PURDUE UNIVERSITY

Davidson School of Chemical Engineering

GSO

29th Annual Graduate Research Symposium

Abstracts

August 20th 2020

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Preface

It is with great pleasure that I welcome you to the Davidson School of Chemical Engineering for the 29th Annual Graduate Research Symposium. Despite shifting Symposium virtually, we still would like to preserve this event's long history of strengthening the relationships between our department and industry, and your virtual attendance and presence today continues this tradition. Our senior graduate students benefit greatly from the feedback they receive from our industrial partners and become better prepared for the hiring process as a result.

Furthermore, your financial contributions help to support the Graduate Student Organization's mission of building a flourishing and enriching community for our students. With your generous support, we are able to host a variety of professional development, service, and social events, ranging from teaching local third graders after-school science lessons and conducting highway cleanups to hosting Jeopardy and boardgame nights.

We hope you take this opportunity to listen to the oral presentations from our graduate students and help them with the important transition from academia to industry. We also encourage you to spend some time viewing the virtual elevator pitch sessions to become more familiar with the research of our rising graduate students.

I would like to personally extend my sincere gratitude to all in attendance today. Your continued support is greatly appreciated by the graduate student body, and we look forward to a continued partnership in the years to come.

Wei-Lee Wu

President, Graduate Student Organization

2020-2021

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Sydney Scheirey .....Presentation Coordinator

Daniel Hayes .....Judging Coordinator

Apurva Pradhan ..... Industrial Packet Coordinator

Carly Battistoni ..... Industrial Liaison Head

Jonathan Turnley .....Slack Coordinator

Daniel Gribble .....Slack Coordinator

Schedule of Events

Thursday, August 20, 2020

8:30AM – 12:00PM	**Student Research Seminars** *Davidson School of Chemical Engineering* *Session A – Room G124* *Session B – Room B124*
12:45PM – 2:30PM	**Poster Showcase** Davidson School of Chemical Engineering *Virtual*
3:15PM – 4:15PM	Keynote Address **Dr. Upma Sharma** **President of Arsenal Medical** *Davidson School of Chemical Engineering* *FRNY G140*

Keynote Speaker

Dr. Upma Sharma, PhD
President and CEO
Arsenal Medical

Webex Link
Meeting Number: 120 393 1394
Password: catdog68

Dr. Upma Sharma is President and CEO of Arsenal Medical. She has led Arsenal's lead product, ResQFoam, from concept to the clinic, including management of the product development process, establishment of GMP contract manufacturing, and receipt of a FDA IDE approval. Previously, at Lyra Therapeutics, Upma advanced the company's innovative drug delivery depot from concept through a Phase I clinical study. Under Upma's leadership, Arsenal Medical and Lyra Therapeutics have been awarded more than $50M in government funding to support product development efforts. Upma earned a Ph.D. from Princeton University in Chemical Engineering and a B.S.E. from Purdue University. During a post-doctoral fellowship in Bioengineering at Rice University, Upma was awarded a NIH Training Grant in Nanobiology. Upma has authored more than 20 peer-reviewed scientific publications and is an inventor on more than 40 issued or pending patents worldwide, including 20 US issued patents.

Student Research Seminar Schedule

Session A – Room G124

Webex Meeting Room

Meeting ID: 120 369 7909 **Password:** catdog68

8:30 AM – 8:50 AM	**Influence of Copper Site Structure and Proximity in Cu-CHA Zeolites on Partial Methane Oxidation to Methanol** Laura Wilcox *Prof. Rajamani Gounder*
8:55 AM – 9:15 AM	**Structural Interconversion Between Agglomerated Pd Domains and Isolated Pd Cations in Chabazite Zeolites** Trevor Lardinois *Profs. Rajamani Gounder and Fabio H. Ribeiro*
9:20 AM – 9:40 AM	**Effects of Dioxygen Pressure on Rates of NO_X Selective Catalytic Reduction with NH_3 on Cu-CHA Zeolites** Casey Jones *Profs. Rajamani Gounder and Fabio Ribeiro*
9:45 AM – 10:05 AM	**Pyrolysis-based processing of biomass and shale gas sources for the production of chemicals and fuels** Abhijit D. Talpade *Prof. Fabio Ribeiro*
10:10 AM – 10:30 AM	**Density Functional Theory Analysis of Conversion of Light hydrocarbons into Fuels and Chemicals** Ranga Rohit Seemakurthi *Profs. Jeffrey Greeley and Fabio Ribeiro*
10:35 AM – 10:55 AM	**Propylene Epoxidation on Au/TS-1: Deconvoluting the Catalytic Contributions of Gold Active Sites** Jeremy Arvay *Profs. W. Nicholas Delgass and Fabio H. Ribeiro*
11:00 AM – 11:20 AM	***Designing Multi-functional Catalyst Models using First Principles and Machine Learning*** Pushkar Ghanekar *Prof. Jeffrey Greeley*
11:25 AM – 11:45 AM	**Understanding selectivity in NO electroreduction on Pt_3Sn alloys via a first principles approach** Siddharth Deshpande *Prof. Jeffrey Greeley*

Student Research Seminar Schedule

Session B – Room B124

Webex Meeting Room

Meeting ID: 120 969 2081 **Password:** catdog68

8:30 AM – 8:50 AM	**The Role of Adhesion and Stiffness on the Sensitivity of Energetic Materials to Vibration and Impact** Jason Wickham *Profs. Stephen Beaudoin and Steven Son*
8:55 AM – 9:15 AM	**Relationship of various interfacial tensions of oil/water interfaces to oil recovery efficiency** Jaeyub Chung *Profs. Bryan W. Boudouris and Elias I. Franses*
9:20 AM – 9:40 AM	**Solution Phase Fabrication of $Cu(In,Ga)(S,Se)_2$ Thin-Film Solar Cells Using Amine-Thiol Solvent System** Swapnil D. Deshmukh *Prof. Rakesh Agrawal*
9:45 AM – 10:05 AM	**Silver Indium Diselenide: An Intriguing Absorber Layer Candidate for Low-Cost, High Efficiency Printable Photovoltaics** David J. Rokke *Prof. Rakesh Agrawal*
10:10 AM – 10:30 AM	**Identifying Energy-Efficient Distillation Configurations: Advances in Modelling and Optimization** Tony Joseph Mathew *Prof. Rakesh Agrawal*
10:35 AM – 10:55 AM	**Electrohydrodyanmic Equatorial Streaming** Brayden Wagoner *Profs. Osman A. Basaran and Michael T. Harris*
11:00 AM – 11:20 AM	**Green Synthesis of Metal Nanorods Exploited Novel Biological Templates: Barely Stripe Mosaic Virus Virus-Like Particles** Yu-Hsuan Lee *Prof. Michael T. Harris*

Influence of Copper Site Structure and Proximity in Cu-CHA Zeolites on Partial Methane Oxidation to Methanol

Laura N. Wilcox

Prof. Rajamani Gounder

Copper-exchanged zeolites have received renewed attention as materials that facilitate partial methane oxidation (PMO), with many proposals for the structure of the active site that include mononuclear and polynuclear Cu species [1-3]. We interrogate Cu-zeolites with well-defined Cu speciation and proximity, prepared using judiciously chosen synthetic and treatment procedures, to facilitate identifying PMO active sites. The distribution of framework Al (Al–O(–Si–O)$_x$–Al) between isolated ($x \geq 3$) and paired ($x = 1,2$) arrangements in CHA influences the speciation of Cu^{2+} at paired Al sites (Z_2Cu) and $[Cu(II)OH]^+$ at isolated Al sites (ZCuOH) [4]. Here, we synthesized Cu-CHA to contain only Z_2Cu (Si/Al=4.5, Cu/Al=0.08, 0.21) or ZCuOH sites (Si/Al=15-25, Cu/Al=0.06-0.30) of varying density, or a mixture of Z_2Cu and ZCuOH sites (Si/Al=15-25, Cu/Al=0.10-0.40). The number of Z_2Cu and ZCuOH sites on each sample was consistent with the direct quantification of residual Brønsted acid sites with NH_3, given 2:1 or 1:1 H^+:Cu^{2+} exchange stoichiometry [4]. This suite of Cu-CHA samples was studied for stoichiometric PMO reaction cycles (oxidative treatment: 20 kPa O_2, 723 K, 6 h, methane exposure: 21 kPa CH_4, 473 K, 0.5 h, methanol extraction: 2.5 kPa H_2O, 473 K, 1 h). Methanol yields (per Cu) do not depend systematically on total Cu or Z_2Cu content but increase systematically with ZCuOH density. ZCuOH sites are precursors to polynuclear Cu-oxo structures that form after O_2 treatments [5] and behave as PMO active sites [6]. *In-situ* X-ray absorption spectroscopy showed that inert (He, 723 K) and reducing (CH_4, 473 K) environments led to increasing fractions of Cu(I) with ZCuOH density. *In-situ* UV-Visible spectroscopy identified mononuclear Cu^{2+} species from d-d transitions (~8,000-16,000 cm^{-1}) and binuclear Cu^{2+} di-oxo from LMCT (24,000-30,000 cm^{-1}), and spectral changes were monitored while reducing Cu di-oxo species by CO (523 K) [5] and CH_4 (473 K). O_2 activation of Cu-CHA forms bis(μ-oxo) dicopper(II), trans-1,2-peroxo dicopper(II), and μ-(η^2:η^2)peroxo dicopper(II) intermediates identified by Raman spectra, whose assignments were confirmed with computational modeling. Multivariate curve resolution-alternative least squares was used to extract time-resolved contributions from Raman spectra to investigate O_2 activation kinetics, which reveal two Cu site types with distinct kinetic behavior.

References:

[1] Ipek, B. et al., ACS Catal., 2017, 7, 4291.

[2] Grundner, S. et al., Nature Comm., 2015, 6, 1.

[3] Ravi, M. et al., Angew. Chem. Int. Ed., 2017, 56, 16464.

[4] Paolucci, C. et al., J. Am. Chem. Soc., 2016, 138, 6028.

[5] Li, H., et al., Chem. Sci., 2019, 10, 2373.

[6] Pappas, D. K. et al., J. Am. Chem. Soc., 2017, 139, 14961.

Structural Interconversion Between Agglomerated Pd Domains and Isolated Pd Cations in Chabazite Zeolites

Trevor Lardinois

Profs. Rajamani Gounder and Fabio H. Ribeiro

The majority of NOx (x = 1,2) emissions from mobile engine sources occurs during cold-start when exhaust aftertreatment systems are below (<450 K) their effective operating temperature window. Incorporating palladium-exchanged zeolites in the aftertreatment system can help mitigate cold-start NOx emissions by passively adsorbing NOx at low temperatures and desorbing NOx once downstream catalytic converters function effectively. Isolated Pd cations are the purported precursor sites to store NOx, rather than agglomerated PdO or metallic Pd domains. Yet, the influence of post-synthetic treatments and zeolite material properties on the interconversion between cationic Pd^{2+} and agglomerated Pd species remain incompletely understood. Here, a combination of spectroscopic (in situ diffuse reflectance UV-Visible, X-ray absorption, infrared) and site quantification (H_2 temperature programmed reduction) techniques were used to quantify the distribution of cationic and agglomerated Pd species as a function of treatment conditions and material properties.

After ion-exchange or incipient wetness impregnation methods to introduce Pd-amine precursors onto zeolite supports, they contain predominantly isolated $[Pd(NH_3)_4]^{2+}$ complexes. During subsequent air temperature treatments intended to remove NH_3 ligands (473-723 K), in situ formation of H_2 from NH_3 decomposition was observed, causing Pd reduction and agglomeration. Progressive treatments of Pd-exchanged zeolites to higher temperatures (723 to 1023 K) in air increased the extent to which agglomerated Pd domains were converted to exchanged Pd^{2+} cations through a solid-state ion-exchange process. Pd-CHA zeolites (Si/Al = 12, Pd/Al = 0.24) treated in air to 773 K to re-disperse agglomerated Pd metal particles formed after reduction in H_2 (5 kPa H2, 573 K) were found to reversibly form the same number of exchanged Pd^{2+} ions (0.11 Pd^{2+} / Al) after three consecutive cycles. After treatment to 1023 K in air, however, a higher fraction of exchanged Pd^{2+} ions (0.15 Pd^{2+} / Al) was formed, which was also recovered after a subsequent H_2 reduction and lower temperature (773 K) air treatment. These findings demonstrate that Pd-CHA zeolites retain memory of a 1023 K air treatment and suggest higher temperature air treatments facilitate Pd cation exchange more uniformly throughout zeolite crystallites. A series of Pd-CHA zeolites were synthesized with similar bulk Pd and framework Al content (Pd/Al = 0.18, Si/Al = 14) but varying numbers of 6-membered ring (6-MR) paired Al sites (Al-O-(Si-O)x-Al, x=1,2), providing evidence that 6-MR paired Al sites can stabilize exchanged Pd^{2+} cations and nominally isolated Al sites can stabilize $[PdOH]^+$ species (□(OH) = 3656 cm^{-1}). Together, these results help explain the chemical mechanisms responsible for Pd agglomeration and re-dispersion to isolated Pd^{2+} ions and the effects of framework Al siting on the structures of exchanged Pd^{2+}.

Effects of Dioxygen Pressure on Rates of NO_X Selective Catalytic Reduction with NH_3 on Cu-CHA Zeolites

Casey Jones

Profs. Rajamani Gounder and Fabio Ribeiro

The abatement of nitrogen oxides (NO_X, x=1,2) from automotive exhaust remains an important challenge because NO_X will invariably be formed during the combustion of fuels at high temperatures and the presence of atmospheric NO_X, even at low concentrations, is harmful to the environment.[1] The selective catalytic reduction (SCR) of NO_X with NH_3 using Cu-CHA zeolites emerged over a decade ago as the prevalent NO_X abatement strategy for lean-burn diesel engines because of the ability of the catalyst to remain stable after withstanding the harsh hydrothermal environments of automotive exhaust.

The SCR of NO with NH_3 over Cu-CHA zeolites at low temperatures (<573 K) proceeds via a redox cycle of NH_3-solvated Cu^{II}/Cu^{I} ions. At O_2 pressures relevant for practical operation (10 kPa O_2), both $NO+NH_3$-assisted single-site Cu^{II} reduction and O_2-assisted dual-site Cu^{I} oxidation are kinetically relevant steps. Due to the different site requirements for each half-cycle, SCR rates (per g, 10 kPa O_2) show a complex dependence on Cu density, transitioning from an apparent second- to first-order dependence on Cu density with increasing Cu density.[2] Steady-state SCR rates (per Cu, 473 K) measured over a wide range of O_2 pressures (1-60 kPa) on Cu-CHA show a Langmurian dependence on O_2 pressure, enabling the quantification of apparent rate constants that are first- and zero-order in O_2 pressure.[3] *In operando* X-ray absorption spectra are consistent with the kinetically-relevant step transitioning from Cu^{I} oxidation to Cu^{II} reduction with increasing O_2 pressure. First-order rate constants increase systematically with Cu density, consistent with the dual-site requirement for the Cu^{I} oxidation step. Zero-order rate constants increase more gradually with Cu density, primarily reflecting changes in the fraction of Cu ions that are able to participate in the SCR redox cycle. These findings are corroborated by transient Cu^{I} oxidation experiments, which show that both the Cu^{I} oxidation rate and the fraction of Cu^{I} sites that oxidize increase with Cu density. The combination of steady-state and transient kinetic measurements provides a methodology to quantify rate constants that describe the SCR reduction and oxidation half-cycles, and can be used to determine how catalyst properties affect rates of each half-cycle individually.

References:

[1] Cox, L. Nitrogen oxides (NOx) why and how they are controlled. Diane Publishing (1999).

[2] Paolucci, C. et al. Dynamic multinuclear sites formed by mobilized copper ions in NOx selective catalytic reduction. Science 357, 898–903 (2017).

[3] Jones, C. B. et al. Effects of dioxygen pressure on rates of NOx selective catalytic reduction with NH3 on Cu-CHA zeolites. Journal of Catalysis 389, 140–149 (2020).

Pyrolysis-based processing of biomass and shale gas sources for the production of chemicals and fuels

Abhijit D. Talpade

Prof. Fabio Ribeiro

Fast-pyrolysis of biomass to fuels is considered a promising technology due to the higher yields to liquid fuel products, but suffer from carbon losses to bio-char, accounting for 25-40 wt.% of the product stream depending on the biomass type [1]. Using a combination of biomass pretreatments and mass spectrometric analysis coupled with lab-scale reactors, the char contribution from the individual lignocellulosic components, cellulose, hemicellulose, and lignin was found to follow the order: Lignin > Hemicellulose > Cellulose. Addition of inorganic salts (K, Na and Ca) to cellobiose, a model compound for cellulose, was found to catalyze additional dehydration reactions on stable pyrolysis products (e.g., levoglucosan) to yield secondary products (e.g., 5-HMF), and produce more char. This knowledge of char formation contributors, through a combination of pre-treatments and fast-pyrolysis, can enable optimization of the bio-refining process sequencing and thus achieve higher carbon efficiency.

While biomass has been viewed as a future energy source, there is a need for a transition fuel with the lowest possible CO2 footprint. Shale gas, consisting primarily of methane, is a potential candidate due to its large availability. Recently, single-atom catalysts have shown promise as stable and non-coking catalysts for non-oxidative coupling of methane (NOCM) to higher hydrocarbons [2]. This work uses homogenous (Chemkin simulations, gas phase kinetics) and heterogeneous reaction tools (reaction orders, steady state kinetics) coupled with microscopy to understand the role of the solid materials during NOCM. Under similar NOCM conditions (975 0C, Space velocity=30 L hr-1 gcat-1), single-site Pt supported on CeO2 (Pt SAs) and Pt nanoparticles (~2 nm) supported on SiO2 (Pt NPs) show similar ethylene formation rates (TOR=1.5E-03 mol s-1 (mol Pt)-1) (assuming all Pt are active) (methane conversion ~ 1.5 %) and gas phase selectivity to reaction products like ethylene (~60%), ethane (~20%) and higher hydrocarbons. Also, transmission electron microscopy analysis on the post reaction samples reveals that the Pt-based materials (Pt SAs and Pt NPs) sinter to 5-7 nm particles. These results indicate that the single atoms are not active for NOCM. Additionally, power rate law reaction orders with respect to methane, ethylene and hydrogen show similar results for all the non-catalytic and the catalytic systems (nCH4=1, nC2H4=0 and nH2=-0.5), indicating similar NOCM reaction mechanism in these cases. The gas phase reaction mechanism, however, is unable to match the reaction orders obtained experimentally. This indicates that the surface catalyzed reactions are important for NOCM, with the desorption of methyl radical from the surface identified as the rate-determining step. In conclusion, the surface plays a role during NOCM, however, single atoms are not the active sites, negating the claims in the literature.

References:
[1] D. Carpenter et al., Green Chemistry. 16 (2014) 384-406
[2] X. Guo et al., Science. 344 (2014) 616-619

Density Functional Theory Analysis of Conversion of Light hydrocarbons into Fuels and Chemicals

Ranga Rohit Seemakurthi

Profs. Jeffrey Greeley and Fabio Ribeiro

The recent shale gas boom led to large abundance of light alkanes, especially ethane and propane. These low value alkanes can be converted to higher value alkene products through dehydrogenation and oligomerization processes. However, the shale reserves are highly dispersed across US, hence transporting the alkanes to a centralized facility is both difficult and costly. The vision with the CISTAR [1] is to transform the alkanes to higher value alkene products locally using modular plants. This mandates the catalysts to be highly selective and stable to minimize the separation processes upstream. Therefore, this study focuses on molecular understanding of the dehydrogenation reactions on alloy catalysts and oligomerization on metal exchanged zeolite catalysts, using DFT and microkinetic modeling, with the aim of obtaining structure-property relationships towards selectivity and stability of the materials.

Non-oxidative propane dehydrogenation (PDH) on intermetallic alloys is a promising technology to convert the propane available in the shale gas to propylene. We focus, in particular, on PdIn alloys, for which the experimental results from our collaborators have shown to have high selectivity to propylene. Through this analysis, the step surfaces of 1:1 alloys are found to be highly active than terraces (5 orders of magnitude higher rates), while maintaining the high propylene selectivity. Moreover, a comprehensive microkinetic analysis along with the simplified rate analysis pointed to useful descriptors for activity, selectivity and stability. To test the validity of the computationally obtained selectivity descriptors, catalytic experiments were performed on a series of intermetallic Pd alloys [2] (Pd_3Fe, Pd_3Mn, Pd_2Ga, and PdZn). The comparisons with experiments show that the selectivity descriptor could qualitatively distinguish between the highly selective 1:1 alloys, with the partly less selective 3:1 alloys which have 3-fold Pd ensembles. With these descriptors as a starting point, the high-throughput screening of intermetallic alloy structures, including both steps and terraces, is being performed to identify reactivity trends across active alloys for PDH and, ultimately, find improved catalysts for this chemistry.

The olefins (ethylene, propylene) formed from direct dehydrogenation reactions can be converted to higher molecular weight linear alpha olefins on Ni exchanged zeolite (BEA) catalysts. With the help of DFT and AIMD methods, the active site structure and reaction mechanism for ethylene dimerization on Ni-BEA has been studied. Furthermore, microkinetic analysis was used to predict the isomer distribution of the products. Finally, the effect of pressure has been studied by increasing the ethylene coordination on Ni^{2+}, which showed increased mobility of the Ni complex inside the framework. The mechanistic implications of increase in ethylene coordination, on isomerization and deactivation pathways will be discussed.

References:

[1] NSF Center for Innovative and Strategic Transformation of Alkane Resources, cistar.us

[2] Purdy, S.C‡., **Seemakurthi, R.R**‡., *Chemical Science*, 2020, *11*(19), 5066-81. ‡equal contribution

Propylene Epoxidation on Au/TS-1: Deconvoluting the Catalytic Contributions of Gold Active Sites

Jeremy Arvay

Profs. W. Nicholas Delgass and Fabio H. Ribeiro

Propylene oxide is a key ingredient in the industrial production of polyurethane, ultimately leading to a variety of industrial and consumer products such as functional fluids and polymer structural components for vehicles [1]. The presence of allylic hydrogen in propylene necessitates the use of a 'soft' oxidant, such as hydrogen peroxide, to avoid the selective production of acrolein and instead attack across the double bond in propylene to form propylene oxide (PO). Current methods for producing PO involve *ex situ* production of the oxidant and are often unselective and/or generate environmentally hazardous byproducts, whereas Au/Ti catalysts, such as Au/TS-1, allow for the highly selective epoxidation of propylene with an oxidant generated *in situ* from hydrogen and oxygen and offer a potential path to a more efficient and greener process.

Efforts to design and synthesize improved Au/Ti catalysts for propylene epoxidation are largely limited by a lack of understanding of the different roles filled by gold nanoparticles and what makes some better suited for selective propylene epoxidation than others. Although much focus has been given to the effect of Au nanoparticle size on PO production kinetics, some recent studies have focused on using kinetics to differentiate the various Au active sites present under reaction conditions [2] and correlating the prevalence of under-coordinated Au atoms to rates of propylene epoxidation [3]. Although these recent studies suggest that differences in catalytic rates for propylene epoxidation, unselective hydrogen oxidation, and minor C1-C3 byproduct formation can potentially be explained by differences in the populations of differently coordinated Au atoms, the question of whether PO active sites on Au nanoparticles change significantly as a function of nanoparticle size still remains.

To answer this question, we have synthesized Au/TS-1 catalysts with exclusively large Au nanoparticles (>3 nm) and measured the intrinsic reaction orders and activation energy for propylene epoxidation, unselective hydrogen oxidation, and the minor C1-C3 byproducts. We find that the measured kinetic parameters for propylene epoxidation on both large Au nanoparticles and small Au clusters are similar, with both capable of being explained by a 'simultaneous' reaction mechanism requiring Au and Ti active sites to be within molecular distances of one another. Furthermore, the similarity of the PO production rates for both samples, when normalized to estimates of the number of Au atoms with Au-Au coordination numbers less than 7, implies that the intrinsic catalytic rates of the PO active sites for both larger Au nanoparticles and small Au clusters (< 1 nm) are similar and suggest that the significant increase in the catalytic efficiency of Au for small size particles is driven primarily by the increased fraction of undercoordinated gold surface atoms.

References:

[1] Nijhuis et al. / *Ind. Eng. Chem. Res*. 2006, 45, 10, 3447–3459

[2] J.W. Harris et al. / *Journal of Catalysis* 365 (2018) 105–114

[3] X. Feng et al. / *Journal of Catalysis* 317 (2014) 99–104

Designing Multi-functional Catalyst Models using First Principles and Machine Learning

Pushkar Ghanekar

Prof. Jeffrey Greeley

Computational catalyst models have been instrumental in the developing fundamental understanding of structure-function relationships for catalyst materials. These insights have had direct impact in the areas of renewable energy production and storage, production of fine chemicals, and environmental remediation. However, real-world catalysts are known to dynamically respond to the external reaction environment[1]. Water-gas shift reaction is one such chemistry wherein the coverage of carbon monoxide (CO), as determined by gas pressure in the reactor, is expected to have mechanistic implications on the preferred reaction pathway[2]. By combining first-principles calculations and microkinetic modeling we show that explicit consideration of CO interactions at the catalyst interface is central to correctly determining reaction mechanisms, rate determining steps, and reaction orders when compared to experiments. This analysis shows that modeling strategies which incorporate this atomic-scale detail would lead to improved understanding of the underlying structure-catalyst function relationships.

Now, despite having the ability to generate catalyst models for complex chemistries, as shown in the previous case, first-principles based electronic structure optimization routines are ill-suited to virtually screen through all possible catalyst models. Furthermore, the possible configurational space for multi-component catalyst models is especially large when considering adsorbate coverages on the catalyst surface. Adsorbates can occupy various sites on the surface resulting in high configurational degree of freedom. A surrogate model to rank and sequentially identify candidates to perform expensive computational calculations on would prove beneficial when navigating the complex material search space. To this end, we present a machine-learning (ML) based approach to model the complex adsorbate interactions on the catalyst surface. We use a graph theory-based method[3] to convert catalyst surface models to undirected crystal graphs. The crystal-graph allows us to account for the local environment around each adsorbate species thereby incorporating adsorbate-adsorbate interactions implicitly during the model development. Special attention is given to ensure ML model's flexibility with respect to number of adsorbates on the surface, thereby providing a generalized framework to handle variable adsorbate coverage. High coverage configurations of NO on Pt_3Sn are investigated using the crystal-graph ML model with promising reduction in calculation time and low prediction errors.

Understanding selectivity in NO electroreduction on Pt_3Sn alloys via a first principles approach

Siddharth Deshpande

Prof. Jeffrey Greeley

Nitrogen cycle electrochemistry is an upcoming area of interest in the chemical and environmental engineering communities, with applications ranging from removal of nitrates from wastewater streams to the development of fundamental understanding of NO electrochemistry. In spite of a significant amount of fundamental research for this chemistry on single crystal surfaces, however, the mechanistic details of the reactions are not fully known.[1]

In this work, we begin by describing a detailed analysis of the reaction mechanism of NO electroreduction on PtSn alloys. These alloys are of interest because they have been experimentally shown to be selective to products such as hydroxylamine (NH_2OH) in acidic solutions, which is a more valuable product compared to NH_3, the only product formed on pure platinum surfaces. In spite of this interest, however, little is known about the structural and electronic features of the PtSn that cause this selectivity change.[2]

To elucidate these features, we make use of periodic Density Function Theory calculations combined with theoretical electrochemistry analyses. [3] We first present our analysis for low coverages of NO present on the $Pt_3Sn(111)$ surface and derive preliminary conclusions about the reaction mechanism. Subsequently, we introduce an in-house graph theory based tool [4] to efficiently estimate higher coverage structures of adsorbed NO on the $Pt_3Sn(111)$ surface, and we extend the kinetic analysis to the limit of higher NO coverages, resembling the state of a real catalyst under continuous reaction conditions. Further, we compare the mechanistic insights for NO electrochemical reduction on Pt-Sn alloys with that on Pt(111) and Pt(100) surfaces, [5,6] to understand the role of 'Sn' in promoting the selectivity to NH_2OH. We close by suggesting design strategies to tune the selectivity of NO electroreduction to desired products, including N_2 and hydroxylamine, on other transition metals and alloys.

References:

(1) Duca, M.; Koper, M. T. M. *Energy Environ. Sci.* **2012**, *5* (12), 9726–17.
(2) Yang, J.; Kwon, Y.; Duca, M.; Koper, M. T. M. *Anal. Chem.* **2013**, *85* (16), 7645–7649.
(3) **Deshpande, S.**; Greeley, J. *ACS Catal.* **2020**, acscatal.0c01380.
(4) **Deshpande, S.**; Maxson, T.; Greeley, J. *npj Computational Materials* **2020**, *6*, 79.
(5) Chun, H.-J.; Apaja, V.; Clayborne, A.; Honkala, K.; Greeley, J. *ACS Catal.* **2017**, 3869–3882.
(6) Clayborne, A.; Chun, H.-J.; Rankin, R. B.; Greeley, J. *Angew. Chem.* **2015**, *127* (28), 8373–8376.

The Role of Adhesion and Stiffness on the Sensitivity of Energetic Materials to Vibration and Impact

Jason Wickham

Prof. Stephen Beaudoin and Prof. Steven Son

Energetic materials such as propellants and explosives fulfill a variety of roles in addressing modern engineering and scientific challenges. Traditionally, sensitivity of a given energetic material has been characterized by the response to friction, impact, and electrostatic shock. Recent developments including the expectation of operating at more extreme conditions and demands for performance have led to the discovery of a sensitivity to acoustic excitation or vibration. This new excitation mode has been proven to be sufficient to force energetic materials to violently decompose over relatively short timeframes demonstrating an immediate need for the reevaluation of sensitivity testing and the incorporation of designs to mitigate the possibility of rapid unplanned decomposition of energetic materials.

This study aimed to explore the role of adhesion and stiffness as two material properties that might substantially contribute to the heating observed during acoustic excitation. Further impact excitation tests were carried out in order to explore how changing one material property may result in different outcomes in the sensitivity response. High frequency acoustic excitation was provided in the form of ultrasonic excitation and non-shock mechanical excitation was applied via drop weight impact. A variety of polymers were utilized in order to explore a range of elastic moduli and works of adhesion.

Ultrasonic testing demonstrated that elastic modulus and the work of adhesion played no role in of the degree of heating of the samples. As delamination of the material appeared to be the most significant factor for determining sensitivity to ultrasonic excitation, safer energetic materials can potentially be designed by preventing this separation from occurring in the first place. The impact study suggested that stiffer composite energetic materials were more sensitive to impact than more pliable materials which has implications for future energetic material design. The shape of the drop energy vs the sensitivity also suggested that a new mechanism may be responsible for the dramatic change in sensitivity over the range of the tested properties. Ultimately, these facets of sensitivity will need to be addressed and further investigated in order to limit the possibility of an unintentional and violent decomposition event.

References:

[1] Field, J.E., *Hot spot ignition mechanisms for explosives.* Accounts of Chemical Research, 1992. 25(11).

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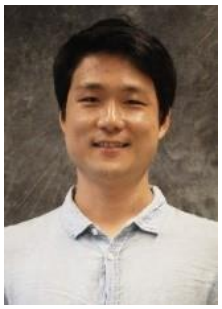

Relationship of various interfacial tensions of oil/water interfaces to oil recovery efficiency

Jaeyub Chung

Professor Bryan W. Boudouris and Professor Elias I. Franses

Enhanced oil recovery (EOR) processes aim to increase the oil production of mature oil fields by using optimized chemical (surfactant/alcohol/polymer) formulations to mobilize trapped oil. It is generally assumed that, for a formulation to be most effective, the interfacial tensions (IFTs) between the aqueous solution, the oil phase, and other possible phases formed (e.g., "middle phase" microemulsions) should be ultralow ($< 10^{-2}$ mN·m^{-1}). Nevertheless, phase behavior tests have received much more attention than developing robust protocols for obtaining IFTs that are relevant for identifying surfactant formulations result in high recovery efficiency. To fill the gap between the importance of IFT and lack of robust protocol for determining IFTs, we define five types of equilibrium IFTs (EIFTs) and developed several robust protocols for evaluating chemical formulations: (i) the un-pre-equilibrated equilibrium IFT ($EIFT_{up}$);[1] (ii) the un-pre-equilibrated EIFTs in the presence of rock ($EIFT_{up,rock}$); (iii) the pre-equilibrated EIFTs ($EIFT_{p}$);[2] (iv) the pre-equilibrated EIFT in the presence of rock and oil ($EIFT_{p,rock}$); and (v) the effluent EIFT ($EIFT_{eff}$). The $EIFT_{up}$ is the EIFT of the aqueous surfactant/brine solution against an oil drop without any pre-equilibration steps. The $EIFT_{up,rock}$ is the EIFT between an oil drop and the pre-equilibrated surfactant solution with a rock sample to consider adsorption losses. Similarly, the $EIFT_{p}$ and $EIFT_{p,rock}$ is the EIFT between the pre-equilibrated water and oil phases from surfactant/brine/oil and surfactant/brine/rock/oil mixtures, respectively. Lastly, $EIFT_{eff}$ is the EIFT from the effluent of the laboratory-scale core flood tests.

Among the five types of EIFTs, the $EIFT_{p,rock}$ was the better parameter for identifying surfactant formulations with high oil recovery performance of core-flood tests than the $EIFT_{up}$, $EIFT_{up,rock}$, and $EIFT_{p}$, because the $EIFT_{p,rock}$ could embrace the most critical surfactant partition processes: partitioning to the oil phases and adsorption losses on the rock surfaces. More specifically, among the three surfactant formulations tested with core-flood experiments, the one that had the lowest $EIFT_{p,rock}$ (~0.01 mN·m^{-1}) had the highest oil recovery ratio (78%), and the one had the highest $EIFT_{p,rock}$ (~0.2 mN·m^{-1}) had the lowest oil recovery ratio (55%). The other EIFTs did not have a strong correlation between the EIFT values and the oil recovery performances. Hence, prior to the core flood tests, it is strongly recommended to identify surfactant formulations that could maintain low/ultralow $EIFT_{up}$ and $EIFT_{p,rock}$, which is relevant to the initial and later stages of the oil mobilization abilities of the injected surfactant formulation, respectively. Therefore, the EIFT values based on the proposed robust protocols can serve as critical parameters to evaluate, screen, and optimize chemical formulations with target field conditions and predict their oil recovery performance in field tests.

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Solution Phase Fabrication of $Cu(In,Ga)(S,Se)_2$ Thin-Film Solar Cells Using Amine-Thiol Solvent System

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Prof. Rakesh Agrawal

$Cu(In,Ga)(S,Se)_2$ (CIGSSe) is one of the high-efficiency thin-film photovoltaic materials with lab-scale cell efficiencies reaching beyond 23%. While such efficiencies have been achieved for vacuum-based batch processes, the solution processing route which has potential for continuous fabrication has demonstrated efficiencies up to 18%.[1] Although this is a promising performance, it involves the use of highly explosive and toxic hydrazine solvent which makes its scalability difficult. While researchers have investigated various non-hydrazine solvent systems, most of them utilize precursors like metal halides, oxides, acetates etc. which could introduce detrimental impurities like O, Cl, Br in the final film.[2] Also, many of these solvent systems produce multilayer film morphologies with the formation of carbon-rich fine grain layer especially when film thickness is increased beyond ~1µm which leads to the reduced current collection in solar cell.[3] To address these issues, amine-thiol solvent system was investigated as a better alternative.

Amine-thiol solvent mixture can dissolve pure metals like Cu, In, Ga, and Se, which provides an opportunity for impurity-free ink formulation. In order to understand the organometallic complexes formed when such metals are dissolved in amine-thiol solution, various chemical analyses including X-ray absorption, Raman, NMR and FTIR spectroscopy along with mass spectrometry were performed on the solutions. These analyses confirmed the oxidation of metals in respective ionic state with the formation of metal thiolate and H_2 gas as a byproduct of dissolution. This further allowed for redesigning the inks in benign solvents like DMSO, DMF by utilizing a rather reactive amine-thiol mixture as only a reactant and not as a solvent. Metal thiolates formed via metal dissolution were then subjected to heating which realized their clean conversion to phase pure metal sulfide besides volatile H_2S and thiirane. CISSe films fabricated using this new ink gave carbon and other impurity-free films with preliminary efficiency beyond 12%.

After resolving impurity issues and achieving promising efficiencies, challenges with obtaining single layer morphology for films with thicknesses above 1µm was addressed. By comparing hydrazine versus amine-thiol based films, the importance of Se in precursor film was realized. With chemical analysis of Se-amine-thiol solutions showing similarities with Se-hydrazine solutions, the extent of Se addition in the ink was controlled in order to alter the film growth mechanism from traditional liquid assisted growth to bulk sintering growth giving for the first time thicker films with the absence of multilayer morphology. In addition to getting uniform film morphology, grains with a couple of hundred-nanometer sizes were converted to desired micron size by controlling the temperature which improved the optoelectronic properties of the film like carrier lifetimes showing further promise for utilization of amine-thiol system.

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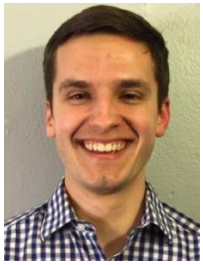

Silver Indium Diselenide: An Intriguing Absorber Layer Candidate for Low-Cost, High Efficiency Printable Photovoltaics

David J. Rokke

Professor Rakesh Agrawal

With photovoltaic deployment on the rise, significant research has been dedicated to increasing manufacturing throughput to accelerate the transition to renewable energy. Solution processing of PV materials has emerged as an exciting candidate for high throughput, low-cost manufacturing. Among the most prominently researched inorganic PV materials are the chalcogenides $Cu_2ZnSn(S,Se)_4$ and $Cu(In,Ga)(S,Se)_2$. However, both materials suffer from intrinsic drawbacks, albeit to different extents. Cation disorders in the crystal lattice introduce detrimental electronic defects, a phenomenon which becomes harder to control at larger areas and is exacerbated by the complex stoichiometry of these systems. A line of research in recent years has been to partially replace the copper content of these materials with silver: the large ionic radius increases defect formation energies in the material, lowering defect concentrations. However, this further complicates device stoichiometry, which we anticipate will lead to challenges when trying to maintain uniformity on large-scale commercial devices.

Instead of further complicating the material stoichiometry in hopes of mitigating defects, we propose synthesizing $AgInSe_2$; a comparatively simple material that has been shown to have a low concentration of intrinsic defects and high carrier mobility[1]. Despite promising material properties and a band gap well suited to collect light from the solar spectrum, research on this material has been sparse.

In this work I demonstrate the synthesis of $AgInSe_2$ from the versatile amine-thiol solvent system. This approach avoids the use of contaminating metal salt precursors used in other common solution chemistries for photovoltaic device fabrication. In addition, it avoids the use of hydrazine, a solvent which has given record solution processed efficiencies for both $Cu_2ZnSn(S,Se)_4$ (12.6%[2]) and $Cu(In,Ga)(S,Se)_2$ (17.3%[3]) but is dangerously toxic and explosive. This synthesis enables more detailed electronic characterization on device-relevant thin films which are of greater relevance than the larger wafer samples used in previous characterization studies. This will enable more definitive conclusions to be made about $AgInSe_2$ as a potential photovoltaic material.

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Identifying Energy-Efficient Distillation Configurations: Advances in Modelling and Optimization

Tony Joseph Mathew

Prof. Rakesh Agrawal

When a mixture is to be separated into three or more components, a distillation configuration is needed, comprising multiple distillation columns with multiple streams transferring between them. The various types of connections between columns (e.g. basic and thermal coupling), and types of splits (e.g. sharp and sloppy) that can be performed in each column, lead to a myriad of possible configurations. For example, there are 6,128 different distillation configurations for a five-component separation, and the number grows combinatorially with the number of components [1]. Determining which configuration is the best for a given separation is challenging, as optimizing even a single configuration in a process simulator (such as Aspen Plus, Aspen HYSYS, PROII and ChemCAD) can take days, and so optimizing all possible configurations could take decades! This is where shortcut models hold promise; they are used to screen through the entire search space of configurations, quickly evaluating each one to generate a handful of attractive configurations in days rather than decades. However, the development of such models has its own challenges that have limited their use.

Three big challenges that we have successfully addressed are: 1. The simpler a model is, the easier it can be applied; with constant relative volatility and constant molar overflow being common assumptions during model construction for this very reason. However, most real mixtures do not obey these assumptions. 2. Most shortcut models employed in optimization [2] are developed for high purity products with high recovery; however, in several industrial applications, impurities in the products are traded for reductions in energy consumption. 3. One of the advantages of running distillation by heat is that the heat it releases may be re-used in the configuration (heat integration), potentially reducing the net energy consumption. However, this re-use is conditional on the right temperatures, and the calculation of temperatures can cause convergence difficulties during optimization due to the complex equations needed. Through a thorough analysis of the fundamental equations involved in distillation, we derived new mathematical insights which enabled us to come up with creative solutions to the aforementioned challenges. The solutions were implemented in our optimization formulation [2] to widen both the scope of separations that it can be applied to, and the distillation features that it takes into account. In this talk, we briefly discuss the resulting first-of-its-kind shortcut model, which is empowered in its ability to quickly and systematically identify those distillation configurations which energetically perform better than the rest in the vast search space for any non-azeotropic separation.

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Electrohydrodyanmic Equatorial Streaming

Brayden Wagoner

Profs. Osman A. Basaran and Michael T. Harris

Four hundred years ago, William Gilbert, Queen Elizabeth's personal physician, reported that static electricity from rubbed amber could "attract" water. The science behind this coupling between fluid flows (hydrodynamics) and electric fields---electrohydrodynamics (EHD)---was subsequently rigorously established by three seminal papers: Rayleigh's discovery [1] that highly charged drops can become unstable, Taylor's analysis [2] of the instability of conducting drops subjected to electric fields, and Taylor's discovery [3] that imperfectly conducting or leaky dielectric (LD) drops can be deformed parallel (prolate) or perpendicular (oblate) to the applied electric field.

These theoretical analyses and numerous experimental studies on jet emission from the conical ends of pendant or free droplets (tip streaming) laid the foundation for widely used applications including electrospray ionization mass spectrometry, electrospinning, and printing of biological cells *and* advanced materials. While the past century of research and application development have been centered on highly conducting prolate drops which emit a stream of droplets in the direction of the applied field, a new EHD streaming phenomenon---equatorial streaming [4]---has recently been observed experimentally.

Motivated by these recent experiments, we, for the first time, develop simulations that can capture the emission of an unstable liquid sheet from the equator of an electrified LD droplet (equatorial streaming). We thereby uncover both the necessary conditions for this streaming instability to occur and the dominant physics at play by performing bifurcation analysis and scrutinizing the stresses imparted upon the drop by the applied electric field. By exploiting the understanding gained here, we propose feasible routes towards electro-emulsification and thin film production without the need for moving parts.

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Green Synthesis of Metal Nanordos Exploited Novel Biological Templates: Barely Stripe Mosaic Virus Virus-Like Particles

Yu-Hsuan Lee

Prof. Michael T. Harris

The synthesis of nanoscale materials of uniform morphology and monodisperse quality is of substantial interest recently. Exploiting natural biomolecules as templates to nanoscale material synthesis have drawn tremendous attention for decades. A variety of biomolecules have been used as biotemplates to display functionalities for nanomaterial fabrication. Utilizing virus particle as biotemplates is an emerging field due to their features of the precise dimension, the diversity of architecture and the amenability to genetic/chemical engineering for a variety of applications.

Motivated by the previous study of biotemplating plant-produced Barley stripe mosaic virus (BSMV) for direct nanomaterial synthesis demonstrated in our group, recent work has focused on the development of the production of BSMV virus-like particles (VLPs) from a heterogeneous system without the restrictions of *in-planta* production. Through genetic engineering, nanorod-shaped BSMV-VLPs were successfully produced from a microbial-based expression system. To further control the stability of BSMV-VLP, internal protein interactions within a virion was decoupled into protein-nucleic interaction and protein-protein interaction. The several amino acid residues involved in BSMV virion protein oligomerization were studied and identified. The results provided ways to modulate and enhance virion stability without incorporating nucleic acid-protein interaction. Furthermore, the bacterial assembled BSMV-VLP was further successfully utilized as a biotemplate to synthesize dense metal nanorod in the absence of an external reducing agent.

Collectively, *in vivo* and faster production of a novel biotemplate, BSMV-VLP, from bacterial expression system was developed. The synthesized BSMV-VLPs has been demonstrated the viability as a promising biotemplate for metal nanorod direct synthesis. This study provides a simple manipulation for BSMV-VLP production and enables full capacity of genetic engineering for unique features, serving as a springboard for biotemplate design in future bionanotechnology.

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Individual Research Poster Pitches

Category	Title Links to Pitch	Author links to Webex	Advisor(s)
Biotech	Bioinspired Elastin-Based Surgical Adhesives	Paulina Babiak	Julie Liu
Biotech	Mitochondrial DNA: Ancient molecule learning new tricks	Han Zhao	Chongli Yuan
Biotech	Epigenetic Mechanism of Accupucture Mediated Pain Management	Kyle Wettschurack	Chongli Yuan
Biotech	Bilirubin-Coated Radioluminescent Particles for Radiation-Induced Photodynamic Therapy	Dhushyanth Viswanath	You-Yeon Won
Biotech	Polymer Lung Surfactant as a Novel Lung Surfactant Replacement Therapy	Daniel Fesenmeier	You-Yeon Won
Biotech	Optogenetic Control in hPSCs for Cardiac Patterning	Peter Hellwarth	Xiaoping Bao
Biotech	Chemically Defined Hematopoietic Cell Generation from hPSCs	Juhyung Jung	Xiaoping Bao
Catalysis	Influences of Al distribution on propene oligomerization	Elizabeth Bickel	Raj Gounder
Catalysis	Effects of Ni Site Density on Deactivation Rates and Mechanisms During Ethene Oligomerization on Ni-Beta Zeolites	Arunima Saxena	Raj Gounder
Catalysis	First Principles Analysis of Selectivity and Durability of Pt-based Alloys for Light Alkane Dehydrogenation	Yinan Xu	Jeff Greeley, Jeff Miller
Fluids	Relationship of Interfacial Tensions of Oil/Water Interfaces to Oil Recovery Efficiency	Jaeyub Chung	Bryan Boudouris, Elias Franses
Fluids	Cross-stream migration of non-spherical particles in general quadratic flows of second-order fluid	Cheng-Wei Tai	Vivek Narsimhan
Mat. Sci.	Facile Chemical Route for Synthesis and Manipulation of Lead Chalcogenide Microstructures	Swapnil Deshmukh	Rakesh Agrawal
Mat. Sci.	Solution Processed Synthesis of Copper Arsenic Sulfide Absorber Layers for Photovoltaic Applications	Apurva Pradhan	Rakesh Agrawal
Mat. Sci.	In-Situ Thermal Runaway Monitoring of Lithium-ion Batteries via Internal Sensor	Mihit Parekh	Vilas Pol
Pharma.	MiniPharm: A Miniaturized Pharmaceutical Manufacturing Platform for Process Development	Jaron Mackey	Zoltan Nagy
Pharma.	End to End Drug Product Synthesis using Dropwise Additive Manufacturing	Varun Sundarkumar	Gintaras Reklaitis, Zoltan Nagy
Pharma.	Two-zone ligand-assisted displacement chromatography for producing…	Yi Ding	Nien-Hwa, Linda Wang
Pharma.	An atomic level perspective on the mechanism of NaCl nucleation from highly concentrated solutions	Pelin Bulutoglu	Doraiswami Ramkrishna

Group Research Poster Pitches

Category	Title (Link to Pitch)	Author(s) (Link to Webex)	Advisor(s)
Mat. Sci.	Sustainable Electrode Materials for Next Generation Energy Storage Devices	Daniel Gribble, Ethan Adams	Vilas Pol
Mat. Sci.	Two-Dimensional Hybrid Perovskites: Design, Synthesis, and Applications	Zitang Wei	Letian Dou
Mat. Sci.	Cost-Driven Manufacturing & Design of 3D-Hybrid Additive Composites	Alex Reichanadter	Jan-Anders Mansson
Mat. Sci.	Solution-Processed Thin Film Photovoltaics via Nanocrystal Inks and Molecular Solutions for Scalable, Low-Cost Manufacturing	Jonathan Turnley	Rakesh Agrawal
Mat. Sci.	Sustainable Coproduction of Food and Solar Energy	Varsha, Jonathan Turnley	Rakesh Agrawal
Process Eng.	Advances in Optimization of Distillation and Membrane Separations	Zewei Chen	Rakesh Agrawal
Process Eng.	Process and Equipment Design for the Center for Innovative and Strategic Transformation of Alkane Resources (CISTAR)	Edwin Rodriguez	Rakesh Agrawal
Biotech.	The Path of Neural-Engineering: From Human Brain to Synthetic Neuron	Junkai Xie	Chongli Yuan
Biotech.	Radioluminescent naoparticles for multimodal treatment of locally advanced head and neck cancers	Kaustabh Sarkar	You-Yeon Won
Pharma.	Crystallization and Particle Technology Systems Engineering (CryPTSys)	Wei-Lee Wu	Zoltan Nagy
Pharma.	Modernization of Pharmaceutical Manufacturing	Yan-Shu Huang, S. Kumar, R. Lagare	Gintaras Reklaitis, Zoltan Nagy
Catalysis	Accelerated Discovery of Multimetallic Oxygen-Cycle Electrocatalysts using Machine Learning	Pushkar Ghanekar, Gaurav Deshmukh	Jeffrey Greeley
Catalysis	First Principles based Catalyst Design for Selective Light Alkane Dehydrogenation and Olefin Oligomeirzation	Ranga Seemakurthi, Yinan Xu	Jeffrey Greeley

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