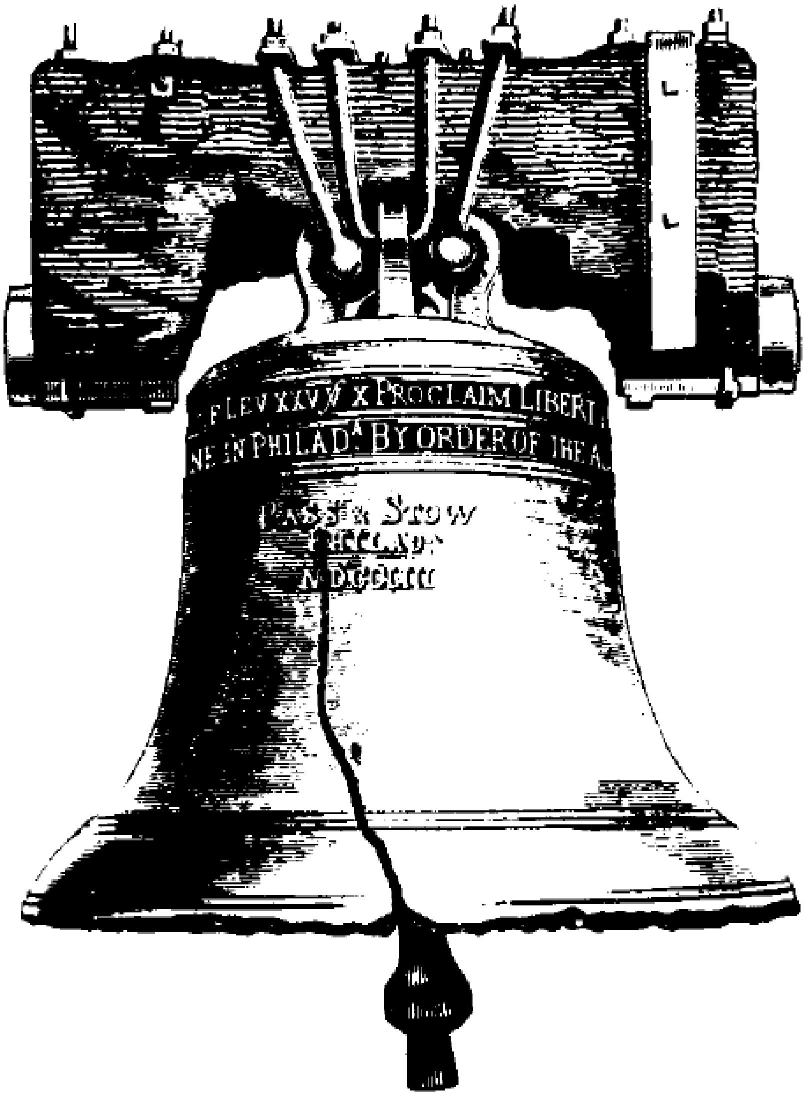
Catalysis Club of Philadelphia

2026 Spring Symposium Program



Promoting the science of catalysis since 1949

Thursday, April 16th, 2026

2026 Catalysis Club of Philadelphia Annual Symposium & Student Poster Joint Conference

Thursday, April 16th, 2026 @ Golf View Room, Springfield Country Club
400 W Sproul Rd, Springfield, PA 19064

Symposium chair: Dr. Weijian Diao (Villanova Univ., Weijian.diao@villanova.edu)
Student poster chair: Dr. Jun Hee Jang (Rowan Univ., Jang@rowan.edu)

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Symposium Speakers

Dr. Udayshankar Singh
Senior Principal Scientist
W.R. Grace

Prof. Enrico Tronconi
Professor
Politecnico di Milano, Italy

Prof. Chao Wang
Professor
Johns Hopkins University

Prof. Jason Bates
Assistant Professor
University of Virginia

Nate Roeckel
Senior Research Chemist
Technip Energies/Zeolyst International

Jackie Ngu
PhD Candidate
University of Delaware

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2026 Spring Symposium
Schedule of Events

Thursday, April 16, 2026

8:00 AM	**Breakfast and Social Hour**
8:50 AM	**Opening Remark**
9:00 AM	**Dr. Udayshankar Singh, W.R. Grace** “Overcoming Contaminant Metal Challenges in FCC: Catalyst Design and Passivation Strategies”
9:45 AM	**Prof. Enrico Tronconi, Politecnico di Milano, Italy** “A Decoupled Transient Kinetic Approach Unravels the Standard NH_3-SCR Redox Chemistry over Cu-CHA Catalysts”
10:30 AM	**Coffee/tea Break**
10:35 AM	***Sponsor Presentations – Tom Ormsbee, Malvern Panalytical Inc***
10:45 AM	**Prof. Jason Bates, University of Virginia** “Intended and Unintended Consequences of Electrolyte Composition for Electrocatalysis”
11:30 AM	**Nate Roeckel, Technip Energies/Zeolyst International** “Catalytic Pyrolysis of Polyolefins with Industrially Relevant Zeolite Catalysts”
12:15 PM	**Lunch (Buffet)**
1:25 PM	**Afternoon Program Opening Remarks**
1:30 PM	***Sponsor Presentations – Greg Thiele, Anton Paar***
1:40 PM	**Prof. Chao Wang, Johns Hopkins University** “Advanced Catalysts for Ammonia Synthesis and Conversion”
2:25 PM	**Jackie Ngu, PhD student, University of Delaware** “Enhancing Ethylene and Propylene Production from Polyethylene Deconstruction via Rapid Pulse Joule Heating”
2:45 PM	**Symposium Closing Remarks and Student Poster Session Introduction**
2:50 PM	**Student Poster Session and Social Hour**
4:50 PM	**Conference Closing**

Overcoming Contaminant Metal Challenges in FCC: Catalyst Design and Passivation Strategies

Udayshankar Singh

Refining Catalysts, W.R. Grace & Co., Columbia, MD.

Resid processing within Fluid Catalytic Cracking (FCC) units is a key strategy for upgrading low-value vacuum residua into high-value transportation fuels and petrochemical feedstocks. This approach significantly improves refinery economics. The growing prevalence of heavier global crude slates, combined with the economic appeal of opportunity crudes, is driving increased demand for resid FCC operations. However, these feedstocks introduce severe challenges due to high concentrations of contaminant metals (Na, Ni, V, Fe), Conradson carbon, and asphaltenes. These contaminants accelerate catalyst deactivation through mechanisms such as zeolite destruction, pore blockage, and increased non-selective hydrogen transfer reactions. The resulting loss of catalytic activity elevates yields of undesirable products, including coke and dry gas, leading to disruptions in unit heat balance and overall operations, which ultimately compromise unit reliability and profitability.

This presentation systematically delineates the unique poisoning mechanisms associated with individual metal contaminants and outlines the advances in catalyst-design strategies to mitigate their impact, sustain catalytic performance, and enable efficient resid processing. Data show that nickel contamination accelerates hydrogen transfer reactions, driving elevated hydrogen and coke formation and thereby diminishing FCC unit efficiency. Sodium and vanadium, by contrast, interact destructively with the zeolitic framework, leading to structural degradation and a corresponding loss in intrinsic catalytic activity. Iron exhibits fundamentally different behavior, in the presence of other metal species, it facilitates the formation of low-melting eutectic, dense surface phases that block pore structures and severely impair catalyst accessibility and overall unit performance. Effective mitigation requires advanced catalyst systems that integrate robust metals-passivation technologies, large-pore architectures, and high matrix activity, complemented by optimized operational strategies.

Udayshankar Singh

W.R. Grace

Udayshankar Singh is a Senior Principal Scientist, and R&D Lead for the Light Olefins Business segment in the Performance Catalyst Solutions Business at the W.R. Grace. His job responsibilities include development and scale-up of new catalysts for application in refining industry, and providing technical support for customer related unit problems. Since joining Grace in 2007, he has made numerous high-impact contributions to the Refining Technologies portfolio, particularly in the areas of emission-control catalysts, propylene-maximization technologies, and innovations in fluid catalytic cracking (FCC) catalysts. Among his recent achievements is the invention and successful commercialization of the ZAVANTI® technology, a catalyst engineered to enhance propylene yields in high-severity FCC operations. This innovation resulted in a granted patent recognizing the novelty of the technology and earned him Grace's highest technical honor, the Grace Award for Technical Excellence (GATE). In addition, he is a five-time recipient of Grace's Premiere Award, reflecting the broad industrial relevance and significant value created through his research and technological innovations.

Beyond his scientific accomplishments, Dr. Singh is deeply committed to serving the catalysis community. He currently serves as Treasurer of the Northeast Corridor Zeolite Association (NECZA) and as a Co-Chair for the North American Catalysis Society Meeting. Previously, he led the Catalysis Club of Philadelphia (CCP), serving both as Chair and Co-Chair.

Udayshankar Singh obtained PhD degree from The University of Exeter in England while studying the synthesis, characterization and sorptive properties of functionalized MCM 41 materials. He subsequently conducted postdoctoral research at the University of California, Santa Barbara, investigating the synthesis, characterization, and mechanistic behavior of diesel CO-oxidation catalysts for automotive emissions control. Dr. Singh has more than 22 years of experience in heterogeneous catalysis and has contributed extensively to the field through patented technologies and numerous publications in peer-reviewed scientific journals.

A Decoupled Transient Kinetic Approach Unravels the Standard NH_3-SCR Redox Chemistry over Cu-CHA Catalysts

A. Gjetja, G. Contaldo, C. Negri, N. Usberti, M. Maestri, I. Nova, **E. Tronconi**

Laboratory of Catalysis and Catalytic Processes, Dipartimento di Energia,
Politecnico di Milano – Via La Masa, 34, Milan, 20156, Italy

Decoupling the reduction and oxidation half-cycles of the low-temperature Standard-SCR redox mechanism over state-of the-art Cu-CHA catalysts is crucial to elucidate the elementary steps governing the DeNOx activity and to develop predictive kinetic models. This talk will illustrate the application of Transient Response Methods to independently study the Reduction Half-Cycle (RHC), where Cu^{2+} is reduced to Cu^{+} by NO and NH_3, and the Oxidation Half-Cycle (OHC), where Cu^{+} is re-oxidized to Cu^{2+} by O_2. Our approach builds upon previous advances in transient kinetic analysis of Cu-CHA systems [1-3]. Catalyst samples differing in Cu loading (0.5-2.7 wt%), SAR (10-25), and hydrothermal aging level were tested under varying NO (300-500 ppm), O_2 (1-8 %), H_2O (0-2 %), and T (150-500 °C) conditions. From these data we have derived intrinsic rate equations and bed-averaged oxidized Cu fractions using an integral plug-flow model of the test reactor.

For all the catalyst samples, we first show that RHC and OHC rate constants independently estimated from low-T transient runs can be combined to predict steady-state NO conversions and oxidized Cu fractions in excellent agreement with experimental data collected under Standard-SCR conditions [3]. Our decoupled approach further highlights that H_2O exerts a mild inhibiting effect on the RHC at high SAR, but significantly promotes the OHC at all SARs, consistent with mechanistic insights on water-assisted Cu redox chemistry from DFT and *operando* UV-Vis spectroscopy studies [4,5]. Mild hydrothermal aging has a negligible impact on RHC, but markedly depresses OHC: accordingly, the original DeNOx activity can be recovered by suitably incrementing the O_2 partial pressure. At temperatures above 250 °C, our results reveal that the characteristic “seagull” shape of the SCR lightoff curves over Cu-CHA originates exclusively from a sharp drop of the OHC rates between 250 and 350 °C, while the RHC rates retain the Arrhenius-type monotonic trend with increasing temperature. This confirms the central role of Cu oxidation kinetics in limiting medium-temperature SCR performance.

Overall, the redox-decoupling framework provides mechanistic clarity on the interplay between Cu^{2+}/Cu^{+} species during both low- and high-temperature Standard-SCR and offers a powerful tool for guiding the rational design of more active and durable Cu-CHA catalysts for automotive emission control.

Acknowledgments

This work was financially supported by Johnson Matthey and Cummins, Inc.

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Enrico Tronconi

Politecnico di Milano, Italy

Biography

Enrico Tronconi is Professor of Chemical Engineering at Politecnico di Milano, where he leads the Laboratory of Catalysis and Catalytic Processes. He is an internationally recognized expert in catalytic reaction engineering, structured catalysts, and reactor technologies for process intensification and electrification. His work has had major impact on environmental catalysis (NH_3-SCR for NO_x abatement), advanced reactor design, and decarbonized hydrogen production, bridging fundamental science and industrial application. He is the recipient of an ERC Advanced Grant and the winner of the 2023 Air Liquide Scientific Challenge. Prof. Tronconi has authored over 330 peer-reviewed publications, holds 15 international patents, and is a frequent invited plenary and keynote speaker at leading international conferences. He has collaborated extensively with industry, investigating DeNOx aftertreatment technologies for vehicles with Mercedes Benz, Johnson Matthey, Corning, Cummins and other leading Companies.

Intended and Unintended Consequences of Electrolyte Composition for Electrocatalysis

Jason S. Bates

Department of Chemical Engineering, University of Virginia, Charlottesville, VA 22903

Electrocatalysis underpins a variety of proposed sustainable chemical technologies. In this context, reaction rates and selectivities are governed not only by the catalyst surface but also by the local microenvironment at the electrode–electrolyte interface. The identity and organization of ions, local electric fields, and the structure of interfacial water have all been proposed to control the stabilities of key surface intermediates and transition states. Despite their importance, general principles for electrolyte design remain poorly defined. Here, we discuss how changes in electrolyte composition can cause both intentional and unintentional modifications to electrocatalytic reactivity. Taking the hydrogen evolution reaction on polycrystalline platinum in alkaline media as a canonical example, we show how electrolyte impurities can lead to both promotion and poisoning of catalysis, complicating mechanistic interpretation and undermining reproducibility. Controlling these unintended effects is a prerequisite for interpreting the kinetic consequences of intentional electrolyte modifications, as we show for the case of organocation additives. Together, these examples illustrate how electrolyte composition couples surface chemistry and interfacial structure, highlighting both the importance of rigorous and reproducible protocols for kinetic measurements, and opportunities for rational electrolyte design.

Jason S. Bates
University of Virginia

Jason Bates received his B.S. in Chemical Engineering at the University of Kansas in 2014, where he conducted research under Bala Subramaniam in the Center for Environmentally Beneficial Catalysis, with summer research experiences under Robert J. Davis at the University of Virginia and under Joshua Schaidle at the National Renewable Energy Laboratory. He received his Ph.D. in Chemical Engineering at Purdue University in 2019, under the supervision of Rajamani Gounder. He completed an NIH postdoctoral fellowship at the University of Wisconsin–Madison in the Department of Chemistry, under the supervision of Shannon S. Stahl. He started his independent career at the University of Virginia in fall 2023. His research explores the fundamentals of heterogeneous thermal and electrocatalysis in areas relevant to decarbonization of the energy and chemical industries. His research has been recognized with the NSF CAREER award, a Young Talent award at the 18th International Congress on Catalysis, and the Virginia Space Grant Consortium New Investigator Award. He has served the catalysis community as the chair of the 2024 Gordon Research Seminar on Catalysis, and is currently vice president of the Southeastern Catalysis Society and a member of the *Journal of Catalysis* early career advisory board.

Catalytic Pyrolysis of Polyolefins with Industrially Relevant Zeolite Catalysts

Nate Roeckel

Zeolyst International

Global plastics production is expected to triple by 2060 relative to 2019, yet currently less than 10% of end of life plastics are recycled. Achieving a circular carbon economy will require advanced recycling technologies that address the limitations of mechanical recycling. Pyrolysis has emerged as a leading method for cracking contaminated, multilayer, and otherwise difficult to recycle polyolefins into liquid hydrocarbons. Further cracking of waste plastic pyrolysis oil into light olefins, and the subsequent polymerization back to polyolefins, enables a circular polyolefin value chain.

This presentation will cover the use of industrially relevant zeolite catalysts for the catalytic cracking of polyolefins into liquid hydrocarbons, as well as the key zeolite properties that enable effective performance in this application.

Nate Roeckel
Zeolyst International

Biography

Nate Roeckel has spent 18 years developing zeolite catalysts in the Product Development Group at Zeolyst International. He currently leads catalyst development for advanced recycling of polyolefin waste. Nate's background includes zeolite synthesis, post synthetic modifications, characterization, and catalysis for advanced recycling and selective catalytic reduction (SCR) of NOx. He holds an M.S. in Chemistry from Villanova University and a B.S. in Chemistry from Temple University.

Advanced Catalysts for Ammonia Synthesis and Conversion

Chao Wang*[1,2]

[1] *Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD 21218*
[2] *Ralph O'Connor Sustainable Energy Institute, Johns Hopkins University, Baltimore, MD 21218*

ABSTRACT

Ammonia represents a promising liquid fuel for hydrogen storage, but its large-scale application is limited by the need for precious metal ruthenium (Ru) as catalyst. Here we discuss our recent efforts on developing advanced catalysts for ammonia-related chemical transformations. Topics include transition metal nitrides for ammonia synthesis and high-entropy alloy catalysts for ammonia cracking and oxidation. Atomic structures of these catalysts are characterized by using state-of-the-art electron microscopy and X-ray spectroscopy techniques. Surface structures and adsorption properties of the catalysts are probed by measuring temperature- or potential-programed chemisorption of small molecules (e.g., *N, *H). Kinetic analysis is performed to discern the rate-determining factors and reaction pathways. The established structure-property-performance correlations are further subjected to computational simulations to develop fundamental understanding of the catalytic mechanisms.

Chao Wang
Johns Hopkins University

Biography

Dr. **Chao Wang** holds a Professor position in the Department of Chemical and Biomolecular Engineering at Johns Hopkins University. His research interests are primarily in carbon capture and conversion, electrochemical energy conversion and storage, and heterogeneous catalysis for green chemical engineering. He received his bachelor's degree from the University of Science and Technology of China in 2004, and doctorate from Brown University in 2009. He was a postdoctoral fellow at Argonne National Laboratory until joining Johns Hopkins University as Assistant Professor in 2012. He was promoted to Associate Professor in 2019 and Professor in 2025. Dr. Wang is a recipient of AFOSR Young Investigator Award (2014), ARO Young Investigator Award (2015) and R&D100 Award (2020). He also received the Johns Hopkins University Catalyst Award (2015) and Discovery Award (2016). He is currently serving as Associated Editor for Science Advances (from 2023). He has co-founded two startup companies HighT-Tech (2018) and EDAC Labs (2022).

Enhancing Ethylene and Propylene Production from Polyethylene Deconstruction via Rapid Pulse Joule Heating

Jackie Ngu
University of Delaware
Advisor: Prof. Dionisios Vlachos

The growing volume of plastics waste, compounded with a low recycling rate, has led to an alarming amount of plastics ending up in landfills or being incinerated. While pyrolysis offers a route for plastic waste deconstruction, its product distribution is often broad and poorly controlled due to unselective radical chemistry at high temperatures. We recently demonstrated that rapid pulse Joule-heated catalytic cracking over HZSM-5, combined with small fractions of steam, can achieve high selectivity (>80 %) toward C_2-C_4 olefins, while significantly reducing coking compared to continuous Joule heating. Here, we investigate how acid catalyst properties, such as silica/alumina ratio, zeolite topology, and catalyst porosity, influence light olefin selectivity during polyethylene deconstruction via rapid pulse Joule heating. We demonstrate that silica-to-alumina ratios of ~30 yield high light olefin selectivity, and small-pore zeolites favor light olefins at the expense of increased coke formation. To mitigate coking, we synthesize HZSM-5 nanosheets and hierarchical zeolites (MFI, FAU, and CHA). These catalysts achieve an ethylene selectivity of approximately 35 %, a twofold increase over prior catalytic pyrolysis. Additionally, co-feeding steam and incorporating hierarchical porosity reduce coke formation and enhance catalyst stability.

Jackie Ngu

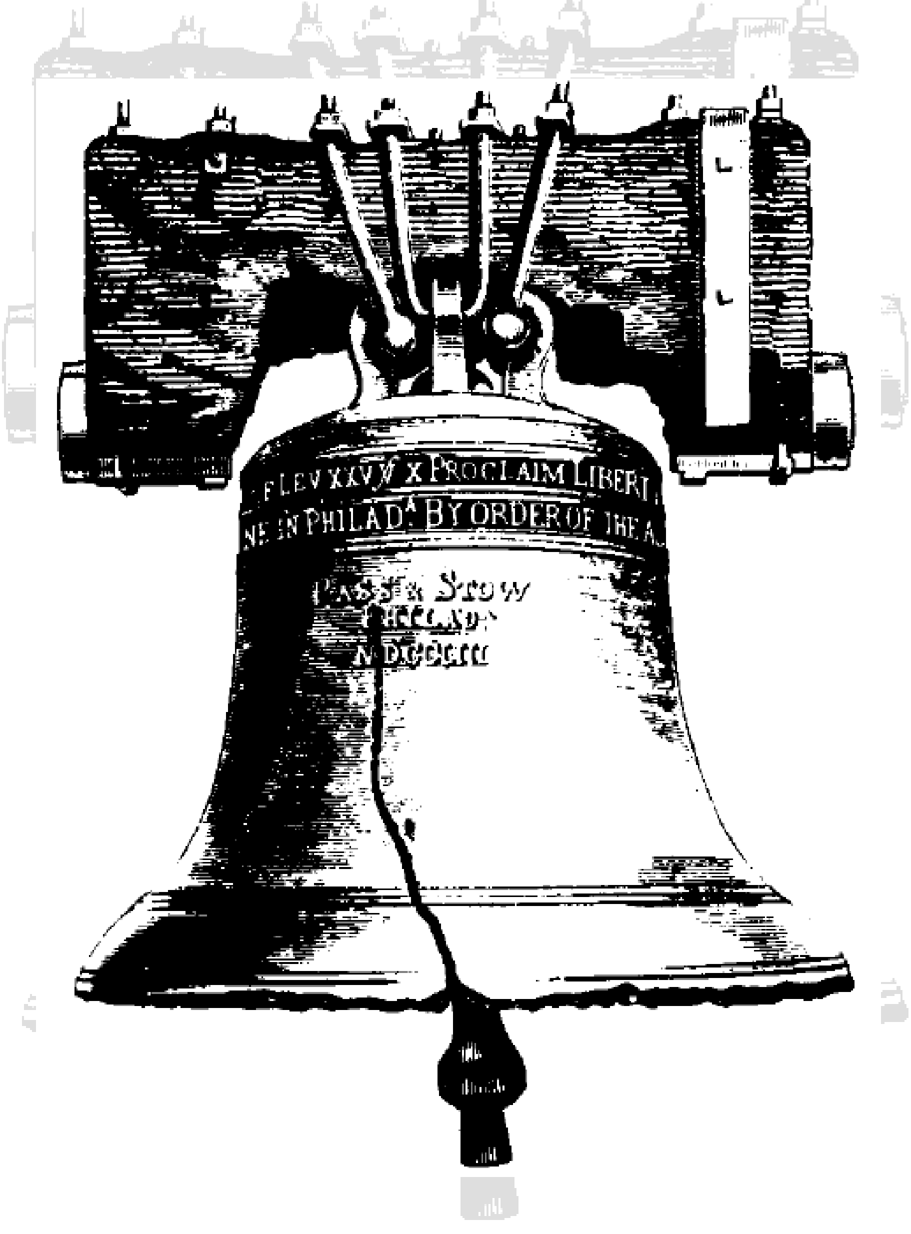
University of Delaware

Biography

Jackie Ngu is currently a fourth year Ph.D. candidate at the University of Delaware. She is currently advised by Prof. Dionisios Vlachos and is working on deconstruction of polyolefins using electrified reactors. Jackie completed her undergraduate degree in chemical engineering at Case Western Reserve University.

Catalysis Club of Philadelphia

2026 Student Poster Session



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Thursday, April 16th, 2026

#	Presenter	Institution	Title
1	Emmanuel Aransiola	Lehigh University	Probing Mo-leaching induced Structural Reconstruction and Electrocatalytic Activity of $CoMoO_4$ for Oxygen Evolution Reaction at Tunable Mo loadings
2	Damilola Awotoye	Lehigh University	Unraveling the Dynamic Surface Architecture and Gas-phase Dynamics of Bimetallic Na-WO_x Catalysts for Selective OCM
3	Emma Battista	Temple University	Cross-aldol Condensation of Benzaldehyde and Acetone to Benzalacetone Catalyzed by Metal Oxyhydroxides
4	Maxwell P. Bobbin	University of Delaware	Multiscale modeling of packed-bed microwave reactors and estimation of intrinsic materials' permittivity
5	Enerelt Burentugs / Charles C. Fields	University of Delaware	Enhancement of Rapid Alternating Polarity Kolbe Coupling for Renewable Chemical Production
6	Emily C. Cunningham	Princeton University	Engineering Framework Defects and Metal Sites in UiO-67
7	Sharan Dhar	Temple University	Framework-free in-situ derived metal (IV) oxyhydroxides outperform MOF in peptide hydrolysis
8	Johari A. Dramiga	Lehigh University	Understanding the Energetics of CO_2 Electroreduction and Sulfur Deposition on Low Index Ni Facets and Ni/YSZ(111) Using DFT
9	Hashini S. Fransiscus	Temple University	Group (VI)- W(0) and Mo(0) Complexes as Efficient Catalysts for Z-Selective Alkene Isomerization
10	Reynold Gao	University of Delaware	Synthesis and Evaluation of Novel Ga-containing CHA Zeolites for Near-Ambient Hydrogen Storage
11	Nicholas M. Houck	University of Delaware	Oxidative Dehydrogenation of Ethane via NO
12	Mikyung Hwang	Pennsylvania State University	A Predictive Framework for the Design of Doped Oxide Hydrogenation Catalysts
13	Neelesh Kumar	Lehigh University	Effect of Surface VOx Coverage on CH_3OH Oxidation by Supported VOx/CeO_2 Catalysts: Heterogeneity of Surface Sites and Reactivity
14	Rajas M. Mehendale	University of Delaware	Molecular insights on branching effects in catalytic upcycling of mixed polyolefin waste

#	Presenter	Institution	Title
15	Joshua L. Miller	Princeton University	Assessing impact of oxidant identity on reactivity, selectivities, and defect generation during MOF-catalyzed oxidations
16	Oscar J Moreno-Piza	University of Delaware	Impact of Alkali Cations on the electrochemical oxidation of Furfural on Gold Electrodes
17	Pedro Moura	University of Delaware	Hydrolysis of a commercial polyamide 6 multilayer film over TiO_2 to enable hydrocracking and chemical recycling
18	Christine M. Oberhausen	University of Delaware	Tandem Catalysts for Hydroconversion of Polyethylene-EVOH Multilayer Plastics
19	John V. Piorkowski	Princeton University	Impacts of Surface and Pore Interactions on Rates and Selectivities of Polyolefin Decomposition with Zeolites
20	Arthur Prewette	Villanova University	Supported Catalytically Active Liquid Metal Solutions for Energy Applications
21	Thanuka S.R. H. Ralalage	Temple University	Are Defects Always Beneficial in Photocatalysis? Insights from Organophosphate Detoxification
22	Jessie A. Sun	University of Delaware	Elucidating the roles of polymer diffusion and active site location in polyolefin hydrocracking using metal encapsulated zeolites
23	Oamfah Suwannapong	Princeton University	Impacts of Coordination Spheres on Alkylation Reactions in Varied Aluminosilicate Environments
24	Shuting Xiang	Lehigh University	Acrolein Synthesis from Oxidative Coupling of Biomass-Derived Methanol and Ethanol by Supported Monolayer $MoOx/Fe_2O_3$ Catalyst
25	Jianbo Yang	University of Delaware	Effect of Reactor Configuration on Radical initiated Low-temperature Polystyrene Pyrolysis
26	Azad Yilmaza	University of Delaware	Catalytic Glycolysis of Polyester-Spandex Blends
27	An Zhang	Villanova University	Bimetallic CuPd Catalysts Supported on AlOOH with -OH-riched Surface for C_2H_2 Semi-Hydrogenation

2026 CCP Poster Abstract
Type: (Graduate)
Consideration in poster competition: (Yes)

1

Probing Mo-leaching induced Structural Reconstruction and Electrocatalytic Activity of $CoMoO_4$ for Oxygen Evolution Reaction at Tunable Mo loadings

Emmanuel Aransiola,[1] Charlie Vo,[1] Juliane Weber,[2] Jonas Baltrusaitis[1,*]
[1] *Department of Chemical and Biomolecular Engineering, Lehigh University, 111 Research Dr., Bethlehem, PA 18015, USA*
[2] *Oak Ridge National Laboratory, Chemical Sciences Division, Oak Ridge, TN 37831, USA*

With the urgent global shift toward sustainable energy systems, electrochemical water splitting has continually been identified as a promising route for long-term green hydrogen (H_2) production to replace depleting fossil fuels and mitigating CO2 emissions.[1,2] Efficient water splitting relies critically on the development of robust, active, and durable electrocatalysts to lower kinetic overpotentials for both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER).[3,4] However, OER remains the kinetic bottleneck of overall water splitting owing to its multistep, four-electron transfer pathway and sluggish surface intermediates, prompting intensive efforts to develop highly active and stable OER electrocatalysts.[5] RuO_2 (and IrO_2) remains the state-of-the-art OER benchmark and has already been implemented in commercial proton-exchange-membrane electrolyzers, however, the scarcity and high cost of Ru-based catalysts, together with their mediocre long-term durability under harsh operating conditions, severely constrain large-scale deployment.[6,7] To meet growing energy demand, durable, low-cost $CoMoO_4$ electrocatalysts are considered for efficient oxygen evolution reaction (OER). Mo incorporation and dissolution in Co-based electrocatalysts tune the electronic environment of Co active sites and modulate their activity, contributing to improved OER performance. However, the chemistry of Mo dissolution and evolution of Co active sites under catalytically relevant regions remains elusive in terms of method of synthesis and extent of Mo incorporation.

To address this research gap, in this work, $CoMoO_4$ was synthesized by electrochemical and hydrothermal methods to probe compositional and synthesis-dependent effects towards OER. Using *in-situ* spectroscopy we examined whether Mo dissolution is also evident in the binder-free electrodeposition method, which may improve electrocatalyst stability. The structure–activity relationships of $CoMoO_4$ catalysts prepared by the two synthesis routes and with different Mo contents (Co/Mo = 1/4, 1/1, and 6/1) in electrodeposition method were established. Electrochemical and spectroscopic characterizations revealed that the Co:Mo stoichiometry strongly influences OER activity. Low Mo incorporation promotes the formation of catalytically active Co sites, whereas high Mo content reduces the density of Co active sites and lowers OER performance. *In-situ* Raman, *ex-situ* XPS, and ICP-OES indicate that distorted MoO_4 tetrahedra accelerate Mo dissolution and reconstruction of $CoMoO_4$ into CoO_6 units in $Co(OH)_2$, followed by transformation into active CoOOH for OER.

This integrated approach enables us to correlate structural reconstruction pathways with activity and stability, providing mechanistic insights into how Co–Mo coupling at varying molar ratios can be harnessed to design next-generation $CoMoO_4$-based OER electrocatalysts.

References

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2026 CCP Poster Abstract **# 2**
Type: Graduate
Consideration in poster competition: Yes

Unraveling the Dynamic Surface Architecture and Gas-phase Dynamics of Bimetallic Na-WO$_x$ Catalysts for Selective OCM

<u>Damilola Awotoye</u>,[1] Nils Hansen[2], Christopher Jesse Kliewer[2], Srinivas Rangarajan[1] and Jonas Baltrusaitis[1,*]
[1] Lehigh University, Department of Chemical and Biomolecular Engineering, Bethlehem, PA, 18015.
[2] Sandia National Laboratories, Livermore, CA, 94550.

The oxidative coupling of methane (OCM) offers a transformative route for natural gas valorization; however, the reaction's dual nature and competing kinetic pathways impose a formidable trade-off between conversion and selectivity. Achieving commercial viability requires the rational design of catalysts capable of navigating these mechanistic limitations. This research focuses on the controlled synthesis and characterization of model Na-WO$_x$/SiO$_2$ catalysts to interrogate the nature and selectivity of dispersed Na-WO$_x$ sites versus crystalline Na$_2$WO$_4$ sites for ethylene production. Utilizing in situ and operando spectroscopic techniques, including Raman, XRD, and near-surface MBMS, this work correlates surface vibrational signatures with real-time gas-phase product distributions and establishes definitive structure–activity relationships. Our findings demonstrate that maintaining high active-phase dispersion is critical for optimizing C$_2$ selectivity. These insights provide a strategic framework for the rational design of bimetallic catalysts, emphasizing the necessity of stabilized surface architectures to drive efficient ethylene production in industrial OCM applications.

2026 CCP Poster Abstract
Type: ([✓ Undergraduate], Graduate, Postdoc)
Consideration in poster competition: (Yes or [✓ no])

 # 3

Cross-aldol Condensation of Benzaldehyde and Acetone to Benzalacetone Catalyzed by Metal Oxyhydroxides

Emma Battista, Sharan Dhar, Thanuka Ranatunga, Eric Borguet
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Cross-aldol condensation reactions play significant roles in pharmaceutical production, food production, and in the synthesis of biofuels from biomass-derived molecules.[1] [2] However, this type of reaction is often characterized with low selectivity due to a high susceptibility for reactants to undergo self-adol condensation at high temperatures. Metal-organic frameworks (MOFs), such as UiO-66, can drive this reaction for a desired result through their active metal nodes. Here, we aim to determine if the metal notes alone can drive the reaction. Furthermore, we aim to understand the relationship between the Lewis acidity and conversion yield using the metal oxyhydroxides formed through hydrolysis in water (i.e. ZrCl4, HfCl4, Ce(NH4)2(NO3)6). Our hypothesis is that the catalytic sites in the metal nodes can function as a base and are more accessible to the substrate than the catalytic sites in the MOF, and therefore using just the metal oxyhydroxides should improve catalytic efficiency and selectivity, and increase the yield of benzalacetone. To identify the products, the reaction was analyzed through gas chromatography coupled with mass spectrometry. Subsequently, the reaction was monitored through 1H-NMR. Based on previous research using MOF metal oxyhydroxide precursors as catalysts, increasing Lewis acidity increased catalytic efficiency.[3] Thus we anticipate that metal oxyhydroxides will provide a more comparable yield of selectivity and conversion to benzalacetone and as obtained with the UiO-66 MOFs.[4] This strategy could provide a route supporting the use of more cost effective, efficient, and selective heterogeneous catalysts for cross-aldol condensation reactions.

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2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

4

Multiscale modeling of packed-bed microwave reactors and estimation of intrinsic materials' permittivity

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Modeling of packed-bed microwave reactors relies on an accurate representation of particle size, shape, and distribution within the bed, as well as the particles' dielectric properties. The measured permittivity of microwave susceptors (powders or structured materials) depends on the geometric features of the particles and the porosity of the bed, as well as the specific form factor of a structured material. These are effective properties and cannot be used to analyze other reactor configurations unless the geometric effects are removed. Therefore, we introduce a methodology for extracting the intrinsic particle permittivity from experimentally measured effective permittivity by combining cavity-based measurements with multiscale simulations and machine learning. Further, we develop the first multiscale model of packed-bed microwave reactors that incorporate particle effects (geometric features, random packing, and particle contact). This approach bridges macroscopic observables with mesoscopic physics, enabling analysis of local hotspots, arcing, and contact effects that control reactor performance. Using polymer-based spherical activated carbon (PBSAC) and silicon carbide (SiC) as examples, we demonstrate that the inferred particle permittivity is consistent with independent experimental heating profiles we collect from microwave reactors without adjustable parameters. This methodology establishes a foundation for predictive, multiscale design of microwave packed-bed reactors that explicitly accounts for particle-scale effects, enabling the estimation of intrinsic permittivity for the first time.

2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

5

Enhancement of Rapid Alternating Polarity Kolbe Coupling for Renewable Chemical Production

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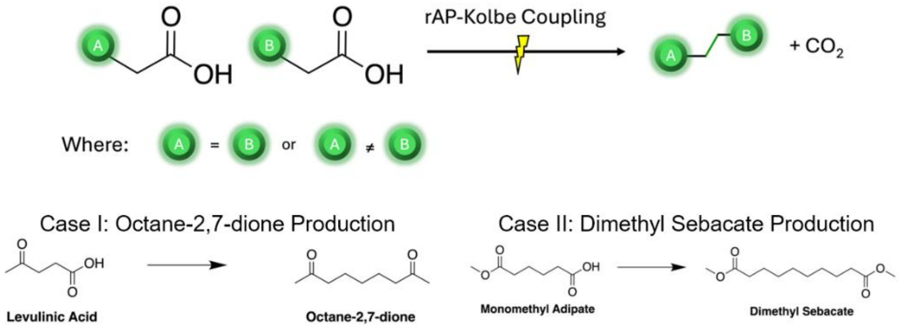
Despite being established in 1849 as one of the earliest carbon–carbon (C–C) bond-forming reactions, Kolbe coupling has yet to achieve broad industrial adoption due to several key limitations. The reaction typically requires high current densities to initiate and relies on expensive precious metal electrodes (e.g., Pt) to promote dimerization, while also suffering from electrode passivation. As a result, its practical utility in large-scale applications remains limited despite its promise for upgrading biomass-derived feedstocks. [1,2]

Recent studies have shown that rapid alternating polarity (rAP) waveforms can overcome these challenges by enabling the use of sustainable carbon-based electrodes in place of traditional precious metals[3]. By rapidly switching between anodic and cathodic potentials, rAP mitigates electrode passivation while enhancing both reactivity and chemoselectivity.

Herein, we systematically investigate rAP Kolbe electrolysis on reticulated vitreous carbon (RVC) electrodes across two carboxylic acid substrates. Using monomethyl adipate, we synthesize the platform chemical dimethyl sebacate (DS) in 83.0 ± 2.8% yield at 2.2 F/mol—a 27.7% improvement over conventional direct current systems employing Pt electrodes[4]. Extending this approach to the biomass-derived substrate levulinic acid, optimization of alternating frequency, applied voltage, and co-solvent composition achieves 83.4% yield at 98.7% conversion, and 73.2% Faradaic efficiency. Screening across tetraalkylammonium hydroxide bases shows that base identity does not significantly affect performance, providing flexibility in electrolyte selection. Methanol serves as an effective co-solvent, and RVC electrodes can be reused without loss of performance.



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2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

 # 6

Engineering Framework Defects and Metal Sites in UiO-67

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Metal-organic frameworks (MOFs) are a versatile class of high-surface-area, crystalline porous materials whose modular synthesis enables exceptional tunability of structure and function for catalytic and adsorptive applications. Variation of metal clusters and organic linkers along with post-synthetic modification strategies allows for manipulation of active-site identity, density, and environment, making MOFs powerful model systems for probing catalytic mechanisms. In this work, the influence of two structural variables, missing linker defects and post-synthetic Ti incorporation, on MOF activity in both liquid-phase and non-thermal plasma environments is examined. Missing linker defects generate undercoordinated Lewis acidic Zr(IV) sites and introduce additional porosity while Ti incorporation is expected to create stronger Lewis acid centers. UiO-67 was selected as the MOF for this study due to its high thermal and chemical stability, allowing it to accommodate substantial defect densities and post-synthetic modifications. A suite of UiO-67-derived materials with systematically varied defect concentrations and/or Ti loadings was synthesized and rigorously characterized using PXRD, N_2 physisorption, TGA, and elemental analysis to quantify textural properties, defect density, and metal incorporation. Reactivity was evaluated using two mechanistically informative Lewis-acid catalyzed probe reactions: styrene oxide ring opening with isopropanol in the liquid phase and dry methane reforming under dielectric barrier discharge plasma. The combined results reveal how structural alterations such as defect formation, framework disorder, and Ti incorporation affect catalytic behavior in different reaction environments. More broadly, this work demonstrates how systematic modification of MOF structure can be leveraged to elucidate the roles of active-site chemistry, porosity, and dielectric behavior in complex catalytic systems.

7

Framework-free *in-situ* derived metal (IV) oxyhydroxides outperform MOF in peptide hydrolysis

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Abstract: Zirconium-based metal-organic frameworks (MOFs) are widely studied as artificial proteases where the hydrolytic activity is commonly attributed to Lewis acidic Zr centers embedded within Zr_6 oxo-cluster nodes. Here, we show that such framework-confined nodes are not required for efficient peptide hydrolysis. Instead, simple zirconium salts generate highly active zirconium oxyhydroxide/oxo species in aqueous solution that outperform both a Zr-MOF and an isolated ligand-capped Zr-oxo cluster at pD 7 and 60 °C. Comparable hydrolytic activity was observed across four distinct Zr-containing starting materials, $ZrCl_4$, $ZrOCl_2 \cdot 8H_2O$, $ZrO(NO_3)_2$, and ZrOOH, indicating that the identity of the initial Zr source has little influence on the final catalytic behavior and supporting the formation of a common catalytically relevant Zr oxyhydroxide species under the reaction conditions. This is supported by the EXAFS analysis which further reveals that under neutral to basic conditions, the in situ formed Zr species are more consistent with ZrO_2-like local environments than with MOF-type Zr_6 nodes for all types of Zr-catalyst. Under acidic conditions, however, GlyGly concentration-dependent Zr_6-type clusters emerge, and at higher substrate concentrations their local structure increasingly resembles the Zr_6 nodes found in MOFs. Product selectivity is also strongly pH-dependent: highly acidic conditions favor cyclization, whereas milder conditions produce both cyclic and hydrolytic products. To mimic site-isolated inorganic centers without a MOF linker environment, ZrOOH was deposited onto a catalytically inert covalent organic framework to form ZrOOH@COF. This material showed similar intrinsic reactivity to bare ZrOOH but lower overall conversion because of reduced Zr loading, indicating that the framework itself does not promote hydrolysis. Extending this framework-free strategy across related metal oxyhydroxides revealed a Lewis acidity-dependent activity trend of $Ce^{4+} > Zr^{4+} > Hf^{4+}$, consistent with the higher activities of CeOOH and CeOOH@COF relative to their Zr analogues. Together, these results identify accessible, framework-free metal oxyhydroxide/oxo species as the dominant drivers of peptide hydrolysis in water and establish active-site accessibility, local metal speciation, and Lewis acidity as key design parameters for hydrolytic catalysis.

2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: No

8

Understanding the Energetics of CO2 Electroreduction and Sulfur Deposition on Low Index Ni Facets and Ni/YSZ(111) Using DFT

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Solid Oxide Electrolysis Cells (SOECs) represent a transformative technology for the high-efficiency conversion of CO2 into value-added chemical feedstocks. However, the commercial viability of Ni/YSZ-based cathodes is often compromised by complex surface kinetics and rapid degradation in the presence of trace impurities. In this work, we employ a multiscale approach—combining Density Functional Theory (DFT) with a potential-dependent framework—to delineate the competition between CO_2 activation and SO_2-induced inhibition at the Ni/YSZ triple phase boundary (TPB).

Our investigation into the structure-sensitivity of the Ni catalyst reveals a significant disparity in catalytic performance across different crystallographic orientations. While the close-packed Ni(111) and stepped Ni(211) surfaces are hindered by prohibitive thermochemical dissociation barriers (>190 kJ/mol), the Ni(100) facet emerges with a notably lower activation energy of 139.35 kJ/mol. Crucially, we utilize work function modulation via halide co-adsorption to demonstrate that these metallic facets are electrochemically inactive, meaning their reaction rates do not respond to applied cell polarization. In contrast, the Zr sites at the TPB serve as the primary electrochemically active site. We identify the kinetic limit of Y-doped sites reach a thermochemical plateau at low overpotentials, whereas Zr-interfacial sites maintain potential sensitivity and rate control up to -2.0 V.

Furthermore, we quantify the catastrophic impact of SO_2 impurities in the feed gas. We find that SO_2 undergoes a competitive, two-step reduction mechanism that is both thermodynamically and kinetically favored over CO_2. With a primary dissociation barrier of only 43 kJ/mol, SO_2 effectively titrates out active interfacial sites. Under cathodic bias, this poisoning is electrochemically accelerated, leading to the persistent deposition of atomic sulfur.

2026 CCP Poster Abstract
Type: (Undergraduate, [✓ **Graduate**], Postdoc)
Consideration in poster competition: ([✓ **Yes**] or no)

 # 9

Group (VI)- W(0) and Mo(0) Complexes as Efficient Catalysts for Z-Selective Alkene Isomerization

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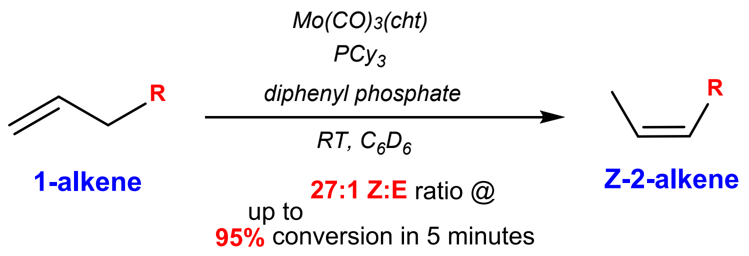
The synthesis of Z-alkenes remains challenging due to their thermodynamic instability and purification difficulties. Catalytic systems capable of converting terminal alkenes to internal Z-2 alkenes are therefore highly valuable for synthetic chemistry. Previously in our lab, cis-Mo(CO)$_4$(pip)(PCy$_3$) was identified as an active pre-catalyst for Z-selective alkene isomerization. The tungsten analogue exhibited good selectivity but lower rates and greater air sensitivity. Guided by prior DFT studies on cis-Mo(CO)$_4$(pip)(PCy$_3$), which suggest that the active species contains three carbonyl ligands, we targeted ML$_3$(CO)$_3$-type precatalysts. Cycloheptatriene molybdenum tricarbonyl (Mo(CO)$_3$(cht)) combined with tricyclohexylphosphine (PCy$_3$) and diphenyl phosphate (dpp) forms an efficient catalytic system, achieving 95% conversion of 1-octene within 5 min with high Z-selectivity (Z:E > 20:1) and turnover numbers up to ~4600. The Z-selectivity is maintained across a broad substrate scope, although catalytic efficiency decreases with strongly coordinating substrates. Other monodentate phosphines were also tested with the precatalyst and revealed that ligands with steric and electronic properties similar to PCy$_3$ provide good activity, whereas less sterically demanding and weaker electron-donating phosphines result in reduced catalytic activity and lower Z-selectivity. Kinetic studies of the Mo(CO)$_3$(cht) /PCy$_3$ system show zero-order dependence on alkene concentration and second-order dependence on total catalyst concentration, suggesting the involvement of two catalyst molecules in the mechanism. This system represents a significant improvement over previously reported catalysts for Z-selective alkene isomerization.



2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

 # 10

Synthesis and Evaluation of Novel Ga-containing CHA Zeolites for Near-Ambient Hydrogen Storage

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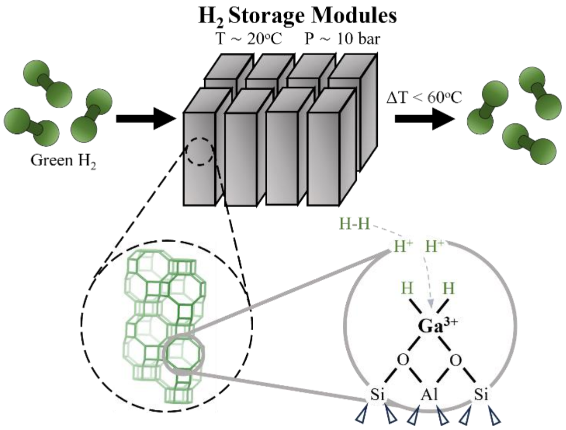
Hydrogen is essential to addressing our energy challenges and the current climate emergency. It can be generated from water via electrolysis and used in lieu of fossil fuels or as a form of long-term energy storage to support renewable energy resources. However, a critical barrier to the widespread deployment of hydrogen is its inefficient storage. Compared with the presently used physical storage methods of hydrogen, material-based methods for hydrogen storage have the potential to be more safe, cost-effective, transportable, and space-efficient[1-3]. Through chemisorption and physisorption, hydrogen could be stored with high volumetric and gravimetric densities at ambient or near-ambient conditions. Yet, no material has been able to meet all the requirements to be competitive.

In this study, we investigate the fundamental mechanisms and synthesis of a novel Ga-containing CHA zeolite (GaCHA) that can reversibly form Ga hydrides at near-ambient conditions. Compared with other material-based methods, Ga hydrides are potentially more practical, as they can reversibly store hydrogen with high density at more reasonable conditions. Reductive solid-state ion exchange (RSSIE) introduces Ga^+ cations into the extra-framework sites of the CHA framework. These cations coordinate to the negatively charged aluminate centers of the zeolite which can form $[GaH_2]^+$ in the presence of hydrogen. To maximize hydrogen storage capacity, GaCHA with low Si/Al ratios must be synthesized, but at such low ratios, the zeolite framework is much less stable. N_2 physisorption (77K), XRD, and H_2-TPR validate the synthesis of and further elucidates the formation mechanism of a stable GaCHA with a Si/Al ratio of two. In-situ FTIR verifies that hydrogen is stored within the material and quantifies the amount stored. A peak at 2036 cm^{-1} for the Ga-H bond is evident in the IR spectra when the GaCHA material is exposed to a hydrogen environment.



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2026 CCP Poster Abstract
Type: (Graduate)
Consideration in poster competition: (Yes)

11

Oxidative Dehydrogenation of Ethane via NO

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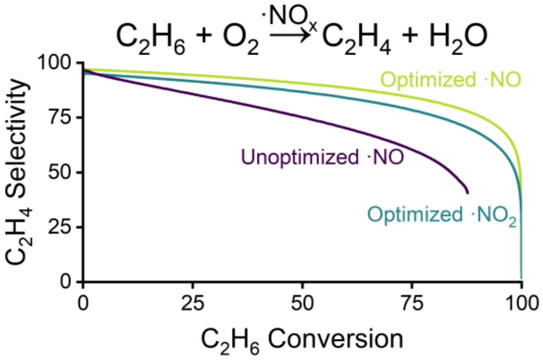
A tubular reactor model was developed to simulate the kinetics and thermodynamics of the oxidative dehydrogenation of ethane. The model was used to investigate ethylene selectivity when using NO/O_2 mixtures. OH radicals were found to drive the reaction. Two major OH-producing reactions were identified from the model: a reaction between NO and HO_2 to form HO radicals at NO volume fractions of ≥5% and H_2O_2 homolysis at NO volume fractions <5%. The reaction conditions were optimized for C_2H_6, with a maximum ethane conversion of 53% with 90% ethylene selectivity being achieved (a near 3x increase in conversion from unoptimized simulations). CO, CO_2, H_2O, He, and N_2 were explored as feed additives to control the selectivity and reaction kinetics but had a negligible impact. NO_2 was also explored as an alternative to NO; the optimizer found a maximum ethane conversion of 38% with an ethylene selectivity of 90%.[1]



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2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

12

A Predictive Framework for the Design of Doped Oxide Hydrogenation Catalysts

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Chemoselective hydrogenation of unsaturated carbon bonds can upgrade compounds into value-added chemicals.[1] Reducible metal oxides can perform selective hydrogenation of unsaturated moieties.[2] Under hydrogenation reaction conditions, oxygen vacancy sites (O_{vac}) can form on the reducible oxide surface, inducing repulsive strains between neighboring Lewis acids (i.e., metal cations). On these energetically strained cation sites, metal-bound hydrogen, a hydride, has been identified.[3] These hydrides on the oxygen vacancy sites serve as crucial intermediates in C–H bond formation, offering a kinetically feasible pathway.[2]

To further enhance catalytic performance, we investigate the modification of Lewis acid sites within oxide structures through transition metal cation substitution (i.e., doping). Employing density functional theory methods, we analyze how doping promotes surface reduction, providing active sites for hydrogenation reactions, and influences hydride species formation on the reduced sites. We further investigate doping effects on the activation barriers associated with the hydrogenation of unsaturated C–C or C–O bonds. First-principles-based microkinetic modeling (MKM) is performed to assess selectivity changes induced by doping. Starting with benzoic acid and anatase TiO_2 surfaces, we extend our scope to explore various unsaturated reactants and metal oxides, using density functional theory and thermodynamic data from open databases to guide material selection. This approach identifies descriptors for catalytic performance and develops descriptor-based kinetic models. The derived models establish a rational design framework that links the electronic behavior of reducible metal-substituted oxide catalysts to their potential for facilitating C-H bond formation in reactants of interest.

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2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: (Yes)

13

Effect of Surface VO_x Coverage on CH_3OH Oxidation by Supported VO_x/CeO_2 Catalysts: Heterogeneity of Surface Sites and Reactivity

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Introduction: Supported VO_x/CeO_2 catalysts attracted much interest because of their high redox specific activity (TOF) for alcohols/light alkanes ODH reactions. During ethane ODH, surface VO_x and CeO_x sites were proposed to undergo redox ($V^{5+} \leftrightarrow V^{4+}$and $Ce^{4+} \leftrightarrow Ce^{3+}$) for ternary supported $V_2O_5/CeO_2/SiO_2$.[1] DFT calculations, however, concluded that isolated surface VO_4 sites on model $CeO_2(111)$ thin films do not undergo redox during methanol ODH and that redox is being performed by exposed surface CeO_x sites.[2] Experimental investigations at steady state ethanol ODH conditions also suggested that only CeO_x undergoes redox.[3] In contrast, transient studies during ethanol ODH observed that both surface VO_x and CeO_x undergo redox.[4] To address this conundrum, the roles of the CeO_2 support and surface VO_x sites during methanol ODH by supported VO_x/CeO_2 powder catalysts with varying surface VO_x coverage (0.3-8 V/nm^2) were investigated with a suite of *in situ*/*operando* spectroscopic techniques.

Results & Discussion: *In situ* Raman and IR spectroscopy confirmed that multiple surface VO_x mono-oxo sites were present on the CeO_2 support at 0.3-8 V/nm^2. CH_3OH TP-IR demonstrated the different reactivity for the distinct CH_3OH-derived species. CH_3OH-temperature programmed surface reaction (TPSR) identified highly active ($T_p \sim 120$ ^{0}C) and mildly active sites ($T_p \sim 188$ ^{0}C) reactions that form HCHO upon CH_3OH chemisorption at RT and 110 ^{0}C, respectively. *Operando* DR UV-Vis-MS spectroscopy during CH_3OH-TPSR revealed that rates of HCHO formation and reduction of surface V^{5+} to $V^{4+/3+}$ are kinetically coupled, depicted in Fig.1. Interestingly, the redox CeO_2 support was found to provide lattice oxygen to re-oxidize surface $V^{4+/3+}$ before methanol was completely consumed. Surprisingly, at elevated temperatures the surface V^{4+} sites were oxidized by O* from the CeO2 support lattice (Ce^{4+} to Ce^{3+}). The results also show that supported VO_x/CeO_2 powder catalysts behave differently than the model $VO_x/CeO_2(111)$ thin films where Ce_n-OH and dynamics of V and Ce interactions are the governing factors. *Operando* DR UV-Vis-MS during CH_3OH ODH provided key insights about the redox of supported VO_x/CeO_2 catalysts at different temperatures that explains the apparent conundrum in the literature.

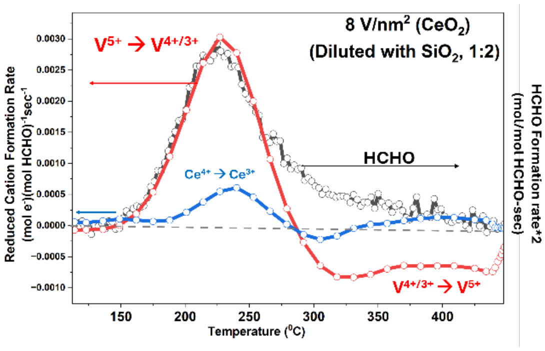

Figure 1. Formation rates of HCHO and $V^{4+/3+}$ & Ce^{3+} reduced cations *vs*. temperature for monolayer supported VO_x/CeO_2 (~ 8V/nm^2) during CH_3OH-TPSR assessed via *operando* UV-Vis-MS spectroscopy (110 ^{0}C chemisorption). The positive and negative curves on the red trace reflect reduction of V^{5+} and re-oxidation of $V^{4+/3+}$, respectively.

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2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

14

Molecular insights on branching effects in catalytic upcycling of mixed polyolefin waste

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The mitigation of the large amount of plastics waste generated today is essential for a sustainable and circular economy. Catalytic hydroconversion reactions, such as hydrogenolysis and hydrocracking, offer powerful routes for chemically upcycling plastic waste into high-value products, including fuels and lubricants. Polyethylene (PE) and polypropylene (PP) together account for nearly half of global plastic waste production, underscoring the importance of developing effective strategies for their upcycling.

Mixed polyolefin (PO) feedstocks present significant complexity, as PE exists in various forms that differ in branching density and branch length. These structural variations not only change the properties of the goods that they are used in but also affect their molecular interactions with the catalyst surface during deconstruction reactions. Enthalpic and entropic tradeoffs control which polymer preferentially segregates to the surface, which in turn determines the sequence of reactions. This competitive adsorption thus affects the product distributions obtained from these reactions.

There is a limited understanding of how polymer branching influences competitive adsorption in mixed plastic waste recycling systems. This knowledge gap hinders the modeling of deconstruction kinetics in mixed polyolefin systems, which are necessary for predicting and tuning product distributions. To address this challenge, we present a combined approach that integrates molecular simulations and isotope-labeled experiments to elucidate competitive adsorption of PE and PP, as well as linear and branched PE species, on catalyst surfaces.

Mixtures of polyolefin surrogate melts were simulated over catalysts using Replica-Exchange Molecular Dynamics (RE-MD). Linear PE preferentially adsorbs over PP on the catalyst surface over a range of molecular weights. Using Fourier-Transform Infrared Spectroscopy (FTIR), we show that the preferential adsorption of polymers in PE/PP mixtures is facilitated by the catalyst. We also show that branching dominates over molecular weight in competitive adsorption and reactivity. These insights will aid in developing a modeling framework to understand and tune product distributions from real-life polyolefin feedstocks.

15

2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: ([✓ Yes] or no)

Assessing impact of oxidant identity on reactivity, selectivities, and defect generation during MOF-catalyzed oxidations

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Metal-organic frameworks (MOFs) have a crystalline structure of metal oxide clusters with high surface areas and a high degree of isolated metal sites, which make them attractive for mechanistic investigation in metal-catalyzed reactions like selective formation of oxygenates. Here, iron-based MIL-100(Fe) is examined for liquid-phase oxidations of styrene with different oxidant identities (hydrogen peroxide (HP) versus *tert*-butyl hydroperoxide (TBHP)) in acetonitrile. HP exhibits ~4x higher oxygenate formation rates normalized by total iron content than TBHP, which is predominantly attributed to differences in the proposed oxidation mechanism across oxidants. Initial rate analysis indicates styrene oxidation by HP follows an Eley-Rideal mechanism with styrene addition to surface-bound HP-derived intermediates, while styrene oxidation by TBHP is governed by the concerted interaction of styrene and TBHP at the iron node. Differences in oxygenate product distribution between HP and TBHP are largely driven by MIL-100(Fe) structural changes during reaction, with greater HP-driven defect generation that promotes the secondary ring opening of styrene oxide to styrene glycol. The mechanism of glycol formation is determined to be Brønsted acid-catalyzed based on *in-situ* MIL-100(Fe) titrations, suggesting the creation of Brønsted acid-type defects during reaction with HP. MIL-100(Fe) pre-exposures to HP before reaction are used to further investigate the interplay between HP-driven defects and MIL-100(Fe) reactivities and oxygenate selectivities. Additionally, other characterizations, including TGA-MS, ICP-OES, and Mössbauer spectroscopy, help to elucidate a more complete picture of the Fe nodal environment during reaction with each oxidant, enabling quantification of open site densities, iron and linker leaching, and formate defects. Altogether, this work utilizes kinetic and spectroscopic techniques to investigate defects in MOF catalysts and the resultant impacts on oxidation reactivities and product selectivities.

16

2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

Impact of Alkali Cations on the electrochemical oxidation of Furfural on Gold Electrodes

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The electrochemical oxidation of furfural (FF) to furoic acid is a promising biomass valorization route,[1] yet the role of electrolyte cations composition in governing reaction pathways remains largely unexplored. Here, we present a mechanistic study of furfural electrooxidation on polycrystalline Au electrodes in alkaline media using cyclic voltammetry (CV), alternating-current voltammetry, EIS, rotating disk electrode (RDE) analysis, bulk electrolysis, and in situ SERS and ATR-SEIRAS complemented by DFT calculations, focusing on the influence of alkali metal cations (Li^+, Na^+, K^+, Cs^+).

Furfural oxidation on Au proceeds via oxygen-anchored intermediates (gem-diol and diolate species formed through a hydration pre-equilibrium) through multiple parallel pathways with distinct kinetic bottlenecks (Ox1–Ox4).[2] Ox1 and Ox2 are diffusion- and adsorption-controlled, respectively, and are selectively enhanced by Cs+, whose weakly hydrated compact double layer[3,4] stabilizes reactive diolate intermediates and substantially reduces charge-transfer resistance relative to Li+. A central finding is the identification of Ox3 as a CE mechanism: a slow interfacial reorganization of the cation–water–adsorbate layer coupled to the Au–OH to oxide (place exchange)[5,6]. In LiOH, the rigid OH_{ad}–$Li^+(H_2O)_x$ network suppresses this process entirely at scan rates above 10 mV s^{-1}, while in CsOH the more labile double layer permits reorganization but renders Ox3 sensitive to forced convection.

In situ SERS confirms oxygen-mediated adsorption through the gem-diol dianion (~1040 cm−1) and adsorbed furoate (~1395 cm−1) signatures, with markedly stronger signals in CsOH consistent with a higher-coverage ordered adlayer. ATR-SEIRAS further reveals a potential-driven structural reorganization of the furoate adlayer — from monodentate to bidentate binding — kinetically coupled to the surface oxide–hydroxide transition. Taken together, the cation effect in furfural electrooxidation arises from a complex interplay of double-layer structure, interfacial water orientation, and surface redox chemistry. These findings provide guidelines for electrolyte engineering in biomass electrooxidation: weakly hydrated cations ($Cs^+ \geq K^+$) promote intermediate stabilization and enhance activity, while hydrodynamic conditions should be tuned to preserve the interfacial configuration required by slower CE pathways.

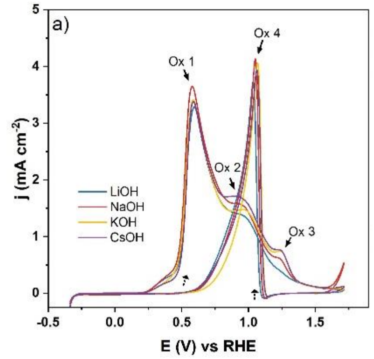

Figure 1.CVs of FF oxidation (15 mM) on Au in 0.1 M alkali hydroxides.

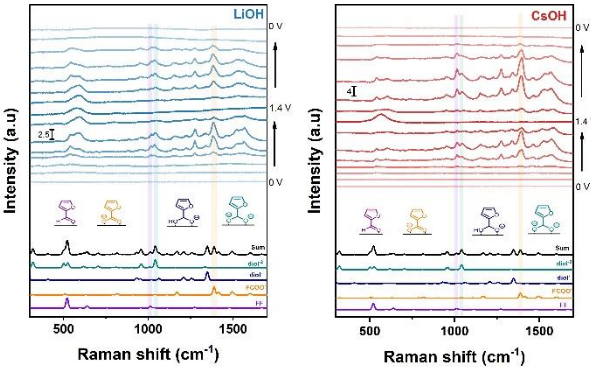

Figure 2. In situ SERS spectra recorded during furfural oxidation in LiOH and CsOH. DFT calculations are presented at the bottom.

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2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

17

Hydrolysis of a commercial polyamide 6 multilayer film over TiO_2 to enable hydrocracking and chemical recycling

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Plastic packaging represents one of the largest fractions of real-world plastic waste [**1**] and, due to its heterogeneity, faces significant challenges in recycling and upcycling. Of particular concern are polycondensation polymers, such as Nylon 6, which can deactivate upcycling catalysts and undermine mechanical recycling [**citation**]. Here, we investigate the hydrolysis of a nylon-based multilayer commercial film over anatase TiO_2 as a nitrogen-removal step to enable subsequent hydrocracking and mechanical recycling. Systematic film characterization elucidates the polymer composition, structure, and changes in the film additive profile before and after hydrolysis, and their implications for hydrocracking and mechanical recycling are discussed. Reaction temperature is shown to be an important leverage to improve hydrocracking tolerance in LLDPE mixtures containing PA6. Hydrolysis fully removes nitrogen in the form of aqueous, polymerizable Nylon 6 products and degrades additives into polyconjugated species, resulting in degraded optical properties. However, key rheological and chemical properties remain unaffected during hydrolysis, preserving the processability of the pretreated films under extrusion-relevant mechanical recycling conditions. Moreover, hydrocracking performance is comparable to LLDPE resins. Overall, this work demonstrates a robust pretreatment strategy for recycling and upcycling complex waste streams containing nylon, with broader implications for waste feedstocks that include polycondensation polymers.

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2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

18

Tandem Catalysts for Hydroconversion of Polyethylene-EVOH Multilayer Plastics

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Chemical recycling of multilayer plastic waste is hindered by oxygen-containing barrier layers such as poly(ethylene-co-vinyl alcohol) (EVOH), which generates deactivating polyaromatics during hydroconversion. This study develops a tandem catalytic strategy enabling efficient hydroconversion of well-defined five-layer polyethylene/EVOH multilayer films into liquefied petroleum gas (LPG, C_3-C_4) and naphtha (C_5-C_{12}) hydrocarbons. Pt loading was tuned to control particle size and proximity to Brønsted acid sites on BEA zeolite, where low Pt loadings produced small, intraporous particles with superior metal-specific hydrocracking activity. A complementary mesoporous hydrogenation catalyst was introduced to suppress deactivation by saturating naphthalene-like species formed from EVOH degradation. Characterization (TEM, XPS, BET) and probe reactions show that MCM-41 (2-4 nm pores) stabilized highly dispersed and reduced Pt particles with high polyaromatic hydrogenation activity. Kinetic studies revealed strong synergy between Pt/BEA and Pt/MCM-41, achieving 98% selectivity to LPG and naphtha with stable performance upon reuse. These results establish a viable catalytic route to convert high-performance EVOH multilayer films into valuable chemicals, demonstrating that multilayer barrier packaging can be engineered to deliver exceptional gas-barrier performance while remaining compatible with end-of-life chemical recycling pathways.

2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

19

Impacts of Surface and Pore Interactions on Rates and Selectivities of Polyolefin Decomposition with Zeolites

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The extensive use of single-use plastic has led to an extremely linear plastics economy, in which only a small fraction of waste plastic is recycled with the remainder landfilled, incinerated, or leached into the environment. To recover value from abundant plastic waste, research has focused on developing catalytic pathways to convert waste polyolefins into valuable hydrocarbons under mild conditions. Zeolites, with well-defined microporous networks and abundant Brønsted acid sites, have been extensively utilized in industrial hydrocarbon conversions and can be applied for the analogous chemistry of selective acid catalyzed cracking of waste polyolefins to gaseous and liquid products. Although prior studies have demonstrated that acid site accessibility[1,2] and framework topology[3] influence reactivity parameters in polyolefin decomposition with zeolites, fundamental aspects of polymer-zeolite surface interactions and reaction pathways remain less clear due to the complexity of the reaction network. In addition, the introduction of metal sites to zeolites forms bifunctional hydrocracking catalysts and introduces de- and rehydrogenation pathways to the acid mediated carbon bond scissions.[4,5] This work seeks to link framework parameters of zeolites to polyolefin decomposition rates and selectivities by using a combination of thermogravimetric analysis, (time-resolved) batch reactors, and post-reaction catalyst characterization. Rates and selectivities of gaseous hydrocarbon products in hydrogen-pressurized batch reactions are strong functions of framework pore limiting diameters. Similarly, variations in polymer molecular weight changes the relative accessibility to micropores, indicated by changes to first-order rate and deactivation constants. Upon the addition of intraparticle metal sites, product distribution saturations can be tuned through the balance of metal and acid sites. This work provides fundamental insights into rate-limiting surface interactions of polyolefins and zeolites and changes to reaction pathways across zeolite frameworks ultimately to control conversion of polyolefins into light hydrocarbon fuels at mild conditions, providing a route for "reuse" of waste carbon streams.

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2026 CCP Poster Abstract
Type: (Undergraduate, [✓ Graduate], Postdoc)
Consideration in poster competition: ([✓ Yes] or no)

 # 20

Supported Catalytically Active Liquid Metal Solutions for Energy Applications

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Supported Catalytically Active Liquid Metal Solutions (SCALMS) represent a new class of heterogeneous catalysts that combine the strengths of both homogeneous and heterogeneous systems. In these systems, transition metals are dissolved in molten gallium droplets deposited on porous supports, creating unique surface ensembles containing atomically isolated active sites that are unconstrained by rigid lattices and responsive to reaction conditions. These features enable exceptional selectivity, activity, and resistance to coking/poisoning at ultra-low noble-metal loadings.

In this work, we are developing a general and scalable synthesis method for Ga-based SCALMS using strong electrostatic adsorption (SEA) of gallium precursors followed by liquid-phase reduction and galvanic displacement to incorporate secondary metals (e.g., Pd, Ni, or Ru). The resulting catalysts will be evaluated in a packed-bed reactor for low-temperature dry reforming of methane (DRM) to probe the origins of CH_4 activation, including apparent activation energies, reaction orders, and rate-limiting steps. Acetylene hydrogenation will serve as an ensemble-sensitive probe reaction to interrogate how liquid-metal surface dynamics and atomic isolation influence catalytic pathways and selectivity toward ethylene. This research aims to establish robust design principles for industrially viable SCALMS while addressing key limitations of traditional solid catalysts in energy applications. We are using a Pt monometallic catalyst system to study the ensemble effect. The XRD and catalyst evaluation data are shown here for the acetylene hydrogenation reaction of Pd with different particle and ensemble sizes.

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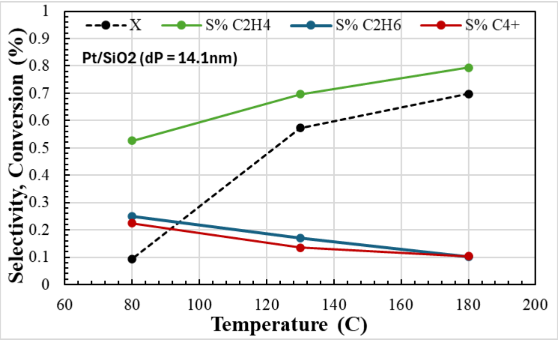

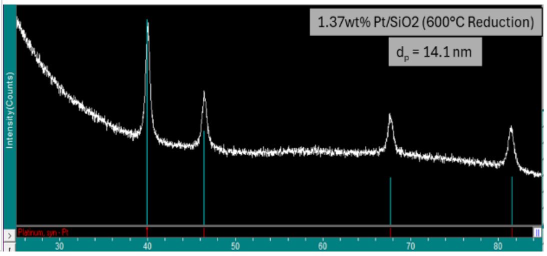

21

2026 CCP Poster Abstract
Type: (Graduate)
Consideration in poster competition: (Yes)

Are Defects Always Beneficial in Photocatalysis? Insights from Organophosphate Detoxification

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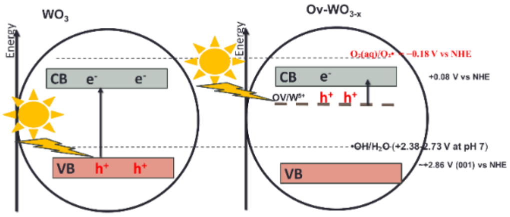
Defect engineering is widely used in catalysis and photocatalysis because defects can enhance adsorption, increase accessible surface area, and improve surface reactivity. However, whether defects always improve photocatalytic performance remains an important open question. Here, we address this issue in the visible-light detoxification of phosphate-based toxic compounds using dimethyl methylphosphonate (DMMP) as a simulant for herbicides, pesticides, and nerve-agent-related organophosphorus toxins. Because these compounds can readily contaminate groundwater and surface water through agricultural use, we focus on a solution-phase detoxification strategy under solar irradiation. Although DMMP degradation has been reported over TiO_2 in the gas phase, its wide bandgap (Eg=3.2eV) limits its efficiency under visible light.[1,2] Here, we investigate tungsten trioxide (WO_3), a visible light active semiconductor (Eg ~2.6 eV), and oxygen-vacancy-engineered WO_{3-x} (OV-WO_{3-x}) as photocatalysts for DMMP detoxification under UV (365 nm) and blue visible light (450 nm), benchmarking their activity against P25-TiO_2.

OV-WO_{3-x} samples were prepared by reduction under 3% H_2:97% N_2 at 350, 400, 450, and 500 °C. The formation of oxygen vacancies was confirmed by Raman spectroscopy and oxygen-uptake studies, together with optical changes observed by solid-state UV-Vis diffuse reflectance spectroscopy. Reaction kinetics and mechanistic pathways were monitored by ^{31}P NMR, while transient intermediates were probed using coupled ^{1}H-^{31}P NMR along with ^{1}H and ^{31}P NMR product analysis. The absence of hydrocarbon signals in ^{1}H NMR and the observation of phosphate as the final phosphorus-containing product in ^{31}P NMR are consistent with near-complete mineralization of DMMP to CO_2, H_2O, and inorganic phosphate.[1] Preliminary results show that WO_3-based catalysts are active under visible-light irradiation. Mechanistic investigations indicate that reactive oxygen species are generated through hole-driven water oxidation and electron-driven O_2 reduction, as further evaluated by methanol substitution and N_2 purging experiments.

Importantly, increasing the reduction temperature of WO_3/increasing OV concentration led to lower photocatalytic activity, demonstrating that defect formation does not always enhance photocatalysis. Solid-state UV-Vis diffuse reflectance spectra reveal the growth of a visible-NIR absorption band at higher reduction temperatures, attributed to polaron-mediated electronic transitions from oxygen-vacancy defect states to the conduction band.[3] These changes are accompanied by an apparent increase in the indirect bandgap from 2.6 eV to 3.0 eV and the formation of lower-power defect-state holes with weaker oxidation power than valence-band holes, thereby suppressing water oxidation and the photocatalytic detoxification rate. PXRD shows that the monoclinic WO_3 crystal structure is largely retained at moderate reduction temperatures, whereas the 500 °C reduced sample exhibits formation of $WO_{2.72}$ and shows no catalytic activity. Overall, this work demonstrates that oxygen vacancies can either enhance or suppress photocatalysis depending on how they modify the electronic structure, while also establishing WO_3 as a promising visible-light photocatalyst for solution-phase detoxification of organophosphorus toxins with no toxic intermediates.



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2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

22

Elucidating the roles of polymer diffusion and active site location in polyolefin hydrocracking using metal encapsulated zeolites

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Hydrocracking offers a promising route for polyolefin upcycling, but its efficiency is hindered by mass transport challenges that inhibit hydrocracking kinetics, independent of intrinsic catalytic activity. To address this, we selectively encapsulate Ni nanoparticles within ZSM-5 zeolite, enabling spatial control over metal and Brønsted acid site placement. This platform enables systematic evaluation of how polymer molecular weight, viscosity, and chain architecture influence diffusion and catalytic performance. Internal metal-acid site proximity enhances activity but increasing polymer chain length and viscosity introduces substantial diffusion limitations. Polymer branching further modulates pore accessibility and product selectivity, particularly toward light alkanes. Moreover, we demonstrate that the metal and acid sites on the external surface play a critical role in facilitating the diffusion of reaction intermediates into the zeolite pore network. Together, these findings underscore the importance of tuning active site distributions and pore confinement to balance activity, selectivity and mass transport, providing design principles for next generation hydrocracking catalysts.

2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

23

Impacts of Coordination Spheres on Alkylation Reactions in Varied Aluminosilicate Environments

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The role of water in zeolite-catalyzed reactions has attracted great interest in catalytic research; water, often present as either a co-feed reactant or a byproduct, can alter the local environment near the active sites and thereby influence the catalytic chemistry.[1] This behavior is more pronounced in aqueous phase environments where the solvation effects complicate the interactions between guest molecules and active sites, as exemplified in industrial biomass conversion processes.[1,2] Here, reaction microenvironments and solvent effects are probed using the liquid-phase Brønsted acid-catalyzed Friedel-Craft alkylation of hydrophobic mesitylene (TMB) and hydrophilic benzyl alcohol (BA), which occurs exclusively on the external surface of medium pore MFI, but can occur within larger micropores of BEA and mesopores of Al-MCM-41.[3] Total and external Brønsted acid site densities of MFI samples with varying aluminum density (Si/Al = 25-140) and other aluminosilicates with larger pores (BEA-13 and Al-MCM-41) were quantified by n-propylamine temperature-programmed desorption (TPD) and TMB-dibenzyl ether alkylation,[4] respectively. Initial rate studies were conducted with varying water loading (0-0.5 M) to evaluate the impacts of water on reactivity and determine the change in reaction microenvironments. At low water loading, the turnover rates of all catalysts decreased to approximately 40 % of their values under anhydrous conditions, suggesting similar water-zeolite-guest interactions across different microenvironments. However, the extent of rate inhibition varies across materials at high water loading, reflecting differences in material hydrophobicity and the interactions under confined/unconfined environments. Complementary water uptake studies further provide evidence of strong competitive adsorption of water to active sites. Together, these water uptake and kinetic studies provide insights into water-zeolite-guest interactions under distinct microenvironments, advancing a fundamental understanding of water's effects in aqueous-phase catalytic systems.

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2026 CCP Poster Abstract
Type: Postdoc
Consideration in poster competition: Yes

24

Acrolein Synthesis from Oxidative Coupling of Biomass-Derived Methanol and Ethanol by Supported Monolayer MoO_x/Fe_2O_3 Catalyst

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The global acrolein market is substantial, with an estimated value of around USD 1,178 million in 2024. Currently, acrolein is primarily produced from fossil-derived propylene. Therefore, it is highly significant to develop sustainable methods for acrolein production from renewable feedstocks for both industrial and environmental interests. Here, we report the selective formation of acrolein from biomass-derived methanol and ethanol oxidation over a model supported monolayer MoO_x/Fe_2O_3 catalyst. In this study, a well-defined surface MoO_x monolayer on Fe_2O_3 was synthesized, characterized, and investigated for acrolein synthesis.

A model supported monolayer MoO_x/Fe_2O_3 catalyst was synthesized by incipient-wetness impregnation. This model MoO_x/Fe_2O_3 catalyst was characterized by Raman spectroscopy, infrared spectroscopy (IR), and high-sensitivity low-energy (HS-LEIS), which confirmed complete surface coverage of Fe_2O_3 by a monolayer of surface MoOx species without formation of bulk crystalline MoO_3 or $Fe_2(MoO_4)_3$ phases. IR results revealed that alcohol adsorption on Fe_2O_3 forms surface Fe-OCH_3/OCH_2CH_3 species. After the MoO_x deposition on the surface of the Fe_2O_3 support, the surface MoO_x monolayer replaced surface Fe-OCH_3/OCH_2CH_3 species with surface Mo-OCH_3/OCH_2CH_3. Temperature-programmed surface reaction (TPSR) demonstrates that methanol selectively forms only formaldehyde on the surface Mo redox sites, indicating that acid-base reactions on Fe_2O_3 were completely suppressed by the surface MoO_x monolayer. During ethanol oxidation, acetaldehyde forms as the redox reaction product. Under mixed methanol/ethanol and O_2 flowing conditions, the dynamic surface MoO_x redox sites enabled C-C coupling leading to acrolein (CH_2=CHCHO) formation. Operando UV-Vis spectroscopy showed that the presence of gas phase O_2 keeps the sample fully oxidized, which is consistent with a surface Mars-van Krevelen mechanism.

By establishing clear structure-function relationships for the well-defined model catalyst of supported monolayer MoO_x/Fe_2O_3, these findings offer significant guidance for the rational design of next-generation oxidation catalysts. Ultimately, this study enables new and sustainable pathways for producing high-value chemicals from renewable biomass-derived feedstocks.

2026 CCP Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

 # 25

Effect of Reactor Configuration on Radical-initiated Low-temperature Polystyrene Pyrolysis

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In 2019, 320 million metric tons of plastic waste were generated;[1] only 9% plastic waste was recycled. Research has focused on physical and chemical recycling strategies for plastic wastes, especially for polyethylene (PE) and polypropylene (PP). Industrial recycling is in practice centered around pyrolysis, which requires high temperature to break the polyolefin backbone for initiation. Radical initiators can theoretically lower the bond breaking energy barrier by decomposing into radicals at low temperature and transfer radicals centers to the polymer chains. It has been shown that dicumyl peroxide (DCP) can promote the low-temperature pyrolysis of PP. This study investigates the low-temperature pyrolysis of PS aided by DCP across three different scales, focusing on the effect of reactor configuration on PS deconstruction.

Initial experiments conducted in a semi-batch Parr reactor showed that extended reaction time and high temperature increased the liquid product yield, but higher initiator load unexpectedly reduced the liquid product yield. We hypothesized that generated radical species can rapidly evaporate and escape the reactor before having sufficient contact with the viscous polymer melt. To mitigate the loss, the reaction was transitioned into a closed batch reactor to prolong the residence time of the radical intermediates. Liquid yield increased around 40% compared to that in the semi-batch system, accompanied by a significant drop in number average molecular weight (M_n). However, decreased selectivity towards styrene monomer was the trade-off. Finally, thermogravimetric analysis (TGA) was employed as an idealized, thin-layer reactor to demonstrate the intrinsic feasibility and potential of the use DCP-initiated low-temperature degradation. These findings suggest future reactor design must prioritize radical-substrate contact and residence time of active species to prevent the loss of chemical driving force.

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2026 CCP Poster Abstract
Type: (Graduate)
Consideration in poster competition: Yes

 # 26

Catalytic Glycolysis of Polyester-Spandex Blends

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The rapid growth of global textile production (>120 million tons annually) and the dominance of polyester (>50% of total fibers) have created an urgent need for scalable chemical recycling strategies[1]. However, nearly 80% of textile waste is still landfilled, largely due to the complexity of blended fabrics and the lack of efficient separation technologies[2]. Among these, polyester-spandex blends represent a particularly challenging and increasingly prevalent waste stream, as spandex is incorporated into up to ~20–30% of garments yet is difficult to detect, separate, and process[3,4]. Conventional recycling approaches often fail, highlighting a critical gap between idealized single-polymer studies and real-world feedstocks.

In this study, we investigate the impact of spandex on the glycolytic depolymerization of polyethylene terephthalate (PET) under microwave-assisted conditions using heterogeneous catalysts. Compared to pure polyester, polyester-spandex blends exhibit a significant reduction in monomer yield, whereas polyester–cotton blends show no such limitation, indicating a distinct inhibitory role of spandex.

Systematic model experiments and spectroscopic characterization demonstrate that this yield suppression originates from interactions between spandex, polyester, and the catalyst. To overcome this limitation, we explore a new class of catalysts with tunable active centers. These materials show improved tolerance toward spandex-containing feeds.

This work bridges the gap between model polymer recycling and realistic textile systems, providing mechanistic insight into catalyst deactivation and guiding the design of robust catalytic processes for complex waste streams.

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2026 CCP Poster Abstract

 # 27

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Bimetallic CuPd Catalysts Supported on AlOOH with -OH-riched Surface for C_2H_2 Semi-Hydrogenation

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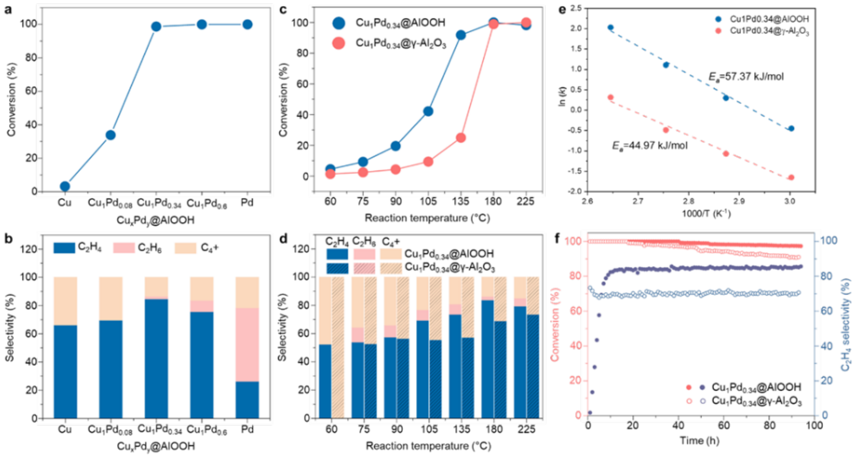
Boehmite AlOOH has been reported as support for C_2H_2 semi-hydrogenation due to its hydroxylated surface and high concentration of OH vacancies, which are conducive to highly efficient hydrogen activation. [1, 2] In this work, ultra-thin AlOOH was prepared by a simple hydrolysis reaction of aluminum. Then, CuPd bimetallic sites were loaded onto AlOOH by the dry impregnation method. First of all, the optimized Cu:Pd ratio was found to reach the balance of conversion and selectivity for the C_2H_2 semi-hydrogenation reaction. Furthermore, as a comparison, CuPd bimetallic system was also loaded onto the commercial γ-Al_2O_3. The differences in catalytic performance show that the conversion of $Cu_1Pd_{0.34}$@AlOOH is at least 3.2 times higher than $Cu_1Pd_{0.34}$@γ-Al_2O_3 when the temperature is below 180 °C. In addition, $Cu_1Pd_{0.34}$@AlOOH has 84% of selectivity for C_2H_4 formation compared to 69% of $Cu_1Pd_{0.34}$@γ-Al_2O_3. Also, during a 95 hr long-run testing, $Cu_1Pd_{0.34}$@AlOOH shows good stability, which proves its potential for practical application.



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