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2019 FALL SYMPOSIUM

Friday, October 18, 2019

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The SWCS officers and I welcome you to the 2nd SWCS Fall Symposium, on Friday, October 18, 2019, in the Historic French House on the campus of Louisiana State University. We hope this event will be an effective venue for academic and industrial catalysis researchers from the region to mix and interact.

We are delighted to have four invited speakers from both industries and academia for this year's symposium. A poster session will be held following the invited talks and several meritorious posters presented by students will be identified with Best Poster Awards and cash prizes.

Registration for the 2019 Fall Symposium is free for students and $10 for professionals (online registration required for both). The price at door is $15. A catered reception will take place concurrently with the poster session.

Members of SWCS and non-members alike are welcome to participate in this event. We hope to see you at the Symposium!

Lars C. Grabow

Department of Chemical and Biochemical Engineering

University of Houston

2019 FALL PROGRAM

Talks and the poster session will be held in the French House at LSU.

1:00 PM	**Registration**
1:25 PM	**Welcoming Remarks – Ye Xu**
1:30 PM	**Cathryn (Gail) Blakley**, W.R. Grace *An Introduction to W.R. Grace and Recent Advances in Determining the Mechanism of Activating Metallocene Catalysts for Olefin Polymerization*
2:10 PM	**Daniel Shantz**, Tulane University, Department of Chemical and Biomolecular Engineering *Designing Composition and Local Structure in Zeolites: Teaching Old Catalysts New Tricks*
2:50 PM	**Intermission**
3:00 PM	**Kewei Huang**, Shell Refining Catalyst Technology *Hydroprocessing Catalyst Basics and Catalyst Manufacture*
3:40 AM	**Kunlun Ding**, LSU, Department of Chemical Engineering *Synthesis of Supported Metal Nanoparticles – New Approaches with Old Chemistry*
4:20 PM	**Reception (Catered) and Poster Session**
5:45 PM	**Poster Awards**
6:00 PM	**Adjourn**

📍 **Meeting site – Historic French House** (co-ordinates: 30.410916, -91.175548)

📌 **Visitor Center**

P **Visitor parking --** https://www.lsu.edu/parking/parking/visitor.php

-- Nearest visitor parking: Union Square Parking Garage (behind Barnes & Noble)

An Introduction to W.R. Grace and Recent Advances in Determining the Mechanism of Activating Metallocene Catalysts for Olefin Polymerization

Cathryn (Gail) Blakley
W.R. Grace

Introducing WR Grace to the local scientific community and their commitment to being a leading global supplier of specialty chemicals by leveraging its talent, technology, and trust. The two industry-leading business segments, Catalysts Technologies and Materials Technologies, provide innovative products, technologies, and services that enhance the products and processes of our customers around the world. Through the combination of high-throughput (< 1 gram) and bench scale (<100 grams) studies at WR Grace's recently acquired facility in Baton Rouge, new insight has been gathered into improving the overall activation efficiency of these single-site initiators with MAO to allow the advancement of catalyst commercialization quicker than previously possible.

Biography

Cathryn (Gail) Blakley is a Research Scientist for WR Grace, which acquired the Albemarle polyolefins business in 2018. She earned her Ph.D. in 2014 from the University of Maryland under Professor Lawrence Sita, where she studied Group 4 post-metallocene living olefin polymerizations. Gail joined Albemarle after completing her degree. Since then she has been working on commercial metallocene polymerization catalysts and the fundamentals of activation with methylaluminoxanes. In addition to coordinating the site's seminar program, she also leads the site's scientific outreach program.

Designing Composition and Local Structure in Zeolites: Teaching Old Catalysts New Tricks

Daniel Shantz
Tulane University

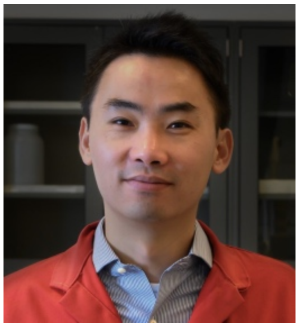
Zeolites are a technologically important class of materials used in applications including fuel production, gas separations, and ion-exchange processes. As such, zeolites are a somewhat mature, albeit societally important class of materials. After a brief overview of zeolite properties relevant to the presented work, this seminar will provide examples of how controlling local structure and composition can be used to improve the performance of zeolites in existing technologies as well as pushing them into new spaces. The first part of the talk will discuss the lab's efforts in iron-containing zeolites. I will show how controlling the mesostructure of a zeolite was essential to realizing substantive improvements in the catalytic oxidation of benzene to phenol. In the best cases phenol yields of 23% with a TON of 82 was observed, making this the best zeolite catalyst reported to date for this reaction. I will follow up these results with a discussion of using iron zeolites to convert methane to methanol using hydrogen peroxide. Here, the key was the presence of framework trivalent atoms in addition to the iron. I will discuss how acid site strength and density can be used to control the activity of the zeolite as well as the product slate observed.

Biography

A native of Muskegon Michigan, Dan obtained his B.S. (ChE, 1995) from the University of Florida and Ph.D. (ChE, 2000) from the University of Delaware. Dan was an Alexander von Humboldt Postdoctoral Fellow for 18 months following his Ph.D. Dan then joined the Chemical Engineering Department at Texas A&M in 2001, starting as an assistant professor and ultimately holding the Ray Nesbitt Professorship and the rank of full professor. In 2012 Dan joined SABIC (Saudi Basic Industries), first as a Chief Scientist and then as a Senior Manager in SABIC's Corporate Research and Innovation Future Feedstocks group playing a leadership role in the inception, technical formulation, and growth of the group. Dan joined the Department of Chemical and Biomolecular Engineering at Tulane in July 2014 as the Entergy Chair in Clean Energy Engineering, and became the Chair of the Department in August of 2018. Dan's lab is internationally recognized for its work in zeolite nucleation, biomimetic materials, and hybrid materials for catalysis and separations.

Hydroprocessing Catalyst Basics and Catalyst Manufacture

Kewei Huang
Shell Refining Catalyst Technology



Shell Catalysts & Technologies (SC&T) is a global catalyst and technology supplier, with a broad portfolio of solutions for the refining industry including hydrotreating, hydrocracking, and residue upgrading. Catalysts are the chemical "engine" of a hydroprocessing unit, increasing reaction rate to allow higher throughput, more difficult feeds, and longer cycles. Hydroprocessing catalysts will be introduced with a focus on their purpose, composition, and function. Commercial production of these catalysts will also be covered using the Port Allen Catalyst Plant as an example. This SC&T facility is fully integrated including powder production, extrusion, and impregnation capability in one plant and is a good example of best-in-class operation.

Biography

Kewei Huang is a research scientist in Shell Refining Catalyst Technology, currently working on catalysts R&D for Resid Upgrading and Hydroprocessing. Kewei earned his Ph.D degree in 2014 from Rice University with Prof. Angel Martí, where he studied the synthesis and application of the transition metal materials and received Harry B. Weiser Research Award in recognition of excellence in chemical research. Before joining Shell in early 2016, he worked one year as a postdoctoral research scientist at Texas A&M University. Kewei has developed three commercialized catalysts at Shell.

Synthesis of Supported Metal Nanoparticles – New Approaches with Old Chemistry

Kunlun Ding
Louisiana State University, Department of Chemical Engineering

Heterogeneous catalysts that contain metal nanoparticles (NPs) are used in many petrochemical processes. In recent years, bimetallic NPs have been used in biomass conversions, electrocatalysis, and many other catalytic processes. Conventional impregnation method usually results in ill-defined NPs with inhomogeneous particle sizes. The synthesis of ultrasmall (< 3 nm) supported metal NPs remains challenging. In this talk, we will demonstrate two new synthesis approaches for supported metal NPs using old chemistry concepts. The first strategy involves the preassembly of well-defined heterometallic compounds on a substrate. The supported heterometallic compounds can be converted to well-defined supported bimetallic NPs upon reduction. This approach can be applied to a large variety of bimetallic NPs, including several bulk immiscible systems. In the second part of the talk, we will discuss a new protocol to deposit colloidal metal NPs onto various catalyst supports by tuning the interaction between colloid metal NPs and supports. This approach is applicable to many types of metal NPs and supports, and can be readily scaled up without affecting the dispersion of NPs. The metal loading can be adjusted by changing the ratio between metal NPs and supports. Furthermore, the adsorption of colloidal NPs mostly occurs on the external surface of catalyst supports, thus eliminating the diffusion control in catalytic reactions.

Biography

Dr. Ding is an assistant professor in Chemical Engineering Department at Louisiana State University. He received his Ph.D. in 2009 from the Institute of Chemistry, Chinese Academy of Sciences. In the same year he joined Prof. Galen Stucky's group at UCSB as a postdoctoral researcher, where he worked on halogen-mediated natural gas conversion in collaboration with Gas Reaction Technologies. After three years of work at UCSB, he joined Prof. Peter Stair's group at Northwestern University in 2013. His work at Northwestern mostly focused on atomic layer deposition and in situ spectroscopies.

Dr. Ding joined LSU in 2016. His research group aims to develop site-specific techniques to achieve atomic level understanding of heterogeneous catalysis. They develop model catalysts to minimize the structural heterogeneities of heterogeneous catalysts, and further calibrate spectroscopies to distinguish the surface structures and discriminate the catalytic performance of different sites. Their targeted reactions include oxidative coupling of methane, partial oxidation of methane, olefin and alkane metathesis, selective hydrogenation of alkynes and olefins, and low temperature CO oxidation and water-gas shift reactions. Dr. Ding has published 48 papers and 5 patents, and his work has been cited more than 3,600 citations.

POSTER ABSTRACTS

1. Synthesis of Supported Metal Nanoparticles By Controlling the Interaction between Colloidal Metal Nanoparticles and Supports

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Supported metal nanoparticles (NPs) play a significant role in the fuel and chemical industry. A large effort has been devoted to the synthesis and characterization of supported metal NPs. The most important industrial methods including impregnation and precipitation of molecular precursors followed by calcination and reduction often yield size polydispersed NPs. Deposition-precipitation, ion exchange, electrostatic adsorption, photodeposition, surface reduction, surface organometallic chemistry, and atomic layer deposition have been developed to improve the uniformity. However, these methods heavily rely on the surface properties of catalyst supports, such as charges, defects, and reactivity of surface hydroxyls. Thus, they cannot be simply extended to different types of supports. In this work, we have developed a strategy inspired by deposition-precipitation to deposit colloidal metal NPs onto a variety of supports. By tuning the interaction between colloid metal NPs and supports, different metal NPs dispersed evenly on metal oxide, zeolites, silica and carbon. The approach can be readily scaled up and the metal loading can be adjusted by simply changing the weight ratio of metal NPs to supports without affecting the dispersion of NPs. Moreover, the colloidal NPs mostly deposite on the external surface of catalyst supports, which eliminates the diffusion control in catalytic reactions. The Pd catalysts synthesized via our strategy show much lower alkane selectivity than the impregnated counterparts in competitive acetylene hydrogenation.

2. Dual Role of Surfactants in Zeolite Synthesis and Catalyst Optimization

Aseem Chawla[1], Noemi Linares[2], Rui Li[1], Rishabh Jain[1], R. John Clark[1], James G. Sutjianto[1], Jeremy C. Palmer[1], Javier García-Martínez[2], and Jeffrey D. Rimer[1]*

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Zeolites are crystalline microporous aluminosilicates with unique properties, such as tunable acidity and exceptional (hydro)thermal stability, which are utilized in commercial processes ranging from ion-exchange and adsorption to catalysis and separations. Surfactant templating has emerged as one of the most effective and versatile strategies for the construction of well-defined porous architectures in zeolites.[1] Despite tremendous efforts to elucidate the mechanisms of surfactant templating in zeolite synthesis, these pathways are not well understood. Here, we will discuss the dual roles of the cationic surfactant cetyltrimethylammonium (CTA) as an organic structure-directing agent (OSDA) and as a mesostructuring agent in the rational design of zeolites.

One of the most common zeolites is ZSM-5 (MFI type), which is used as a catalyst and sorbent in a wide range of industrial applications.[2] In ZSM-5 synthesis it is challenging to identify new and inexpensive OSDAs that can tailor the physicochemical properties of the final product. The most frequently used OSDA in ZSM-5 synthesis is tetrapropylammonium (TPA); however, recent studies have shown that CTA can be used as an alternative.[3,4] Here, we will present the effects of using CTA and TPA as OSDAs in combination with a variety of alkali metals as inorganic structure-directing agents. Our findings reveal that the selection of inorganic/organic combinations has a significant impact on the kinetics of ZSM-5 crystallization, as well as the properties of the resulting crystals. Notably, we show that TPA/Na and CTA/K are optimal combinations of structure-directing agents that can markedly alter the size, morphology, and aluminum distribution in ZSM-5. Using a combination of experiments and molecular modeling, we explore the use of CTA as an alternative OSDA for zeolite MFI and show that we can achieve smaller crystals (ca. 600 nm) in similar time (< 24 h) as syntheses employing TPA.

In addition to OSDA design, the development of mesoporosity in zeolites has been a long-standing goal in catalysis to alleviate the diffusion limitations imposed by micropores.[5,6] One area of research that has garnered considerable interest, yet is not fully understood, is the rearrangement of zeolite crystals post-synthesis to accommodate mesoporosity. Here, we will present *in situ* observations of intracrystalline mesoporosity in USY zeolite (FAU type) assisted by CTA using atomic force microscopy. Our findings capture in real time the structural, morphological, and textural evolution of initially rough crystals to smooth crystals with a uniform distribution of mesopores.

(1) Choi, M et al. *Nature* 461 (2009) 246–249

(2) Chawla, A et al. *Mol. Syst. Des. Eng.* 3 (2018) 159-170

(3) Meng, L.; Mezari, B.; Goesten, M. G.; Hensen, E. J. M.; *Chem. Mater.* 29 (2017) 4091–4096

(4) Moteki, T.; Keoh, S. H.; Okubo, T.;*Chem. Commun*. 50 (2014) 1330–1333

(5) Sun, J.; C. Bonneau, et al. *Nature* 458 (2009) 1154

(6) Chawla, A et al. *Chem. Mater.* (2019) In Press

3. Deconvoluting the Role of Active Sites in MWW-type Zeolite Catalysis

Deependra Parmar, Seunghyeok Cha, Lars C. Grabow, and Jeffrey D. Rimer*
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The topology of zeolite pores can have a profound impact on the performance of zeolite catalysts in numerous commercial processes.[1] The landscape of active sites among the ca. 250 zeolite frameworks can be markedly different owing in large part to confinement effects within their channels and cages. Here, we present studies of the MWW framework, which is used as a commercial catalyst for various alkylation reactions. MWW-type zeolites consist of three independent pore systems: supercages, 10-ring sinusoidal channels, and surface pockets. Since these pore systems have different topologies, they are expected to show different activity and selectivites; therefore, deconvoluting their role(s) in reactions offers a route to optimizing catalyst performance.

Using a model reaction, deconvolution has been done by selectively deactivating the active sites in specific pore systems (i.e. supercages and surface pockets), and then comparing their activity with the fresh catalyst. Deactivation of active sites in supercages has been done by pre-coking the supercages by established procedures.[2] Active sites in the external surface pockets were deactivated by depositing an amorphous silica layer on the external surface.

Our findings indicate that active sites in supercages are often the first to be deactivated during early time on stream. This allows for shape-selective catalysis within the medium-sized sinusoidal channels, leading to distinct changes in product selectivies at later reaction times. Collectively, these studies reveal new insights into the role of active sites for MWW-type zeolites to help guide the rational design of microporous catalysts.

(1) Shen, Y. et al. Deconvoluting the Competing Effects of Zeolite Framework Topology and Diffusion Path Length on Methanol to Hydrocarbons Reaction. *ACS Catalysis* 8, (2018) 11042-11053.

(2) Laforge, S., Martin, D., Paillaud, J. & Guisnet, M. m-Xylene transformation over H-MCM-22 zeolite: 1. Mechanisms and location of the reactions. *Journal of Catalysis* 220, (2003) 92-103.

4. Covalently Functionalized Uniform Amino-Silica Nanoparticles: Synthesis and Validation of Amine Group Accessibility

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Silica nanoparticles with grafted organic functional groups have been extensively studied due to applications such as separations, catalysis, pharmaceuticals, and thin films. However, the majority of the functionalized particles have a significant size increase compared with pristine particles. In a typical synthesis of uniform spheres, tetraethylorthosilicate is reacted with ammonium hydroxide forming nanoparticles that immediately aggregate and are very difficult to subsequently redisperse. To avoid this, amino acid capping groups, such as L-lysine, have instead been used as a base catalyst during synthesis which results in a transparent solution with monodisperse silica spheres around 10 nm in diameter. Applications of these particles could significantly expand by adding covalently bound organic functionalities while maintaining monodispersity, small diameter, and colloidal stability in a wide range of solvents.

In this work, amine functional groups were post-synthetically grafted onto monodispersed silica nanoparticles initially synthesized with L-lysine. The grafted particles could then be resuspended in water up to a concentration of 20 mg/mL while maintaining monodispersity. Particle grafting was completed by precipitating the aqueous suspended particles then transferring to acetonitrile. The particles could then be resuspended with the addition of trifluoroacetic acid and sonication. Amine grafting was then completed with 3-aminopropyldimethylethoxysilane and the resulting particles could be transferred to an aqueous acidic solution. The average diameter was found to be 25 nm by dynamic light scattering, transmission electron microscopy, and small-angle X-ray scattering. The amine grafting was confirmed and quantified by ninhydrin assay with loading calculated to be about 0.2 mmol amine/g silica. The amine grafted nanoparticles were then used to analyze organic acid-amine binding with a suite of solution NMR techniques. It was found that the organic acid hydrophobicity and alkyl chain length was the main factor in binding quantity and strength, which could be determined through analysis of molecular relaxation times and exchange rates. This technique could also be used to analyze many molecular binding/reactions that occur at a functionalized particle interface.

5. Controlling Silicon and Aluminum Zoning in ZSM-5 for Improved Performance in the Methanol-to-Hydrocarbon Reaction

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Methanol-to-hydrocarbon (MTH) is an increasingly important process in petrochemical production from alternative sources. A key factor for improving MTH catalyst performance lies in the design of zeolite catalysts. In recent years, significant efforts have been directed to tailoring the morphology and size of zeolite crystals as a means of improving their mass transport properties and catalytic performance[1,2]; however, less attention has been paid to the control of broad spatial distribution of Al. The aforementioned non-homogenous distributions of Al is known as the zoning phenomena. Al zoning – Al is preferentially concentrated in the exterior rim of zeolite crystals was first reported in large ZSM-5.[3] In contrast, Si zoning – Si is enriched in the exterior rim of ZSM-5 crystals, is less common, but has been reported in prior studies.[4] The latter has been a focus of catalyst design as one major factor influencing MTH catalyst performance is the external surface (S_{ext}) acid sites. Reactions at S_{ext} sites are non-shape-selective[5] and can lead to external coking, i.e., pore blockage due to formation of polyaromatic molecules.[6] An approach to passivating external acid sites was patented by Mobil in 1978[7], followed by various methods of chemical vapor deposition.[5] In this work, we developed a novel strategy to control broad spatial distribution of Al in ZSM-5, and justified the importance of this ability in zeolite catalyst design by illustrating the dominant effect of spatial distribution of Al on MTH performance, evidenced by the significantly improved catalytic lifetime observed for Si-zoned ZSM-5.

(1) Choi M. et al.; *Nature* 461 **(2009)** 7261

(2) Zhang X. et al.; *Science*.336 **(2012)** 6089

(3) von Ballmoos, R. and Meier, W.M.; *Nature* 289 **(1981)** 5800

(4) Aramburo, L.R. et al.; *Chemistry – A European Journal* 17 **(2011)** 49

(5) Reitmeier, S.J. et al.; *J. Phys. Chem. C* 113 **(2009)** 34

(6) Bjørgen, M. et al.; *J. Catal.* 249 **(2007)** 2

(7) Rollmann, L.D.; Mobil Patent **(1978)**

6. First-principles Kinetic Monte Carlo Study of Biomass Conversion over Titania Supported Ruthenium Catalyst

Xiao Li and Lars Grabow*
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Catalytic upgrade of bio-oil to fuels and chemicals requires the selective reduction of its 10-40 wt% oxygen content.[1] Ruthenium supported on titania (Ru/TiO_2) has recently evolved as one of the better performing catalysts for such hydrodeoxygenation (HDO) processes. Commonly proposed HDO mechanisms on oxide containing materials invoke oxygen vacancy sites as catalytically active sites, but the mechanism of their formation remains disputed.

To address this question, we use first-principles kinetic Monte Carlo (kMC) simulations to investigate the HDO reaction of m-cresol over TiO_2(110) in the presence and absence of Ru, with particular focus on the Ru/TiO_2 interface. To eliminate the strong effect of Lewis acid-base pairs on adsorbate-adsorbate interactions, we extract pairwise interaction parameters from a series of co-adsorbed configurations that do not exhibit any electronic artifacts on rutile TiO_2(110). Our kMC results show that the presence of Ru nanoparticles substantially increases the reduction rate of the TiO_2(110) surface attributed to H spillover and a facile, heterolytic H_2 cleavage pathway across the Ru/TiO_2 interface. We also qualitatively reproduce experimental results for water adsorption on TiO_2(110). Under HDO reaction conditions over Ru/TiO_2, the Arrhenius plot exhibits two kinetic regimes at low and high temperatures, corresponding to a coverage transition occurring at around 550 K. The presence of added water in the feed impedes this reaction pathway though vacancies by rapid water dissociation on vacancies, resulting in two hydroxyl groups. Alternatively, we propose proton-assisted HDO reactions occurring at the interface.

Overall, our detailed simulation is capable of capturing coverage effects and mechanistic changes in response to variations in temperature or feed composition, including the addition of water to the feed. To our knowledge, there exist no comparable model with the ability to discriminate between metal, oxide and interfacial activity, and assign a dominant catalytic role to each component. The ability to generate such detailed fundamental insight can be leveraged for the future design of multifunctional catalysts with unprecedented selectivity advantages.

(1) Mortensen, P. M. et al. *Appl. Catal. A: General* **(2011)** 407, 1-19.

7. Tuning Selectivity in the Oxidative Dehydrogenation (ODH) of Ethane over Well-Defined Metal Oxide Catalysts by Controlling Non-Stoichiometric Oxygen Density

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Oxidative dehydrogenation (ODH) of ethane over metal oxides catalysts is an economically attractive alternative to the steam cracking of ethane,[1] with bulk nickel-based oxides, including Ni-Nb-O, Ni-Ce-O, and Ni-W-O emerging as ODH catalysts.[2] Nickel oxide ($Ni_{1-x}O$) possesses nickel vacancies as the predominant defect are proposed to be catalytic relevant structure.[3] Systematic control over the non-stoichiometry of nickel oxide-based catalysts is essential for understanding the C-H activation chemistry on the oxide surface and achieving high selectivity during oxidative dehydrogenation (ODH) of ethane.

In this study, we demonstrate that the ethylene selectivity is positively correlated with the non-stoichiometric oxygen density, which can be tuned by calcining nickel oxides at different temperatures. Nickel oxide was synthesized via a molten salt route (MSR) by decomposing nickel nitrate in the alkali salt media, and the resultant crystals exhibited well-defined, cubic morphology which remained stable up to 1200 °C. The degree of non-stoichiometry is determined by UV adsorption spectra, and the surface and bulk excess oxygen is quantitatively determined by temperature-programmed desorption (TPD) and reduction (TPR). The effect of treatment temperature on nickel oxide ODH performance was assessed. Ethylene selectivity decreased monotonically with increasing treatment temperature, suggesting a positive correlation between non-stoichiometric oxygen density and ethylene selectivity. This finding demonstrates that thermal treatment can be used to tune kinetic performance of bulk oxide catalysts, with implications for a variety of transition metal oxide catalysts for selective oxidation reactions.

(1) Cavani, F., Ballarini, N., & Cericola, A,; *Catalysis Today,* 127(1–4), **(2007)** 113–131

(2) Gärtner, C. A., Veen, A. C. Van, & Lercher, J. A. *ChemCatChem*, 5 **(2013)** 3196–3217

(3) Heracleous, E., & Lemonidou, A. A. *Journal of Catalysis*, 237(1), **(2006)** 162–174

8. Theoretical Investigation of Electrochemical Stability of 2-Phenylethanethiol on Au Surfaces

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A new trend in research on the electrochemical CO_2 reduction (CO_2RR) is the use of organic molecules, particularly organothiols, to modify electrodes such as Au in order to alter the activity and selectivity of the reaction. Recently it has been shown that among others, 2-phenyethanethiol (2-PET) adsorbed on polycrystalline Au can make Au more active and achieve greater Faradaic efficiency for CO evolution than blank Au, and contrary to conventional wisdom, a majority of this ligand persists on the Au surface down to -1 V_{RHE} as evidenced by ATR-IR.[1] To better understand this intriguing electrode system, we theoretically investigate the electrochemical stability of 2-PET adsorbed on Au using density functional theory (DFT) calculations as it would directly influence any surface-based CO_2RR mechanisms. Different states of 2-PET and different adsorption sites are considered and modeled. A surface Pourbaix diagram is constructed for 2-PET on Au surfaces based on the DFT results, which sheds light on observed electrochemical desorption process and on the nature of the surface 2-PET states that affects CO_2RR.

(1) Fang, Y.; Cheng, X.; Flake, J. C.; Xu, Y. *Catal. Sci. Technol.* 9 (2019) 2689.

9. Enhanced Surface Activity of MWW Zeolite Nanosheets Prepared by a One-Step Synthesis Method

Yunwen Zhou[1], Yanyu Mu[2], Ming-Feng Hsieh[1], Bernd Kabius[2], Robert M. Rioux[2], and Jeffrey D. Rimer[1*]
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Zeolites are shape-selective microporous crystals that have been widely used as heterogeneous catalysts in petroleum and chemical industries.[1] However, pore dimensions (4 – 7 Å) of typical zeolites often encounter diffusion limitations, especially in applications that involve bulky molecules. MCM-22 (MWW type) zeolite exhibits properties that improve mass transport by providing accessible acid sites on or near its external surface.[2] Conventional layered MCM-22 precursors lead to the direct condensation of MWW layers during calcination, sacrificing significant accessibility to surface acid sites. In our studies, we have demonstrated a novel approach to obtain disordered MWW-type material with high external surface acid sites via a commercially viable single step protocol.

Disordered MCM-22 was obtained in a one-pot synthesis using a cationic modifier to disrupt the natural alignment of MWW layers. A series of catalysts were prepared with varying Si/Al and a range of layer disorder to assess the degree of impact of external surface area on catalytic performance. Scanning electron micrographs reveal stark differences in the morphology and thickness of ordered and disordered zeolites. Cryo transmission electron microscopy quantified the thickness dependence of the MWW crystallites as a function of cationic surfactant concentration; the control sample (no surfactant addition) were on average a factor of 6-7 times thicker than MWW synthesized in the presence of maximum cationic surfactant, which were mono- or bilayered unit cell. The packing structure of MWW materials and their interlayer distances can be identified from powder XRD patterns in the range $2\theta = 6 - 10°$. The degree of disorder was quantified by the disorder index, which is defined as the ratio between external and total surface areas (varying from 0.3 to 0.7 for ordered and disordered materials, respectively). The impact of modifiers on Al incorporation into disordered MWW materials was explored by solid state 27Al NMR measurements and by varying the synthesis gel Si/Al ratio. We observe notable differences in the locations of Al at tetrahedral sites in the frameworks of ordered and disordered MWW samples. We will describe the distinct differences in physicochemical properties of MWW zeolites prepared with a range of surface areas, Al speciation, and total acid content. We will also discuss catalytic studies of H-MWW for Friedel-Craft alkylation of benzyl alcohol with benzene wherein comparisons are made between our one-pot samples and those previously reported by post-synthesis delamination. This study provides a new approach for the one-pot synthesis of disordered MWW with high surface area and tunable Al density and siting. The ability to selectively tailor the physicochemical properties of zeolites allows for the development of structure-performance relationships of microporous catalysts.

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10. A One-Step Encapsulation of Zeolite Microcrystals in Mesoporous Supports

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Due to its shape and size selective pore structure, zeolites are useful catalysts for a variety of chemical transformations. To maximize access to the interior pores of zeolites, microcrystals in the size range 5-30 nm have been synthesized in our laboratories, but these microcrystals cannot be used as such in packed bed reactors and have to be fabricated into catalyst pellets with inert binders. We show a facile one-step procedure to imbed zeolite microcrystals into 1-10 μm mesoporous supports such as MCM-41. The synthesis procedure maintains the ordered 2-4 nm pores of MCM-41 with zeolite microcrystals inserted throughout the mesoporous matrix. The matrix provides structural stability to the zeolite and also provides a sacrificial layer to coking and poisoning very much like catalysts in an egg yolk configuration. Additionally large molecule access through the mesopores of the zeolite surface is evaluated through probe reactions such as the reduction of nitrophenol over metal impregnated ZSM-5 microcrystals. The results indicate the potential of these catalytic composites for a number of reactions including the zeolite catalyzed fast pyrolysis of biomass.

11. Mechanistic Insights into Solution Phase Oxygen Reduction Reaction and Effect of Metal Cation on Reaction Product

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Non-aqueous metal-O_2 batteries with high theoretical gravimetric energy storage density stands to be one of the potential future battery technologies to replace current Li-ion batteries.[1-3] This has led to a surge of interest in fundamental studies of oxygen reduction reaction (ORR) in non-aqueous electrolytes because they are the central electrochemical processes involved at the metal-air cathodes. Fundamental insights into these reactions are critical to further improvement and eventual commercialization of these technology prototypes.

During discharge, the main fundamental reaction involved is ORR which leads to the formation of discharge products. We show that the formation and solvation of O_2^- open up pathways to thermochemical ORR in the solution phase.[4-5] This leads preferentially to the formation of solid Li_2O_2, NaO_2 and KO_2 at low overpotentials. Reaction pathways are proposed for the formation of alkali superoxide and peroxide in several solvents that explain the observed product selectivity. Furthermore, the electrolyte for such batteries may contain metal cations through added salts. We investigate the effect of foreign metal cations (dopants) on the morphology and electronic structure of the solid discharge product, by using evolutionary algorithms coupled with DFT to explore the formation of bulk solids that deviate from the thermodynamic minimum crystalline Föppl structure of Li_2O_2 as the discharge product. the local microstructures may aid in improving electron conduction and hence reduce the high overpotential for OER which the bulk discharge product is associated with in Li-O_2 electrochemistry.

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12. Organic-Free Route for the Synthesis of Hierarchical Zeolite ZSM-11 Catalysts

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There has been an increased interest to identify new commercially viable routes to produce zeolites with well-defined properties. One such approach is the seeded growth of zeolites. Indeed, it is well known that using zeolite as a seed can expedite zeolite crystallization by reducing the induction time and reducing the formation of unwanted impurities. Seeding also provides a route to eliminate expensive organic structure-directing agents (OSDAs) from the synthesis; however, the theory behind seeded growth is still unclear due to the inherent complexity of zeolite crystallization and the vast number of species in synthesis mixtures. Interzeolite transformation involves the use of a parent zeolite with the different framework as seed or as a sole source of silica/alumina, which transforms into a desired daughter structure.

We will present a unique approach to synthesize hierarchical ZSM-11 (MEL framework) with intergrown nanosheets using a seed-assisted route in organic-free media. To the best of our knowledge, this is the first example of such a complex morphology for a MEL-type zeolite synthesized in the absences of organic structure-directing agents. A recent study by our group has shown that the reduction in HZSM-11 crystal size from 750 to 150 nm significantly extends the time-on-stream (TOS) lifetime in MTH reactions. Ongoing tests of hierarchical HZSM-11 catalysts prepared with a range of properties (e.g., crystal size and Si/Al ratio) are being conducted with the long-term goal to develop more generalized structure-performance relationships in zeolite catalysis.

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13. Effects of Alkaline Earth Cations in the Rational Design and Synthesis of Zeolites

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Zeolites are microporous aluminosilicates that have been widely used as commercial heterogeneous catalysts, adsorbents, and ion-exchange materials due to their unique porosity, acidity and hydrothermal stability. There are currently over 230 known zeolite framework types, and the vast majority of these structures are prepared synthetically under hydrothermal conditions in alkaline media, involving the use of organic structure-directing agents (OSDAs) that mediate the assembly of channels and cages within the porous network of zeolite crystals.[1] Due to the economic and environmental disadvantages of these organics, it is desirable to synthesize zeolites in the absence of organics, but reportedly less than 15 % of zeolite structures have been made in OSDA-free syntheses.[2] Here, we present a study of parameters that influence zeolite crystallization by developing ternary kinetic phase diagrams with respect to the molar composition of primary synthesis components. Moreover, we systematically introduce multivalent ions (e.g. alkaline earth cations) in syntheses, aiming to explore facile and cost-efficient methods to obtain crystal structures without the aid of OSDAs. Our findings reveal that the encapsulation of alkaline earth cations has a remarkable impact on the kinetics of zeolite crystallization (i.e. dramatically reduced times of synthesis) and can effectively tune the formation of zeolite frameworks under mild synthetic conditions (e.g. reduced temperatures). Here, we will present the results of this work, including the introduction of ternary (kinetic) phase diagrams that quantitatively illustrate pure-phase and multi-phase regions of zeolite structures.

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14. Siloxide Podand (SiP) Ligands as a Scaffold for Group VI Catalyzed Alkyne Metathesis and Isolation of a Rare and Dynamic Metallatetrahedrane Intermediate

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Triphenylsiloxide is one of the most successful ancillary ligands for Mo(VI)-alkyne metathesis catalysts. I was proposed that flexible siloxide ligands allow Mo-O-Si bond angles to modulate the electrophilicity of the Mo≡C and thereby promote the catalysis. Introduction of a siloxide podand ligand allows for eludication of the ligand flexibility and the Mo-O-Si angles on the electrophilicity of Mo≡C. The podand also allowed for the islation of a rare metallatetrahedrane of Mo, which was found to be dynamic in solution.

15. Mechanistic Understanding of H_2 Activation across the Au/TiO_2 Interface to Elucidate the Differences in Alkyne and O_2 Hydrogenation Rates

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Preferential oxidation of CO (CO PrOx) and selective alkyne hydrogenation are two industrially important processes involving H_2 in their feed streams. CO PrOx is potentially useful for purifying hydrogen streams from methane steam reforming, due to its improved energy efficiency relative to methanation. Recent studies have shown that the selectivity of Au catalysts towards CO oxidation can be enhanced by poisoning the H_2 activation sites at the metal-support interface (MSI).[1,2] Selective hydrogenation of alkynes in polyolefin feedstocks to alkenes is an important step in the plastics industry to prevent deactivation of the downstream polymerization catalyst. Both reactions are generally considered to be hydrogen coverage limited; however we have observed significantly lower reaction rates for 1-octyne hydrogenation (relative to H_2 oxidation) on the same Au/TiO_2 catalyst.

We explain this phenomena with the help of density functional theory (DFT) calculations. The DFT calculations show heterolytic H_2 activation at the MSI, which results in a support proton and a formal gold hydride, is the most energetically favorable pathway for H_2 activation on Au/TiO_2. The gold hydrides generated by H_2 activation near the interface were shown to be less stable than the support protons, thus resulting in a spillover to the support.[2] Thus the H_2 activation near the interface, either homolytically on just gold sites or heterolytically across the interface would lead to spillover of gold hydrides onto the support resulting in low hydride coverage on gold. The addition of support protons to O_2 is facile, facilitating the use of protons generated by H_2 activation near the interface. Whereas in the case of alkyne hydrogenation, the calculated barriers for proton addition to propyne are twice those of the barriers for hydride addition, suggesting that the hydride addition is the preferred pathway for alkyne hydrogenation. Thus, H_2 activation near the interface which results in support protons because of spillover does not help the alkyne hydrogenation. The relatively strong binding reported for 1-octyne to the support and the Au/TiO_2 interface is also one of the factors that likely limits the role of the interface sites as active sites for hydrogen activation during alkyne hydrogenation.[3] To verify the DFT predictions we performed a particle size study, where we measured the H_2 oxidation and 1-octyne hydrogenation rates on catalysts with different gold particle sizes. For 1-octyne hydrogenation, the turnover frequencies (TOF) were the same between different particle sizes when they were based on surface sites. While for H_2 oxidation, the TOF were the same when they were based on perimeter sites. This is in agreement with the predictions from DFT that the surface gold sites are the active sites for 1-Octyne hydrogenation and the Au/TiO_2 interface sites are the active sites for O_2 hydrogenation.

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16. Impact of Copper Exchange Protocol on Cu-CHA SCR Activity

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One of the major milestones in environmental catalysis is the abatement of environmentally harmful compounds such as hydrocarbons, nitrogen oxides (NO_x), sulfur oxides (SO_x) and carbon monoxide, produced by automobiles and power sources. The discovery of Cu-CHA as a catalyst for selective catalytic reduction (SCR) of NO_x was a breakthrough and lead to a rapid commercialization of the technology for the "lean-NO_x" emissions control. It is a relatively new technology and requires more research on identification of active sites of the catalyst in order to develop next generation catalysts with improved performance, enhanced stability and low cost.

There have been considerable research and progress in molecular-level understanding of the nature of active Cu species and the SCR reaction mechanisms. Unfortunately, many studies were conducted using Cu-CHA prepared via different synthesis methods. Current work investigated several common methods of preparation of copper exchanged zeolites reported in the literature and the NO_x SCR activities were examined using a packed bed flow system. The SCR activities of each sample were considerably different at lower temperature that is relevant to the "lean-burn" engine operational temperature. The differences between catalysts prepared via different protocols were further studied by CO adsorption experiments where it was revealed that each protocol results in different copper species within the zeolite framework. DFT calculations were coupled with CO adsorption spectrum and catalytic results to identify active sites. The poster will show synthesis, characterization and catalytic testing details and results.

17. Computational Study of Carbonate Assisted Electrochemical Methane Activation Using Density Functional Theory

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While being an abundant resource in the U.S., methane has very strong C-H bonds, which makes it energy consuming to be activated. Thus, the development of efficient catalysts to upgrade methane to higher value products is both, challenging and very desirable. Two major issues that current catalysts are facing are that high temperatures (up to 900 K) are required, and the lifetime of the catalysts is limited due to sintering and coking. Inspired by the work of Spinner and Mustain1 we aim to address these challenges and pursue a novel low temperature process, which leverages the use of an electrochemical cell to convert methane to methanol.

The envisioned process uses carbonate anions (CO_3^{2-}) that are produced from CO_2 and O_2 at the cathode and transferred to the anode through an electrolyte. At the anode, carbonate ions serve as activator for methane and the transfer of a single oxygen atom can selectively oxidize methane to methanol. The fact that carbonate anion reduction leads again to CO_2, which readily desorbs into the gas phase, is considered a key advantage of the proposed electrochemical process. By simultaneously controlling the concentration of CH_4 at the anode and the rate of CO_3^{2-} delivery by adjusting the cell potential and current density, we anticipate that the over-oxidation of methane can be prevented, such that a high yield of methanol can be achieved.

To obtain fundamental insight into the feasibility of such process, we have performed density functional theory (DFT) calculations on Ni(111) in VASP and explicitly accounted for the effects of external electric fields. Our results show that the interaction between the adsorbates and the surface forms dipole in between. The external electric field has less impact on the binding energy of the intermediates when there is weak dipole and vice versa. Hence, the reaction enthalpy and activation energy of certain elementary steps exhibit a strong dependence on the applied electric field. We have quantified the electric field effect for two distinct reaction pathways and postulate that a properly tuned electric field can guide the reaction to proceed in the desired direction. While the development of a viable process remains in its early stages, our results suggest that a tunable electric field in an electrochemical cell offers unique advantages for selectively upgrading methane to value-added products.

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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 - 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_4 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).**