of the energy used today is stored in molecules as chemical energy, the vast majority is sunlight captured in the past that we use today in molecules known as fossil fuels; a small fraction has been recently harvested; i.e. biomass. Catalysis is a key enabler to enhance chemical transformation rates and, equally important, to steer chemical reactions in the desired direction, transforming these molecules to the desired products. Shell is heavily involved in this: oil is 'refined' to make transportation fuels and chemicals, which requires a lot of changing molecules. Similarly, the conversion of natural gas to liquids in GTL is also an example of catalysis steering chemical reaction in the right direction. The transformation of (solid) biomass to a liquid transportation fuel also involves a lot of chemistry and catalysis. In this seminar we'll discuss a few examples of what's been done in the past and highlight future challenges in the area of Catalysis

Southwest Catalysis Society Excellence in Applied Catalysis Award

Lynn Slaugh & Richard Mullineaux (Shell Chemical, retired) for the Development of the Shell Phosphine-Modified Cobalt Hydroformylation Process



Lynn Slaugh



Richard Mullineaux

Nanocrystalline CoO as an Efficient Photocatalyst for Total Water Splitting Driven by Visible Light

Jiming Bao

University of Houston, Electrical & Computer Engineering
E-mail: jbao@uh.edu

Current photocatalysts suffer from low efficiency in converting solar energy directly to chemical fuels. By breaking CoO micro-powders into nanoparticles using femtosecond laser pulses, we transformed non-reactive CoO into an efficient photocatalyst. Distinguished from previous catalysts, CoO nanocrystals decompose neutral water at a high rate under visible light without any co-catalysts or sacrificial reagents.

Stoichiometric splitting of water was quantified using mass spectrometry and gas chromatography. At an



irradiation wavelength of 532 nm, the nanocrystals demonstrated an energy conversion of 10% and a hydrogen production rate of $\sim 50 \text{ mmol g}^{-1}\text{-h}^{-1}$. Electrochemical impedance measurement reveals that a significant shift in the band-edge positions is responsible for the photocatalytic activity.

Oxychlorination – Investigation of a Mature Catalyst System

Raghu Menon

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Albemarle is an established global supplier of a variety of catalysts that are used in refining and petrochemical processes such as fluid catalytic cracking (FCC) and hydroprocessing (HPC). Albemarle also supplies catalysts and organometallic components used in polymerization of olefins, such as Ziegler-Natta and Single Site catalysts. Albemarle offers a series of chemical process catalysts for the production of basic chemicals such as hydrogen, ammonia and methylamines. This talk examines a few aspects of oxychlorination, a commercially mature catalytic process for the production of vinyl chloride monomer, and discusses how catalyst design might improve key performance criteria for the balanced process.

Efficient Production of High Purity Phenolic Glycol Ethers

Max Tirtowidjojo*

The Dow Chemical Company, Hydrocarbons, Chemicals, & Energy R&D
E-mail: MMTirtowidjojo@dow.com

Edward Daugs
The Dow Chemical Company, Glycol Ethers R&D



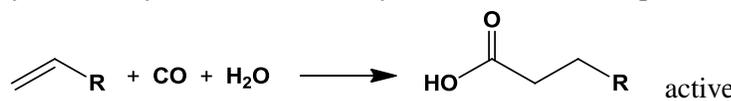
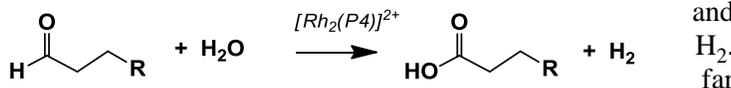
The manufacture of phenolic glycol ethers (also known as alkylene phenolic glycol ethers), e.g., propylene glycol phenyl ether (PPh) and/or ethylene glycol phenyl ether (EPh), is long known and practiced. These glycol ethers are typically produced in a batch process using excess ethylene oxide in presence of an acid or base catalyst. One common process for making phenolic glycol ethers, e.g., PPh and/or EPh, is a batch process in which propylene oxide (PO) and/or ethylene oxide (EO) is reacted with phenol in the presence of sodium hydroxide (NaOH) which serves as a catalyst. In this work, an alternative process for the production of EPh and PPh as a continuous process will be presented that eliminates the need for catalyst neutralization, salt filtration, and long residence times for reaction completion while at the same time improving the selectivity, and hence quality of the products.

POSTER ABSTRACTS

1. 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

A remarkable new catalytic reaction can occur under the proper conditions when water is added to the acetone solvent for our bimetallic hydroformylation catalyst: $[\text{Rh}_2\text{H}_2(\mu\text{-CO})_2(\text{rac-}et,\text{ph-P4})]^{2+}$. Under mild hydrogen deficient conditions the reaction of aldehyde water can occur to produce carboxylic acid and H_2 . This reaction is inhibited by H_2 , which has, so 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 $[\text{Rh}_2(\mu\text{-CO})_2(\text{CO})_2(\text{et},\text{ph-P4})]^{2+}$ as the likely catalyst for the aldehyde-water shift catalysis. We believe that bimetallic cooperativity plays an important role in this catalysis as it does in hydroformylation.



2. Double-Bond Isomerization of Long-chain Olefins

James Bruno and Kerry Dooley
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jbruno8@tigers.lsu.edu (James Bruno)

Positional isomerization of the double bond of long-chain olefins such as 1-hexadecene or 1-octadecene is of industrial importance in the manufacture of paper sizing agents. It is generally agreed that the most desirable isomers are those with the double bond in the 6, 7, or 8 positions. Nafion supported on SiO_2 , a solid superacid catalyst, gives the necessary activity and selectivity to these isomers, but its poor crush strength, high cost and propensity to oligomerize the olefins drives the need for a better catalyst. This project explores other strong acid catalysts such as tungstated zirconias and sulfonated polystyrenes. Supporting Nafion on a support of higher crush strength is also being examined. The catalysts are evaluated on target olefin selectivity, minimal skeletal isomerization, minimal oligomerization, and reusability.

3. Pt/Pd Diesel Oxidation Catalysts (DOCs) with Incorporated Zeolite

Gregory S. Bugosh, Rachel L. Muncrief, Michael P. Harold
Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

Diesel engine exhaust cannot be treated by a typical 3-way catalytic converter due to excess oxygen and particulate matter. To meet increasingly strict emissions requirements the treatment process is completed in several steps, with the diesel oxidation catalyst (DOC) typically first. The primary function of the DOC is to complete the oxidation of carbon monoxide (CO) and unburned hydrocarbons (HCs) to carbon dioxide and water. Heated by engine exhaust and exothermic reactions, the DOC operates at very high conversion once sufficient temperature has been achieved. However, during the "cold start" most of the hydrocarbons pass through unreacted and may exceed allowable limits. A potential solution is to incorporate a component that traps the hydrocarbons at low temperatures and then releases them at high temperature when the catalyst is more active. A series of monolith supported catalysts containing varying precious metal and zeolite content are studied by way of BET surface area measurements, light-off temperature for model reactants (CO, propene), and propene oxidation reaction kinetics. Spatially resolved measurements were also done by way of quartz capillary inserted along the channel of the monolith to examine progression of the reaction along the catalyst length.



4. Cyclohexene Disproportionation Reaction over Pt/SiO₂ Model Catalysts: the Role of Surface Steps on Pt Nanoparticles

Long Chen,^{a*} Xin Wang,^{a,b} Zhen Yan,^a Yunxi Yao,^a Li Liu,^{a*} Mingshu Chen,^{a,b} D. Wayne Goodman^a

^a *Department of Chemistry, Texas A&M University, College station, TX 77843, United States;* ^b *Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, 361005, Fujian, China*

* long.chen@mail.chem.tamu.edu (L. Chen); li.liu@mail.chem.tamu.edu (L. Liu)

Model catalysts of Pt nanoparticles (NPs) supported on SiO₂ thin films were prepared under ultra-high vacuum (UHV) conditions with metal coverage varied from 0.5 to 10 monolayers (ML), corresponding to average particle sizes of 1 ~ 5 nm. The reactivities of these Pt/SiO₂ catalysts were evaluated for cyclohexene disproportionation reaction under near atmospheric pressures (10 Torr) in a batch reactor contiguous to a UHV chamber. Specific reaction rates for the formation of cyclohexane and benzene increase sharply with particle size to a maximum at ~ 3 ML Pt coverage and then decline slightly. Carbonaceous deposition is detected on each catalyst after reaction. Both kinetic data and CO titration experiments using thermal desorption spectroscopy demonstrate that the step sites on Pt NPs are more easily blocked by carbonaceous deposition than terrace sites. The origin of the structure-sensitivity of cyclohexene disproportionation reaction has been rationalized in terms of site selective carbonaceous deposition and surface structure modification as a function of Pt particle size.

5. Role of Ammonia in the lean-rich cyclic reduction of NO_x on a LNT catalyst in the presence of excess H₂O and CO₂

Prasanna R. Dasari, Rachel Muncrief, and Michael P. Harold*

Dept. of Chemical & Biomolecular Engineering, University of Houston, Houston, TX 77204-4004 (USA) mharold@uh.edu

Ground level ozone produced by the NO_x emitted from lean burn and diesel engines is the main driving force for the active research in lean NO_x reduction. Several NO_x reduction technologies, such as selective catalytic reduction (SCR) using urea, lean NO_x traps (LNT) etc., are under development. Considerable research is also being done in developing technologies that combine both LNT and SCR after-treatment systems. The LNT/SCR technology utilizes NH₃ produced during the regeneration of the LNT for storage and reaction with NO_x in the downstream SCR. It is therefore, important to understand the NH₃ formation chemistry and kinetics on the LNT catalyst to develop an optimal design and operating strategy for the LNT-SCR system. LNT operates under cyclic conditions of fuel lean and rich, relative to O₂, environments. During the lean phase NO_x is stored in the form of nitrates and nitrites and during the rich phase the stored NO_x is reduced to N₂, N₂O and NH₃ by a reductant (e.g. H₂, CO, HC's). The production of NH₃ is known to occur by reaction between stored NO_x and H₂ under the rich conditions on a typical LNT catalyst. However, in the presence of CO and excess H₂O during the rich phase, two additional routes are possible. The first is by the water-gas shift reaction of CO and H₂O to give H₂, which then reacts with NO to give NH₃. A second pathway is through reaction between NO and CO forming support bound isocyanate (-NCO) species, which are hydrolyzed to form NH₃. The contribution of both pathways is of significance because each proceeds in the presence of H₂O which is obviously in high concentration in the exhaust (5-10%) but without H₂ in the feed, which is typically low in diesel exhaust. This study focuses on the formation of Ammonia during the lean rich cyclic studies on a LNT catalyst in various reductant environments.

6. The Prospect of Bifunctional Catalysts by Design

Hieu Doan and Lars C. Grabow

University of Houston, Department of Chemical and Biomolecular Engineering, 4800 Calhoun Rd., Houston, TX 77204-4004

Several examples of catalysts that perform multiple site-specific functionalities under steady-state reaction conditions have been reported in the literature [1]. The most common systems are bifunctional catalysts where each of the two distinct sites catalyzes different reaction steps independently. These systems include, but are

not limited to, metal alloys, step and terrace sites on a metal nanoparticle or the metal/support interface. In order to study bifunctional mechanisms systematically, we examine the prototypical CO oxidation reaction, which has O₂ dissociation and CO₂ formation as competing reaction steps [2], on various mixed-site catalyst models. Using density functional theory and microkinetic modeling as main computational tools, our preliminary results indicate that a highly active bimetallic catalyst can be created from less active components. Hence, we want to explore bifunctional catalyst design strategies for reactions where multiple functionalities can improve the overall reaction rate.

1. a) Kim, H. Y., Lee, H. M., & Park, J.-N. *J Phys Chem C*, 114(15), 7128 (2010). (b) Kotobuki, M. *et al. J Catal*, 236(2), 262 (2005) (c) Laursen, S., & Linic, S. *Phys Chem Chem Phys*, 11(46), 11006 (2009).
2. Freund, H.-J., Meijer, G., Scheffler, M., Schlögl, R., & Wolf, M. *Angew Chem Int Ed.*, 10064 – 10094 (2011).

7. Tailored Catalytic Properties of MFI Zeolite through Controlled Surface Modifications: Theory, Synthesis and Catalytic Testing

Arian Ghorbanpour, Lars C. Grabow, and Jeffrey D. Rimer
*University of Houston, Department of Chemical and Biomolecular Engineering,
 4800 Calhoun Rd., Houston, TX 77204-4004*

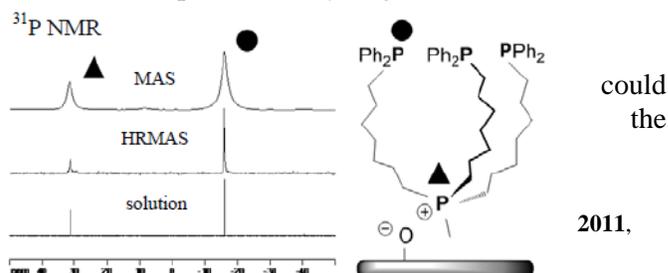
Nanoporous zeolites are utilized in many industrial processes because of their thermal stability, tunable acidity, and shape-selectivity. Notably, the aluminosilicate MFI-type zeolite (termed ZSM-5) is active for various reactions. Much attention has been given to the activity and identity of catalytic sites within the interior pores; however, active sites located on the external surfaces of zeolite catalysts may be equally, if not more important. Nanosized ZSM-5 crystals exhibit increased external surface area, yet differences between the inner and outer surface activity of zeolite catalysts are not well understood, which necessitates increased research efforts to develop an improved fundamental knowledge of active sites. To this end, we have synthesized core-shell MFI-type zeolites composed of an active (ZSM-5) core and a non-active shell of silicalite-1 (siliceous analogue of ZSM-5) with 5 – 10 nm thickness. The silica shell “passivates” external active sites, thus distinguishing differences between the internal and external activity. Initiatives in catalyst synthesis and testing were combined with computational modeling using density functional theory (DFT) to calculate the stability of bulk and surface acidic sites. This unique combination of synthesis, testing and modeling represents a synergistic approach in rational catalyst design that allows us to develop structure-function relationships for zeolite catalysts.

8. Immobilizing Catalysts on Oxide Supports by Chelate Phosphine Linkers with Long Alkyl Chains

Johannes Guenther and Janet Bluemel*
*Department of Chemistry, Texas A&M University, PO Box 30012, College Station, TX 77842,
 jguenther@chem.tamu.edu*

A new class of tridentate phosphine ligands with the general formula [MeP{(CH₂)_xPPh₂}}₃]⁺I⁻ (x = 4, 7, 11), and [MeP(CH₂PPh₂)₃]⁺OTf⁻, have been synthesized and fully characterized.¹ The linkers have been immobilized on silica with their phosphonium moieties via electrostatic interactions, and their mobility and leaching has been studied by solid-state HRMAS (high-resolution magic angle spinning) NMR. Immobilized Wilkinson-type rhodium complexes have been obtained by ligand exchange with the surface-bound linkers.¹ The activities and lifetimes of the catalysts have been tested with respect to the hydrogenation of 1-dodecene. The rhodium catalyst precursor bound by the immobilized linker [MeP{(CH₂)₇PPh₂}}₃]⁺I⁻ led to material with the highest activity and lifetime, and it can be recycled for a record 30 times. For all catalysts formation of rhodium nanoparticles with narrow size distributions around 4 nm has been proven.¹

1. J. Guenther, J. Reibenspies, J. Blümel, *Adv. Synth. Catal.* 353, 443-460.





9. Employing Molecular Modifiers to Tailor the Crystal Morphology of Zeolite Catalysts

Alexandra I. Lupulescu, Jeffrey D. Rimer

*University of Houston, Department of Chemical and Biomolecular Engineering,
4800 Calhoun Rd., Houston, TX 77004*

Zeolite catalysts are ubiquitous in the petrochemical and fine chemical industries due to their exceptional thermal stability, unique shape-selectivity, and high acidity; however, the inability to *a priori* control crystal growth often yields suboptimal materials with limited catalytic performance due to mass transfer limitations. Rational design approaches capable of selectively tailoring zeolite morphology and structure can address these challenges by eliminating long, tortuous internal diffusion pathlengths to dramatically improve catalyst activity and lifetime^{1,2}. We will present a novel synthesis technique that draws inspiration from natural processes, wherein molecular modifiers are employed to mediate anisotropic growth rates of zeolite crystals³. This versatile, facile approach was used to synthesize several zeolite framework types, with silicalite-1 (MFI type) serving as the primary case study⁴. The judicious selection of high efficacy zeolite growth modifiers (ZGMs) resulted in more than an order of magnitude decrease in silicalite-1 platelet thickness, as well as selectively-tailored crystal aspect ratios and surface architecture. Interfacial studies were performed to validate growth inhibition at the microscale; and force spectroscopy was used to probe interactions between ZGM functional groups and zeolite surfaces. In summary, ZGMs are a cost-effective and robust design scheme for achieving unparalleled 3-dimensional control of zeolite crystal morphology.

[1] Choi, M., Na, K., Kim, J., Sakamoto, Y., Terasaki O., Ryoo, R., *Nature* 461 (2009) 246-249; [2] Corma, A., *J. Catalysis* 216 (2003) 298-312; [3] Rimer, J.D., An, Z., Zhu, Z., Lee, M.H., Goldfarb, D.S., Wesson, J.A., Ward, M.D., *Science*, 330 (2010) 337-341; [4] Lupulescu, A.I. and Rimer, J.D., *Angew. Chem. Int. Ed.* 51 (2012) In Press

10. Oxidative desulfurization of diesel with oxygen: Reaction pathways on supported metal and metal oxide catalysts

Andrew M. Madrid, F. Carl Knopf and Kerry M. Dooley

Dept. of Chemical Engineering, Louisiana State University

Catalytic oxidative desulfurization (ODS) has most often used peroxide oxidants with Mo-, V- or Fe-oxides, or Ti-containing silicates. However, oxygen can react with sulfur heterocycles at temperatures above ~340 K. While there is evidence for some oxidation at the catalyst surface, much of the reaction seems to proceed by an autoxidation mechanism through free radical intermediates which are initially surface generated. Therefore the alkylaromatics and nitrogen heterocycles in diesel must also be oxidized to some extent. Here we examine all the oxidation reactions taking place during ODS on two typical catalyst classes: supported Pd (on activated carbons or alumina) and titanium silicates. It is shown that the reaction rate of ODS is heavily influenced by the other oxidizable components present. Temperatures must be kept reasonably low (< ~400 K) in order to minimize co-oxidations. In turn, this requires either higher pressures than typically used for peroxide-based oxidations, or greatly enhanced gas-liquid mixing. Both of these alternatives will be discussed.

11. Surface Chemistry of Gold in Hydrogenation: Ether Synthesis and Chemoselective Reactivity of Propionaldehyde versus Acetone on H-Atom Covered Au(111)

Ming Pan, Adrian J. Brush, Zachary D. Pozun, Graeme Henkelman, and C. Buddie Mullins

Departments of Chemical Engineering and Chemistry and Biochemistry, Institute for Computational Engineering and Sciences, University of Texas at Austin, Austin, TX 78712-0231

Supported gold nanoparticle catalysts have been widely studied in hydrogenation reactions, and, in particular, show exceptional activity for selective hydrogenation processes. However, fundamental studies on the relevant model catalysts are lacking and highly desired in order to an enhanced understanding of hydrogenation reaction mechanisms by gold catalysis. Here we present two studies on hydrogenation reactions on a H-atom covered Au(111) surface under ultra high vacuum conditions. 1) We demonstrate the chemoselective reactivity of acetone and propionaldehyde on H-covered gold. The experimental results indicate that propionaldehyde can be hydrogenated to 1-propanol. In contrast, no hydrogenated product has been detected from the interaction between acetone and hydrogen. Density functional theory calculations predict dissimilar energetic barriers for the individual steps in the hydrogenation reaction and indicate the basis of the chemoselective activity. The



polymerization of $\text{CH}_3\text{CH}_2\text{CHO}$ is also found to play a role in the hydrogenation of propionaldehyde by increasing the concentration of $\text{CH}_3\text{CH}_2\text{CHO}$ at elevated temperatures. 2) We have discovered a new method for ether synthesis. On H covered Au(111), symmetrical and unsymmetrical ethers can be formed via a self-coupling reaction of aldehydes or a coupling reaction between alcohols and aldehydes, respectively. Those two studies demonstrate the unique surface chemistry of gold for hydrogenation reactions from a mechanistic point of view.

12. Synthesis of Au nanoparticles supported on TiO_2 and study of activation conditions for CO Oxidation Reaction

Basu D. Panthi, Johnny Saavedra, Christopher J. Pursell, and Bert D. Chandler
Department of Chemistry, Trinity University, San Antonio, TX 78212-7200

CO oxidation remains an important test reaction for gold nanoparticle catalysts, and preferential CO oxidation in H_2 -rich streams (PROX) is an important industrial reaction. Activation procedures and the reaction conditions have dramatic effects on the high activity of gold catalysts for these reactions. Our recent research has focused on developing synthesis and activation techniques for Au nanoparticle catalysts using PAMAM dendrimers as solution phase nanoparticle templates. Model Au catalysts having particle sizes in the range of 2-4 nm have been prepared using 5th generation PAMAM dendrimers, depositing onto P-25 titania, removing the organic dendrimer template. A detailed investigation into both the nanoparticle synthesis conditions and the conditions required for removing the dendrimer was performed, with a focus on developing low temperature activation conditions. CO oxidation activity in a typical reformate gas mixture was examined using a variety of different activation atmospheres (H_2 , O_2 and O_2+H_2 mixtures). Mild conditions (150^oC, 4 h in H_2 -rich streams) were found to be suitable for Au/ TiO_2 catalysts, improving the activity with respect to conventional "harsher" conditions (300^oC, 16h in O_2 rich streams).

13. Effect of Pd Surface Coverage of Pd-on-Au NPs for Catalytic Reduction of 4-nitrophenol

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Studying how the structure of a bimetallic NP affects its catalytic activity is a growing area of research because these bimetallic catalysts are generally more active than their monometallic counterparts. It is difficult to simultaneously control the composition and size/shape of bimetallic NPs and hence determining how their nanostructure affects their catalytic activity is often not possible. We have shown that 3 nm Pd-on-Au bimetallic NPs can be synthesized with controlled size and surface composition. Here we show that these bimetallic NPs can catalyze room-temperature reduction of nitro compounds to widely applied amino compounds. We used 4-nitrophenol as a model compound and showed that 3 nm Pd-on-Au NPs with 150% Pd surface coverage (100% Pd surface coverage= 1 monolayer) exhibit the highest catalytic activity. Extended x-ray absorption fine structure spectroscopy (EXAFS) analysis revealed that NPs with 150% Pd surface coverage have three-dimensional surface Pd ensembles. The formation of these ensembles on the NP surface may maximize the NP's catalytic activity due to their geometry and/or change in the density of states of the Pd and Au atoms and resulting interfaces.

14. Mixed Rare Earth Oxides (REOs) for the Desulfurization and Tar Reforming of Gasifier Effluents

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The removal of H_2S and tars from syngas generated in biomass or coal/biomass gasification plays an important role in further processing of syngas. Rare earth oxide (REOs, e.g., Ce/ LaO_x)- based materials mixed with transition metals (e.g., Mn, Fe, Ni) have been synthesized by a variety of methods, including templated sol-gel, hydrothermal, and incipient wetness coimpregnation. These materials have been investigated for both H_2S adsorption and tar reforming at high temperatures (~630-750^oC) with a goal of better heat integration in the

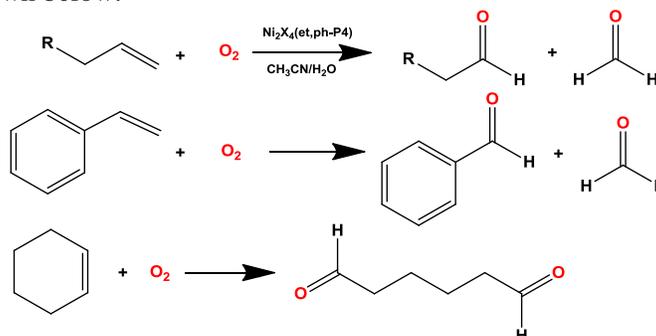
gasification process. Desulfurization tests were conducted using model syngas mixtures. Successive desulfurization-regeneration cycles of some of these materials (e.g., Mn/Ce/LaO_x) demonstrated reasonable sulfur capacities (>0.3 mmol S/g) in the presence of water and CO₂, along with air regenerability. Sulfur capacities at higher temperatures are slightly higher, probably due to more REO reduction and faster diffusion. Naphthalene was used as the model compound for tar reforming/cracking, and the effects of H₂S, CO, H₂O and CO₂ on these reactions were examined. Both H₂S and CO₂ are strong inhibitors, and H₂O also inhibits, while CO is not. Fresh, used and regenerated sulfur sorbents and catalysts have been characterized by BET, TPR, XRD, XANES and EXAFS.

15. Alkene Oxidative Cleavage by O₂ and Bimetallic Nickel Phosphine Complexes

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Bimetallic *meso*- and *racemic*-Ni₂X₄(*et,ph*-P₄) complexes (X = Cl, Br), (*et,ph*-P₄ = Et₂PCH₂CH₂)(Ph)PCH₂P(Ph)-(CH₂CH₂PEt₂) in the presence of oxygen and in water/polar organic solvent solutions show activity as precursors for the oxidative cleavage of unactivated alkenes to cleanly produce aldehyde products as shown below.



Aldehyde and dialdehyde products have been characterized by gas chromatography-mass spectrometry (GC/MS) and NMR spectroscopy. Some monometallic complexes, including NiCl₂(dppe), NiCl₂(dcpe) and NiCl₂(BISBI), show some activity. However, they do not produce as much aldehyde as the bimetallic complexes nor as quickly. Other complexes, including NiCl₂(dppp) and NiCl₂(TPP)₂, are inactive for the oxidative cleavage. Although the current system is not catalytic, spectroscopic studies indicate two main reasons. First, phosphine dissociation from the bimetallic complexes leads to complete oxidation of the tetrakisphosphine ligand to the tetrakisphosphine oxide. This dissociation also leads to the formation of an inactive species, [Ni₂(μ-Cl)(*meso*-*et,ph*-P₄)₂]³⁺, which has been characterized by X-ray crystallography. We believe a new, stronger chelating tetrakisphosphine ligand will allow for a catalytic oxidative cleavage reaction to be realized. Possible reaction mechanisms have been proposed based on DFT computational studies and will be presented.

16. The Role of Functional Groups for Oxygenates Adsorption on Oxides

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Upgrading of highly reactive short oxygenates in bio-oil to valuable chemicals or fuels require development of chemoselective catalysts that convert individual molecules or functional groups while leaving others untouched. Most candidate catalysts for upgrading are oxides or oxide-supported metals; hence it is desirable to investigate the selective interaction of functional groups of representative oxygenates with oxide surfaces. Hydroxyacetone is a good study case because it has two functional groups and is contained in bio-oil in significant concentration. We followed the adsorption and reaction of hydroxyacetone on commonly used oxides, specifically, silica, alumina, titania, ceria and zirconia, by in-situ diffuse reflectance IR spectroscopy (DRIFTS) and pulse thermal analysis (PTA). Low temperature adsorption studies were carried out to estimate the temperatures at which surface reactions occur when hydroxyacetone is adsorbed on the oxide supports. The



monofunctional reference compounds acetone and *n*-propanol, were also adsorbed on these oxides to assess the role of each functionality for reactivity and to generate spectra for comparison. Spectra recorded during temperature-programmed experiments evidence strong interaction of hydroxyacetone with both functional groups and incomplete desorption even after heating to 400 °C. In conclusion, hydrophilic supports may be unsuitable for upgrading highly reactive short oxygenates.

17. Boron Composite Nanoparticles for Enhancement of Biofuel Combustion

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Boron in small amounts (<3 wt%) is a potential candidate fuel additive to improve the combustion of low heating value, difficult to combust fuels, both due to its high energetic density and the ease with which it can be synthesized as nanoparticles of <100 nm. However, complete boron combustion can be difficult, because it forms a B₂O₃ oxide shell of relatively low melting point which tends to stick as a liquid to the pure boron nanoparticles, effectively choking off the oxidation. In this project, we have explored the mechanism of boron combustion in an ethanol spray flame and whether complete combustion can be catalyzed by the addition of rare-earth oxide and iron shells to the boron nanoparticles. These catalysts are applied as coatings to the boron, forming core-shell nanoparticles. A simple mechanical ball milling method can apply the coatings, although wet chemical reductive syntheses have also proven feasible. It has been observed that (especially) the REO coatings enhance the burning behavior of boron by an unknown mechanism. This in turn positively affects the main (ethanol) combustion reaction, significantly reducing the ignition delay, and giving greater overall heat release at a given equivalence ratio (faster combustion).

18. Towards the Design of Optimal Catalysts for Selective Catalytic Reduction of NO_x: A Study of Ammonia Uptake in Cu- and Fe-Zeolites

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Here we examine the influence of metal ion loading in zeolites on the NH₃-uptake capacity and acidity for a family of synthesized Fe- and Cu-exchanged ZSM-5 catalysts using temperature programmed desorption of ammonia (NH₃-TPD). Results reveal that both Brønsted and Lewis acidities were present in Fe- and Cu-exchanged ZSM-5. As the degree of metal exchange increased, the number of Lewis acid sites increased but their capacity to bind NH₃ decreased. The effect of metal loading on the Brønsted acidity is not straightforward, which may be associated with differences in the metal binding and/or the presence of metal (or metal oxide) clusters. Cu-exchanged ZSM-5 exhibited a stronger capacity to store NH₃ at temperature above 500 °C, which may be attributed to Cu Lewis acid sites or an enhanced Brønsted acidity. Moreover, Cu-exchanged ZSM-5 exhibited superior NH₃ uptake capacity than Fe-exchanged samples. The metal loadings resulting in the largest NH₃ uptake were 0.74 (Fe/Al) and 0.94 (Cu/Al) for Fe/Cu-exchanged ZSM-5. A numerical model was used to estimate the thermodynamic and kinetic parameters of NH₃ adsorption and desorption. The heat of adsorption, ΔH_a, for NH₃ on H-ZSM-5 and Fe-ZSM-5 were comparable. In the latter, ΔH_a decreased with increasing Fe loading whereas Cu-ZSM-5 exhibited two desorption peaks. Collectively these studies provide heuristic guidelines for the design of zeolite catalysts for NH₃-SCR.

19. Acetone Assisted Diffusion of Oxygen Vacancies on TiO₂ (110) Surface

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Oxygen vacancies are known dominating the electronic and chemical properties of transition metal oxide surfaces. Using scanning tunneling microscopy, we have studied the interaction between acetone molecules and bridge-bonded oxygen vacancies on the TiO₂ (110)-1 × 1 surface. The STM images from the same area show



that upon the adsorption of acetone molecules at room temperature (RT), the oxygen vacancy pattern changes. The sequential isothermal STM images directly unravel an adsorbate-mediated oxygen vacancy diffusion mechanism. While acetone molecules can diffuse both along the Ti row and along the O row, only the along-O-row diffusion can assist the oxygen vacancy diffusion. The acetone diffusion barriers calculated using DFT agree with experimental results.

20. Dehydrogenation of Propane to Propylene over Supported Ni-Au Catalysts: From Model Systems to Real Catalysts

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Hydrogenolysis and dehydrogenation of propane were studied over model nickel-gold catalysts. The supported model Ni-Au catalysts were prepared by depositing Ni and Au onto a planar silica film. Infrared reflection absorption spectroscopic data showed that isolated Ni sites appeared and became dominant on the surface with the addition of Au to Ni. For the conversion of propane in the presence of hydrogen, the dehydrogenation of propane to propylene was observed on the Ni-Au bimetallic catalysts, whereas only hydrogenolysis products were observed on the monometallic Ni catalyst. A correlation was found between the concentration of isolated Ni sites and the catalytic activity for propane dehydrogenation. The same reactions were also carried out on real Ni-Au catalysts prepared by conventional impregnation methods using high surface-area silica as the support, and the results were in good agreement with those on model catalysts. In addition, the presence of bimetallic Ni-Au nanoparticles was confirmed by TEM/EDX results.

21. CO Oxidation on Inverse Fe₂O₃/Au(111) Model Catalysts

Ting Yan, Daniel W. Redman, Wen-Yueh Yu, David W. Flaherty, C. Buddie Mullins, and Jose A. Rodriguez

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CO oxidation is studied at 10 to 100 Torr between 400 K to 670 K on inverse model catalysts made of Fe₂O₃ nanoclusters grown on Au(111) single crystal. The addition of Fe₂O₃ nanoclusters transformed the inert Au(111) single crystal into an active catalyst for CO oxidation. The catalytic activity increases with iron oxide coverage initially, and then decreases when the iron oxide coverage is greater than 0.5 monolayers. When the iron oxide particles form a continuous film on Au(111) there is no catalytic reactivity. These experimental results strongly suggest that the active sites for CO oxidation are located at the iron oxide/gold interface. Kinetics measurements suggest that CO oxidation at the interface is likely to be the rate limiting step. C-O bond cleavage observed via post reaction Auger electron spectrum suggests that multiple reaction pathways are involved in CO oxidation over Fe₂O₃/Au(111).

22. Mass and Infrared Spectroscopy Study of Acetaldehyde on Clean and Hydrogen-Precovered Au(111) Surfaces

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The surface chemistry of acetaldehyde (CH₃CHO) on the clean and H-precovered Au(111) surfaces is studied using temperature-programmed desorption mass spectroscopy (TPD-MS) and reflection-absorption infrared spectroscopy (RAIRS) under ultrahigh vacuum. At the temperature of 77 K, CH₃CHO molecules weakly bond to the Au(111) surface via the lone pair electrons of oxygen atom. Upon heating to ~120 K, a portion of CH₃CHO molecules polymerize as evidenced by the formation of OCO infrared vibration bands; the remainder desorb as monolayer desorption at ~136 K. The formed CH₃CHO surface polymer is relatively stable and dissociates to CH₃CHO monomers at a temperature > 200 K. Increasing CH₃CHO dosage leads to two additional TPD features for multilayer desorption (~ 106 K) and dissociation of CH₃CHO bulk polymer (150 -

200 K). The precovered hydrogen on the Au(111) surface was found to (1) facilitate the formation of CH₃CHO bulk polymer instead of CH₃CHO surface polymer at 77 K; (2) react with CH₃CHO to produce the hydrogenated counterpart, ethanol (CH₃CH₂OH); and (3) provide a reaction pathway for CH₃CHO coupling into diethyl ether, (CH₃CH₂)₂O. The formed CH₃CH₂OH and (CH₃CH₂)₂O desorb at the temperatures > 180 K, which are higher than their monolayer desorption temperatures, indicating a reaction-limited mechanism.

23. Microwave Assisted Synthesis of Chabazite-type Silicoaluminophosphate and Partial Detemplation used for Enhanced Sr Ion-exchange and CO₂ Adsorption

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Silicoaluminophosphate (SAPO) molecular sieves have been widely studied for catalysis, adsorption and other important applications. A silicoaluminophosphate with a chabazite-type framework (SAPO-34) was synthesized via a microwave heating assisted hydrothermal method. The effect of variables such as crystallization time and aging time on the microwave-assisted synthesis was investigated in detail. X-ray diffraction (XRD), scanning electron microscopy (SEM), inductively coupled plasma mass spectrometry (ICP-MS), solid-state magic angle spinning nuclear magnetic resonance (MAS NMR) measurements, porosimetry and pure component CO₂ gas adsorption were used to characterize the materials structural and textural properties. High purity and small size cubic crystals (0.2–1 nm) of Na-SAPO-34 with large surface area were successfully synthesized by microwave heating after 42 h, compared to 8 days required via the conventional method. It has been discovered that a short aging time of 8 h favors formation of small crystals, plausibly due to an enhanced nucleation. In addition, MAS NMR spectra showed that framework silicon atoms are present mainly as Si(4Al), which evidences a framework with minimal amount of faults. As-synthesized materials were ion exchanged with Sr²⁺ after partial detemplation and afterwards tested for CO₂ uptake at room temperature. Elemental analyses revealed superior Sr²⁺ loadings per unit cell, probably due to the neat crystalline characteristics. As a result, the materials also exhibited superior CO₂ adsorption capacities, particularly at low partial pressures where the sorbent–sorbate interactions are predominant.

24. Adsorption and Diffusion of Acetone on Rutile TiO₂ (110)

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Understanding the surface reaction processes of acetone on metal oxide surfaces is important for photo-oxidation of toxic organic molecules. We have studied the adsorption and the diffusion of acetone on reduced rutile TiO₂(110) surfaces using variable temperature scanning tunneling microscopy (STM). At room temperature we observe that acetone molecules prefer to adsorb on bridging-bonded oxygen vacancy sites. The sequential isothermal STM images show that acetone molecules are mobile at RT. They hop between the unoccupied vacancy sites through both the along-row diffusion and the cross-row diffusion. Images obtained at temperatures below RT show that there are two barriers involved in these diffusion processes. One is the acetone diffusion barrier along the Ti row. The other is the diffusion barrier from vacancy site to the neighboring Ti row. The latter is the rate limiting step. DFT calculations agree with experimental results.

25. Modulating palladium-on-gold catalysis for glycerol oxidation with Pd surface coverage

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Glycerol is a highly functionalized renewable raw material from biodiesel manufacture. Carbon supported Au NPs, Pd NPs and a series of Pd-on-Au NPs with different Pd surface coverages (sc%) ranging from 10 sc% to

300 sc% were prepared. The catalysts have been tested in the liquid phase oxidation of glycerol using oxygen as the oxidant. Pd-on-Au/AC (1.0 wt% Au) had much higher catalytic activities (turnover frequency (TOF) 6076 (h^{-1}) at 80 sc%) over monometallic catalyst materials Au/AC (1.0 wt%) and Pd/AC (1.0 wt%), both of which had TOF of 397 h^{-1} . Catalytic activity and selectivity were also found to be a function of Pd surface coverage, with the highest activity and selectivity to glyceric acid detected at ~80 sc% and ~60 sc%, respectively. XAFS (X-ray Absorption Fine Structure) results have shown that 0 sc%, 60 sc% and 150 sc% catalysts maintained their structures during reaction while Pd/AC did not, indicating the fact that Au can help to stabilize Pd in oxidative environment. Pd atom ensemble formation is proposed to explain the “volcano-shaped” dependence of activity on Pd surface coverage. This catalyst material offers a potential way to convert glycerol into more economically valuable products like glyceric acid, lactic acid and tartronic acid.

26. Epitaxial growth of graphene on a pseudomorphic layer of metal supported on Ru(0001): Tuning the coupling of graphene to substrates

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Department of Chemistry, Texas A&M University

For the purpose of tuning the coupling of graphene to a substrate, a novel method is developed to modify the graphene-metal interaction by introducing a single layer of transition metal to the interface between graphene and substrate. Graphene/Co/Ru(0001) and graphene/Pd/Ru(0001) have been studied by scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and Auger electron spectroscopy (AES). Our experimental findings show that at submonolayer regime, both Co and Pd adapt Ru(0001) lattice to form a pseudomorphic layer, on which self-organized graphene overlayer with high quality can be prepared. An atomic model of such graphene system is proposed, where deposited metal atoms occupy the hcp hollow sites of Ru(0001) with a single layer of intact graphene sheet adsorbed on top. STM measurements show that the corrugation of moiré pattern changes as the single layer of transition metal is intercalated between graphene and Ru(0001). The corrugation follows the following order: Graphene/Co/Ru > Graphene/Ru > Graphene/Pd/Ru. Furthermore, the modification of graphene/Ru(0001) is tested by deposition of Au on three graphene systems and STM results show Au exhibits different morphologies. Overall, our results demonstrate that our method can modify the corrugation of graphene systems, resulting in different morphologies of metal clusters deposited on graphene, which might also change the catalytic activities of metal clusters.

27. Activation conditions and in-situ FTIR studies for Au/TiO₂ catalyst used in CO oxidation

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Activation procedures and reaction conditions have dramatic effects on the high activity of gold catalysts used for CO oxidation catalysis (temperature, time, composition of the gas, etc). A commercial Au/TiO₂ catalyst was treated at elevated temperatures under various atmospheres (H₂, O₂ and O₂+H₂ mixture) and examined with *in-situ* FTIR experiments and CO oxidation activity using a typical reformat gas mixture. Fast and extensive carbonate/carboxylate formation was observed during *in-situ* IR experiments and proposed as the primary reason for deactivation. Activation with H₂ produces a catalyst with a higher tendency to carbonate/carboxylate formation, which agrees with the fast deactivation for this catalyst in the literature and in our own research. An activation method consisting of a short time treatment with mixtures H₂+O₂, produces a catalyst with improved activity and stability compared to conventional activation methods (consisting of higher temperatures and longer times). This activation methodology can be applied in Au-catalysis research as a tool to improve stability and reproducibility of catalysts prepared by different methods and by different research groups.



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 C₄ 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.

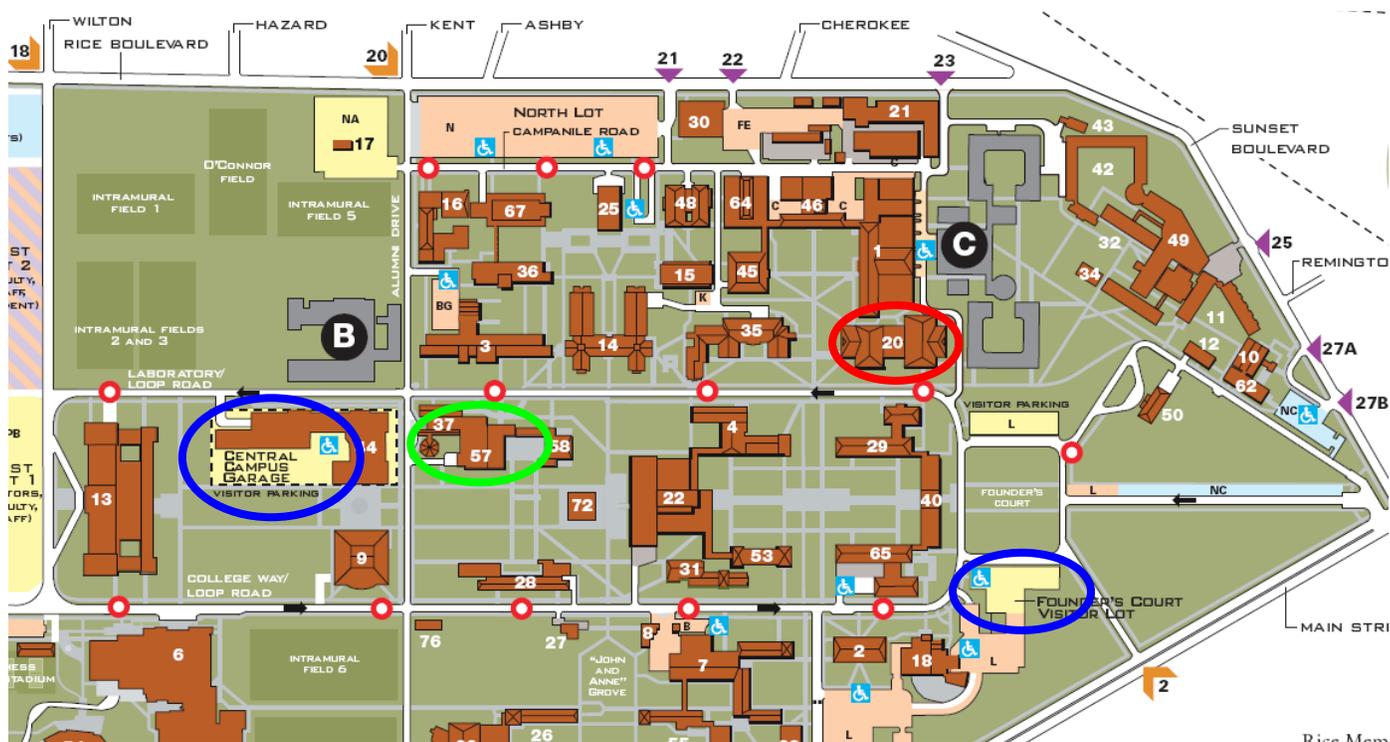


The first thing we did was to organize an NSF-supported workshop at Rice which (not surprisingly) concluded that more funding was needed for research on catalysts for fuels, environmental protection (cat converters), chemicals, etc. At that time, demand was also great for new employees with catalysis 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 Slauch 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 Map (<http://www.rice.edu/maps/maps.html>)



Building numbers

20: Duncan Hall (meeting site)

57: Rice Memorial Center (on-your-own lunch)

44: Central Campus Garage (ample visitor parking)

Founder's Parking Lot (some visitor parking)