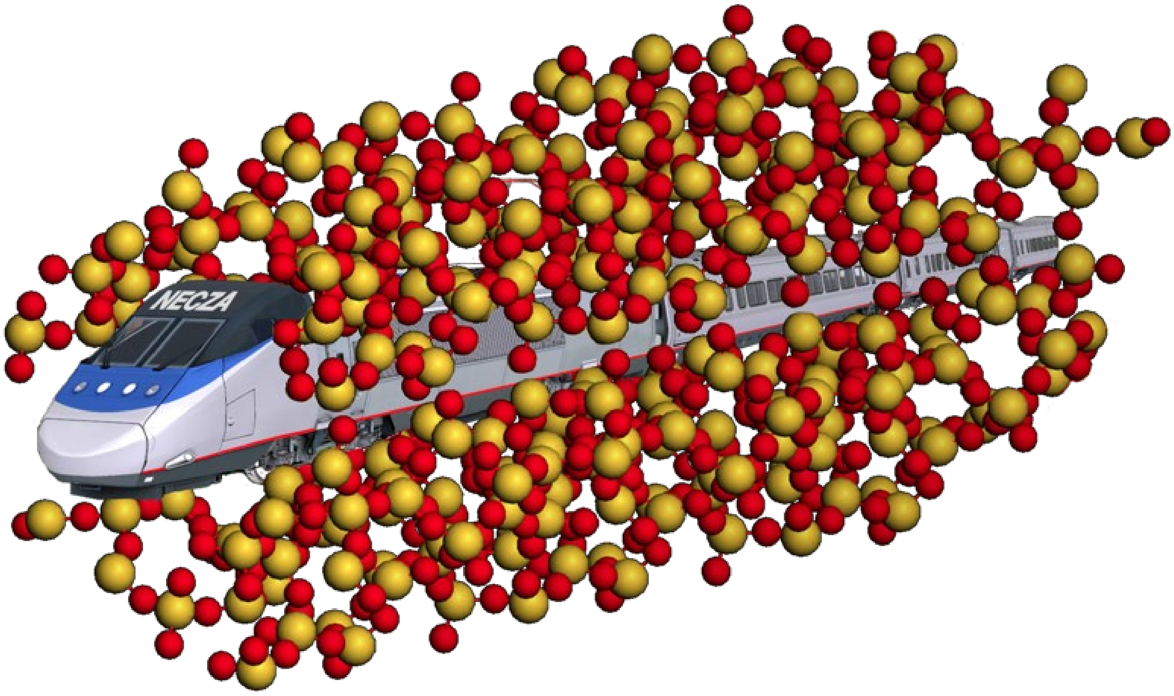
NECZA 2025

The 29th Meeting of the
North-East Corridor Zeolite Association



Friday, December 5, 2025

The Villanova Room

Connelly Center

800 E. Lancaster Ave.

Villanova University

27th Annual NECZA Meeting – Organizing Committee

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8:15 – 8:55	***Registration, Breakfast, Poster Setup***
8:55 – 9:00	***Welcome Remarks***
9:00 – 9:40	Christopher Nicholas (Låkril Technologies) “FAU Frameworks for Catalytic Dehydration, Sustainable Pathways to Bio-Based Acrylics”
9:40 – 10:20	Gennady Gor (New Jersey Institute of Technology) “Coupling Adsorption and Mechanics in Zeolites”
10:20 – 11:00	***Coffee Break – Poster Session I***
11:00 – 11:40	Christopher Paolucci (University of Virginia) “Cation Solvation Effects for Zeolite Catalyzed Oxidation Reactions”
11:40 – 12:20	***Poster Session II***
12:20 – 1:30	***Lunch and Business Meeting***
1:30 – 2:10	Panel Discussion: New Directions in Zeolite Research & Applications: Challenges, Opportunities, and Future Prospects
2:10 – 2:40	Selected Poster Presentations (2 x 15-min each)
2:40 – 3:00	***Coffee Break***
3:00 – 3:40	Sheima Khatib (Virginia Tech) “Designing Stable Mo-Based Zeolite Catalysts for Methane Dehydroaromatization: Linking Active-Site Location, Bimetallic Promotion, and Activation Chemistry”
3:40 – 4:20	Trong Pham (ExxonMobil) “Zeolite Design: From Micropores to Extra-Large Pores”
4:20 – 4:30	***Final Remarks and Meeting Adjournment***
5:30 onwards	***Dinner (for registered banquet participants) at LaScala’s Fire,***

FAU Frameworks for Catalytic Dehydration, Sustainable Pathways to Bio-Based Acrylics

Christopher Nicholas
Låkril Technologies, 2225 W Harrison St. Suite 102, Chicago, IL 60612

ABSTRACT

Acrylic acid and the four primary acrylate derivatives are the cornerstone of a $12B market with broad application across coatings, adhesives, and the super-absorbent polymers industries. AA and acrylate derivatives are currently produced through a petroleum-derived value chain from propylene creating significant CO_2 emissions; about 3.5 kg CO_2 / kg AA. While AA-derived products are an integral part of modern society, more sustainable and eco-friendly production methods are necessary. Consumers increasingly seek sustainable, non-petroleum-based products in a variety of market segments. We focus on the use of feeds derived from lactic acid, a product sustainably fermented from a range of bio-derived sugar sources.

Our novel bifunctional catalytic process converts biomass-derived lactic acid to acrylates and acrylic acid at >90% yield. The FAU zeolite is modified with engineered bases such as amines to achieve these high yields. The catalytic dehydration of lactates to acrylic acid brings a number of challenges we discuss. Among them are A) control of competing reaction mechanisms, with dehydration and decarbonylation favored under certain reaction conditions, B) characterization of oxygenated products produced during reaction, C) impacts of water on catalysis and hydrolysis of alkyl lactates, and D) impacts of the FAU framework composition on catalysis.

BIOGRAPHY

Dr. Nicholas is the Co-Founder and President of Låkril Technologies, the startup he created in mid-2021 to commercialize a catalytic process for bio-based acrylic production. Låkril Technologies was just recognized as one of C&EN's 10 Startups to Watch in 2025. His drive is to catalyze sustainability in chemical processes and has raised over $6M through a multi-agency SBIR and private strategy. Prior to founding a business based on sustainable catalysis, he worked 15 years at Honeywell UOP in technical and managerial roles primarily focused on inventing and catalytically testing new materials and processes. Specific areas included: heterogeneous catalytic processes including olefin oligomerization, synthesis of inorganic materials (primarily metal oxides and zeolites), process engineering, molecular adsorption, and olefin metathesis. He has received the 2020 Herman Pines Award in Catalysis from the Chicago Catalysis Club and the 2022 Award for Excellence in Catalysis from the Southwest Catalysis Society.

Chris earned his Bachelor of Arts from Kalamazoo College and a PhD at Northwestern University. Chris is a 25-year ACS Member and an AIChE Fellow who is an inventor on more than 120 US and foreign patents and coauthor of 35+ peer-reviewed journal articles and a book chapter. Along with responsibilities as a member of the Editorial Advisory Boards of *ACS Catalysis* and *Industrial & Engineering Chemistry Research*, he has been in leadership for the Chicago Catalysis Club and the Chicago AIChE local section.

Cation Solvation Effects for Zeolite Catalyzed Oxidation Reactions

Christopher Paolucci

Department of Chemical Engineering, University of Virginia, Charlottesville, Virginia 22904

ABSTRACT

Ion exchanged zeolites are used in catalytic applications ranging from hydrocarbon upgrading to emissions abatement. Under some conditions, ions can be liberated from the zeolite framework and mobilized by solvent molecules, coupling attractive features of homogeneous and heterogeneous catalysis. Here, I discuss our recent results for metal-exchanged zeolite catalyzed Wacker oxidation and oxidative activation of ethane where we show that metal ions are solvated under reaction conditions, and solvation impacts the reaction mechanism.

The first example, Wacker oxidation, is a well-known redox process involving Cu and Pd ions where the formation of acetaldehyde is speculated to occur on Pd^{2+} ions. While the homogeneous counterpart proceeds by having Cl^- stabilize the metal ions, the anionic AlO_2^- sites of metal-exchanged zeolites can charge compensate Pd, eliminating the need for Cl^-. A major challenge with the heterogeneous catalyst is deactivation due to coking and sintering. We show that the Pd ions are solvated by H_2O and NH_3 under reaction conditions, and relative fractions of these two molecules compete with organic molecules, consequently suppressing oligomerization and coke formation.

Similarly, NH_3-solvated Co ions supported on MFI zeolites catalyze oxidative activation of ethane. Rates measured at different characteristic separations between cobalt ions demonstrate reactions among C_2H_6 and O_2 occur at isolated mononuclear cobalt sites, however, the addition of NH_3 forms oxygen-bridged binuclear cobalt-amine complexes. Computational results and UV-vis spectroscopy show that these binuclear species form by dimerization of mobile Co-amine complexes. Interestingly, confinement within zeolite frameworks stabilizes these complexes relative to their homogeneous analogues.

BIOGRAPHY

Christopher Paolucci joined the Department of Chemical Engineering at the University of Virginia in Fall 2018 and was promoted to Associate Professor in 2024. He received his BS in Chemical Engineering from the University of Notre Dame in 2012, and his PhD in Chemical Engineering from the University of Notre Dame in 2017 under the guidance of William F. Schneider (2012-2017) and as a visiting scholar at Purdue University under the guidance of Fabio Ribeiro, Nicholas Delgass, and Rajamani Gounder (2015). He continued his research in machine learning guided materials screening between fall 2017 and spring 2018 in the group of Jens Nørskov and Thomas Bligaard at Stanford University. Chris' expertise is the application of electronic structure calculations, molecular dynamics, Monte Carlo simulation, and kinetic modeling to problems in materials science and heterogeneous catalysis. His main research areas of interest are catalyst stability and catalyst dynamics under reaction conditions. He received the ACS PRF Doctoral New Investigator award in 2021 and the NSF CAREER award in 2022. He served as a director of the Catalysis and Reaction Engineering Division of AIChE from 2019-2021, was the president of the Southeastern Catalysis Society in 2023-2024. He is currently the fall programming chair for the ACS Catalysis Division and an Associate Editor for Applied Catalysis B: Energy and Environment.

Coupling Adsorption and Mechanics in Zeolites

Gennady Gor
Otto H. York Department of Chemical and Materials Engineering, New Jersey Institute of Technology, 323 Dr. Martin Luther King Jr. Blvd., Newark, New Jersey 07102

ABSTRACT

Most applications of zeolites involve adsorption. Adsorption of guest species is known to affect the host framework, which is particularly manifested as adsorbent deformation [1]. Zeolites are no exception: for example, adsorption of CO_2 in zeolites 13X and 4A induces small but measurable strains on the order of 0.1% [2]. Interestingly, while the CO_2 adsorption isotherms of 13X and 4A are quite similar, their deformations differ markedly -- 4A expands, whereas 13X first contracts and then expands. To elucidate the microscopic origin of this behavior, we performed coupled molecular dynamics and Monte Carlo simulations, which allowed us to capture both gas adsorption and the resulting framework deformation [2].

These studies raised another question: does adsorption also alter the mechanical properties of zeolites, such as their elastic moduli? We addressed this question using molecular simulations [3], which showed that CO_2 adsorption in zeolites 13X and 4A leads to a nearly twofold increase in their elastic moduli. Our group is currently developing an experimental method for measuring the elastic moduli of porous materials during adsorption. I will share details of our sorption–ultrasonic method [4] and present preliminary results for zeolites.

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BIOGRAPHY

Dr. Gennady Gor is an Associate Professor of Chemical and Materials Engineering at the New Jersey Institute of Technology (NJIT). He earned his Ph.D. in Theoretical Physics from St. Petersburg State University in 2009 and conducted postdoctoral research at Rutgers University, Princeton University, and the U.S. Naval Research Laboratory before joining NJIT in 2016.
Dr. Gor leads a research group that integrates molecular simulations, theory, and experiments to study the interactions of fluids with porous and soft materials. His current work spans confined liquids and electrolytes, atmospheric aerosols, and ultrasound propagation in porous media. He is the author of more than 80 peer-reviewed publications, a recipient of the NSF CAREER Award (2020), and serves as Associate Editor of the journal Adsorption.

Designing Stable Mo-Based Zeolite Catalysts for Methane Dehydroaromatization: Linking Active-Site Location, Bimetallic Promotion, and Activation Chemistry

Sheima J. Khatib
Department of Chemical Engineering, Virginia Tech, Blacksburg, Virginia 24061

ABSTRACT

Methane dehydroaromatization (MDA, $6\ CH_4 \rightarrow C_6H_6 + 9\ H_2$) represents a direct route for converting methane into value-added products such as benzene and hydrogen without co-feeds or oxidants. The process offers a promising pathway for distributed valorization of stranded shale gas, enabling modular on-site conversion that mitigates transportation and flaring challenges. Zeolite-supported molybdenum catalysts (Mo/ZSM-5) remain the benchmark systems for this reaction; however, their commercialization is hindered by rapid deactivation and limited control over the active site formation.

Our group has conducted a systematic investigation aimed at uncovering structure–function relationships that govern activity and stability in MDA catalysts. We have shown that the activation protocol used to form Mo carbide species from their oxidic precursors is a decisive factor in achieving long-term catalyst stability. Through in situ/operando X-ray absorption spectroscopy and complementary ex situ characterizations, we have found that the local environment of Mo in the as-prepared state plays a secondary role compared to the conditions under which carburization occurs.

Building upon these insights, we have explored the effects of secondary transition-metal promoters (X = Fe, Co, Ni) and the spatial distribution of active sites within the zeolite. We have employed controlled synthesis strategies to confine or exclude metals from the zeolite channels and external surface. Our findings reveal that promoter effects and the extent of Mo–X synergy depend critically on the relative location and proximity of metal and acid sites: internal sites favor stable benzene formation, while external sites accelerate coke formation. Additional surface modifications through silanation and selective metal extraction confirmed that external Brønsted acid sites are more detrimental than external Mo species, as they predominantly promote oligomerization and coke formation.

Altogether, these studies provide new mechanistic understanding of how metal–acid interactions and the spatial arrangement of active sites within zeolite frameworks govern MDA performance. They also establish rational design principles for tuning metal location and activation chemistry to enhance the durability and selectivity of zeolite-based catalysts for methane valorization.

BIOGRAPHY

Sheima J. Khatib is an Associate Professor in the Department of Chemical Engineering at Virginia Tech. She received her PhD in Chemical Physics in 2007 from the Autonomous University of Madrid and the Institute of Catalysis and Petrochemistry (CSIC) (Spain). She continued her research from 2008-2010 as a postdoc in the Institute of Physical Chemistry “Rocasolano” also in Madrid, and then moved to Virginia Tech for a second postdoc position. She then joined the department of chemical engineering at Texas Tech University in 2015, where she worked for seven years, first as assistant and then as associate professor. She finally moved back to Virginia Tech in Fall of 2022. Her expertise is in studying structure-activity relationships, adsorption microcalorimetry and membrane technology applied to heterogeneous catalysis. Her main areas of interest are natural gas conversion, dehydroaromatization, membrane reactors, catalyst stability, determination of deactivation and regeneration pathways. She received the 2019 NSF CAREER Award for a project combining methane dehydroaromatization with membrane technology. Dr. Khatib is also passionate about exploring new engineering education methods in her classes and places much emphasis on teaching, having received multiple teaching awards and honors including the 2022 Jerry S. Rawls Outstanding Undergraduate Educator Award, 2019 Texas Tech Alumni Association Award, 2017 George T. and Gladys Abell-Hanger Faculty Award at Texas Tech University, and the 2017 and 2018 AIChE student chapter awards, also at Texas Tech. In 2022 she was inducted into the Texas Tech Teaching Academy. She has also taken several leadership roles in the chemical engineering and catalysis communities, including as programming chair for the Catalysis and Reaction Engineering Division (CRE) of the AIChE (2022,2023), chair of the CRE Diversity and Inclusion Task Force (2022), and scientific chair for the 29th North American Catalysis Society Meeting (NAM29) (2025). She currently serves as an editor for the Chemical Engineering Journal (Elsevier).

ZEOLITE DESIGN: FROM MICROPORES TO EXTRA-LARGE PORES

Trong Pham, Allen Burton, Andre Sutrisno, Eugene Terefenko[(a)]
Evgeniia Ikonnikova, Tom Willhammar[(b)]
(a)ExxonMobil Technology & Engineering Company, Clinton, NJ, USA
(b)Stockholm University, Stockholm, Sweden

ABSTRACT

A new aluminosilicate zeolite, EMM-68, structurally related to the CHA framework used in DeNOx and methanol-to-olefins (MTO) catalysis, has been synthesized using 1,2,3-trimethyl-4,5,6,7-tetrahydrobenzimidazolium as the structure-directing agent (SDA). EMM-68 features a 10 × 8 × 8 channel system and a spacious cavity measuring 8.0 × 9.4 × 7.7 Å, as determined by in-house X-ray diffraction using the FOCUS method.

Large and extra-large pore zeolites—defined by channels formed from 12 or more tetrahedral atoms—are critical materials for industrial applications such as shape-selective catalysis, large molecule separation, transalkylation, fluid catalytic cracking (FCC), and hydrocracking of heavy oil fractions. In this study, we report the synthesis of an extra-large pore zeolites: EMM-72 (SFN framework, 6.2 × 8.5 Å), using tetra- and penta-methylbenzimidazolium as the OSDAs. These SDAs are effective across a broad range of aluminosilicate compositions, with Si/Al ratios as low as 15. In EMM-72, the additional methyl group in the SDA enhances fit within the 14-ring pockets, promoting greater molecular spacing in the final framework compared to EMM-57 (DON framework type). By extending benzimidazolium and tetrahydrobenzimidazolium molecules with longer alkyl chains, we successfully synthesized multi-dimensional large-pore zeolites EMM-70, EMM-73, EMM-75, and EMM-76. Stability under hydrothermal conditions and energy optimization calculations highlight the importance of host–guest interactions between SDAs and the zeolite framework in phase selection.

Our results suggest that fused 5- and 6-ring organic compounds are promising SDAs for directing the formation of large and extra-large pore zeolites. These materials will be further explored for catalytic and adsorption applications involving bulky hydrocarbons and shape-selective transformations beyond the limitations of conventional large-pore zeolites.

BIOGRAPHY

Trong Pham's research centers on the synthesis and functional modification of nanoporous materials, including zeolites and metal-organic frameworks (MOFs), with a focus on their applications in separation and catalysis within the petrochemical industry. He earned a B.S. in Chemistry from Vietnam National University and a Ph.D. in Chemical Engineering from the University of Delaware, Newark, DE, under the supervision of Professor Raul Lobo. Following his doctoral studies, he returned to Vietnam and served for two years in the Department of Chemistry at Vietnam National University. Since 2019, he has been working at ExxonMobil Technology and Engineering Company in Annandale, NJ.

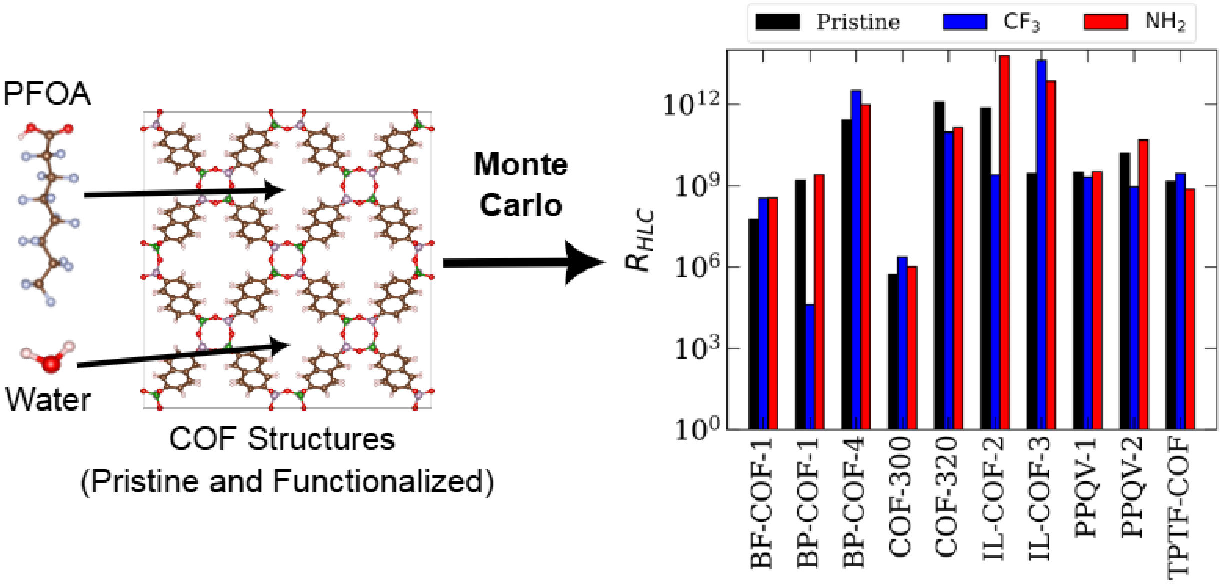
POSTER ABSTRACTS

2025-NECZA Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

Design Principles for PFAS Adsorption in Covalent Organic Frameworks

Mottern, D.D.,[1], Kolesnikov, A.L.,[1,2] Gor, G.Y.,[1] Young, J.[1,3]
[1] Otto H. York Department of Chemical and Materials Engineering, New Jersey Institute of Technology,
323 Dr. Martin Luther King Jr. Blvd., Newark, New Jersey, 07102
[2] Institut fur Nichtklassische Chemie e. V., Permoserstrase 15, 04318 Leipzig, Germany
[3] Matlantis Inc., 1 Broadway, Cambridge, MA, 02142

Recent concerns over the accumulation of per- and poly-fluoroalkyl substances (PFAS) in surface and groundwater sources have stimulated research into novel porous materials for selective PFAS adsorption. Covalent organic frameworks (COFs) represent one of the promising families of materials for this application. Here, we investigated the effects of the chemistry and structure of COFs on the adsorption of perfluorooctanoic acid (PFOA), a commonly seen PFAS molecule. Through Monte Carlo (MC) simulations, we found that nitrogen-based COFs tend to show high potential for PFAS adsorption. We also see that the porosity of a COF has a significant effect on PFOA adsorption, with higher porosity structures exhibiting lower potential for PFAS adsorption than those with moderate porosity. We additionally investigated the effects of COF functionalization with -CF3 and -NH2 functional groups, showing that both functional groups strengthen interactions between the PFOA molecule and COF, but may decrease the porosity needed for effective adsorption of PFOA. For COFs with large enough pores, the addition of these functional groups can greatly improve the adsorption of PFOA and could allow for the improved capture of PFAS from aqueous environments [1].



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2025-NECZA Poster Abstract
Type: Graduate
Consideration in poster competition: (YES)

Mapping Synthesis–Morphology Relationships in Porous Organic Frameworks

Feng K. F., Snyder, M. A.
Department of Chemical& Biomolecular Engineering, Lehigh University, 27 Memorial Dr. W, Bethlehem, 18015

Reticulation of covalent organic frameworks (COFs) results from the assembly and covalent attachment of organic building block monomers.[1] Imine-linked COFs, particularly desirable for their demonstrated stability, benefit from error correction during reticulation, resulting from the reversibility of the associated transimination chemistry. Such error correction enables the formation of bulk crystalline structures, with properties of the specific building blocks—like size, geometry, and chemistry—serving as handles for tailoring COF microstructure, pore size/topology, and function.[2] While bottom-up design and control of microstructure is a hallmark of COF synthesis, the ability to rationally formulate COFs into processable nanostructured particles of morphologies tailored for specific applications remains a challenge. The overarching goal of this work is to develop critical synthesis-structure relations establishing design rules for controlling COF mesoscale morphology and, thereby, assembly. We demonstrate a systematic study of COF nanoparticle synthesis and assembly, linking nanoparticle stability and size (*ca*. 50–250 nm) to solvent choice, reagent concentration, and synthesis time. We show how monofunctional growth modifiers have limited impact on particle size tunability but can improve COF crystallinity.[3] Separately, while acetonitrile promotes colloidal nanoparticle formation, we demonstrate how solvent choice can be employed as a handle for tuning particle morphology beyond 1D spherical nanoparticles.[4] Namely, syntheses in benzonitrile consistently yields flaky, high-aspect ratio plate-like structures, while fine-tuning monomer concentration and catalyst loading in 4:1 dioxane/mesitylene solvent helps traverse a morphological phase space comprising distinct globular, rosette, and extended fibrillar structures.[5]

References

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[5] H. Guo et al., Nano Scale, 11 (2025)

2025-NECZA Poster Abstract
Type: (Graduate)
Consideration in poster competition: (Yes)

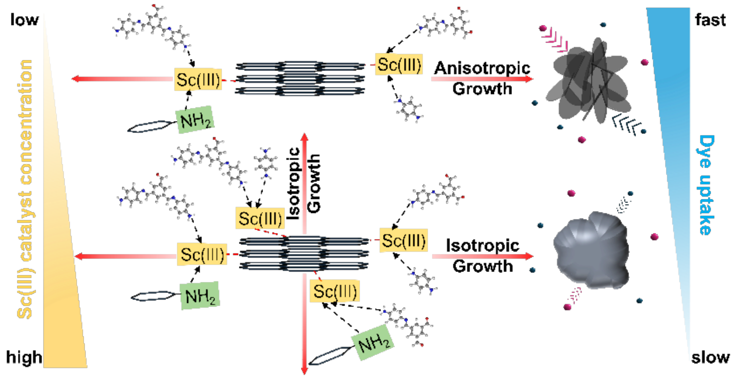
Controlling the hierarchical morphology and crystallinity of 2D imine-based COFs by catalyst, solvent, and temperature choreography

Hao Guo,[1] Joseph Cline,[2] Ryan Thorpe,[3] Kainan Feng,[1] Christopher J. Kiely,[1,2,3] Srinivas Rangarajan[1], and Mark A. Snyder[1,*]

[1] *Department of Chemical and Biomolecular Engineering, Lehigh University, 124 E. Morton St., Bethlehem, 18015*
[2] *Department of Material Science & Engineering, Lehigh University, 5 E. Packer Ave., Bethlehem, 18015*
[3] *Institute for Functional Materials and Devices, Lehigh University, 124 E. Morton St., Bethlehem, 18015*

Two-dimensional covalent organic frameworks (2D COFs), formed through bottom-up covalent assembly of molecular building blocks, are promising materials for catalysis, separations, and other advanced applications due to their tunable pore size, topology, and morphology.[1] In this work, we elucidate synthesis–structure–function relationships, demonstrating how room-temperature catalytic conditions can be exploited to tune COF growth and access unique hierarchical morphologies without the need for secondary templates or structure-directing agents.[2] Using COF-LZU1 as a model imine-based framework, we reveal the dual role of scandium triflate, $Sc(OTf)_3$, as both a highly efficient synthetic catalyst and a growth modifier. $Sc(OTf)_3$ selectively titrates framework defects and terminal amines of varying binding strengths to promote anisotropic crystal growth, yielding rosette-shaped COFs composed of ultrathin, high-aspect-ratio crystalline sheets only a few unit cells thick. These structures exhibit significantly reduced diffusion length scales and increased external surface area and pore accessibility compared to acetic acid–catalyzed analogues, enabling rapid uptake of bulky sorbates.

This new approach to controlling COF morphology exploits framework defects to direct growth from crystalline interfaces. Yet, ensuring high crystallinity of these and other COF products upon activation (*i.e.*, removal of pore-occluded synthesis solvents) is critical for their broad application. While solvent exchange and/or rapid solvent removal can collapse pores and disrupt interlayer stacking,[3] here we describe facile methanol and water-based post-synthetic processing under controlled pH and temperatures that lead to enhancement of 2D imine-based COF product crystallinity. Comprehensive characterization (XRD, BET, FT-IR, XPS, ICP-OES) reveals a mechanistic understanding of how such processing enhances crystallinity across different catalytic conditions. The optimized COF-LZU1 achieves a BET surface area of 1650 m^2/g, approximately 50% higher than the highest reported values.[4] Taken together, this work establishes new synthetic handles for controlling imine-based COF morphology and crystallinity, providing broadly applicable strategies for advancing COF materials in separations, catalysis, and other emerging technologies.



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[2] Hao Guo, *et al.*, *Nanoscale*, **17** (2025), 6488-6504.
[3] Cameron H. Feriante, *et al.*, *Advanced Materials*, **32** (2020), 18637–18644.
[4] Sebastian T. Emmerling, *et al.*, *Chem*, **7** (2021**)**, 1639–1652.

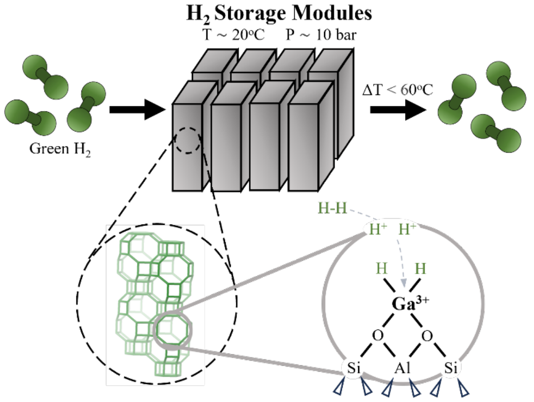
2025-NECZA Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

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

Gao, R.,[1] Lobo, R.F[1,*]
[1] *Chemical and Biomolecular Engineering, University of Delaware, 150 Academy St, Newark, 19716*

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^{-} for the Ga-H bond is evident in the IR spectra when the GaCHA material is exposed to a hydrogen environment.



References

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2025-NECZA Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

Unveiling Structural Insights of RE/Beta Zeolites for Selective Biomass Valorization

Mingze Zheng,[1] **Shivangi Borate,[2] James W. Harris,[2] Brandon C. Bukowski** [1,*]

[1] Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD 21218

2 Department of Chemical & Biological Engineering, The University of Alabama, Tuscaloosa, AL 35487

Rare-earth elements (REEs) incorporated Beta zeolite presents a promising strategy for improving conversion and selectivity specifically in the ethanol-to-olefins (ETO) process for sustainable aviation fuel (SAF) synthesis,[1] while also offering potential applications in other catalytic reactions such as isomerization, hydrogenation, and alkylation.[2–4] In this study, we present computational analysis of yttrium-modified Beta zeolite, examining five proposed Y sites (shown in **Figure 1**) and generating 91 distinct Y-deAlBeta models. Through systematic screening, we identified 18 stable models, closely aligned with experimental data from X-ray spectroscopy and pyridine FTIR, supporting the diversity of observed experimental structures in Y-deAlBeta frameworks. CI-NEB simulations of ethanol dehydration on defect-open and dehydrated defect-open sites reveal Lewis acid catalytic activity, with calculated activation energies closely matching experimental observations. Our findings highlight the potential of Y-modified zeolite Beta for catalyzing reactions requiring Lewis acidity.

Extending this approach, we explored the incorporation of various REEs into the Y-deAlBeta framework using hybrid-GGA HSE06-D3 (BJ) simulations. The results consistently showed structural stability, indicating that the Y open sites accommodate larger REEs while retaining structural integrity. A detailed scaling analysis of REE-O bond lengths and REE-Si-O bond angles further supported their adaptability across different REE sizes. Moreover, pyridine adsorption studies revealed a linear correlation between acid strength and HOMO+LUMO energies, providing predictive insight into the catalytic performance of REE-modified zeolites. These findings provide molecular-level insight into REE incorporation and its role in tuning Lewis acid strength for selective catalytic transformation of biomass-derived oxygenates into chemicals and liquid fuels.

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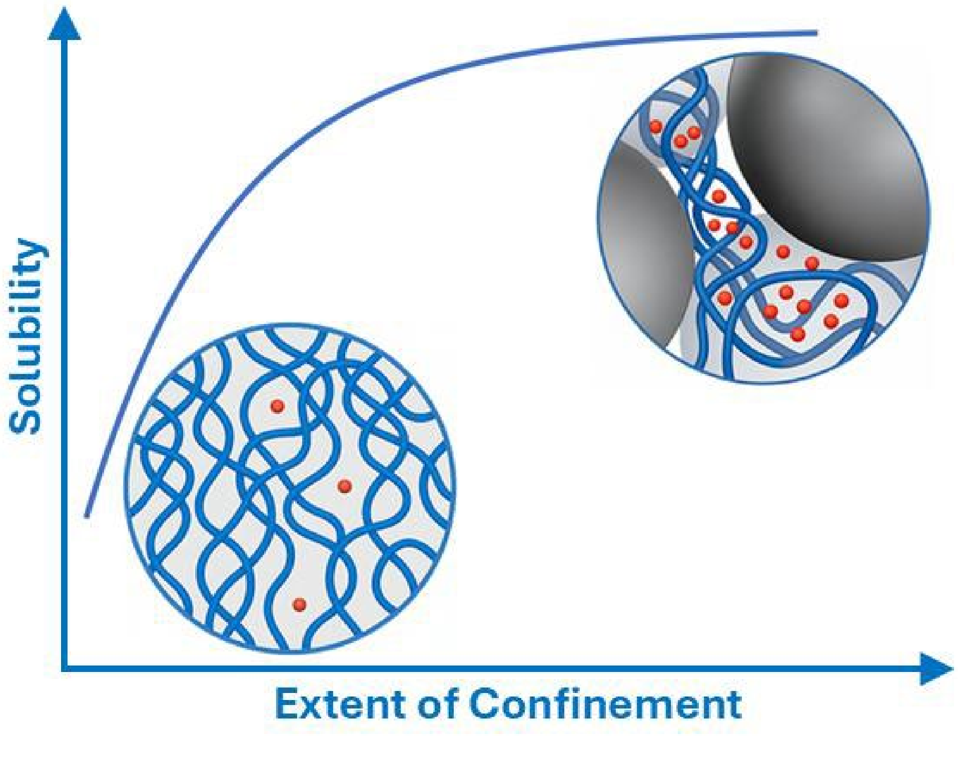
2025-NECZA Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

Dramatic Increases in Small-Molecule Solubility in Non-Polar Polymers under Nanoconfinement

Wang, K. [1], Tapia, J. [2], Ren, T. [1], Gorte, R. [1,*], Vohs, J. [1,*], Bai, P. [2,*], Lee, D. [1,*]
[1] *Department of Chemical and Biomolecular Engineering, School of Engineering and Applied Science, University of Pennsylvania, Philadelphia, 19104*
[2] *Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, 01003*

Understanding how confinement alters gas solubility in polymers is essential for advancing membrane separations, gas-barrier materials, and polymer upcycling technologies. In this work, we investigate methanol and n-hexane solubility in polystyrene (PS) and low-density polyethylene (LDPE) confined within the interstitial pores of disordered silica nanoparticle packings. Using capillary rise infiltration (CaRI), we infiltrate polymers into the nanoporous packings and quantify gas solubility with a quartz crystal microbalance (QCM). We find that confinement dramatically enhances gas solubility—by 10 to 100 times compared to bulk polymers. Systematic studies show that pore size is the primary factor governing this increase, while polymer molecular weight and nanoparticle surface hydrophobicity have only minor influence. Complementary atomistic simulations reveal that both confinement and polymer–surface interactions elevate solubility by modifying polymer packing at the molecular scale. These results demonstrate that nanoscale confinement can be a powerful strategy for tuning gas–polymer interactions and improving the performance of separation membranes and catalytic polymer upcycling processes.



2025-NECZA Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

Molecular Dynamics Predictions on the Elasticity of Confined Methane using Volume Fluctuations: From Mesopores to Bulk Limit

Flores Roman, S. A.[1], Ogbebor, J.[2], Jomon, G.[1], Gor, G. Y.[1,*]
[1] *Dept. of Chemical and Materials Engineering, NJIT, 323 Dr Martin Luther King Jr Blvd, Newark, 07102*
[2] *Dept. of Materials Sciences and Engineering, MIT, 77 Massachusetts Ave, Cambridge, 02139*

When fluids are confined in nanopores, many of their properties deviate from bulk. These include bulk modulus, or elasticity, which determines the mechanical properties of fluid-saturated porous solids. Such properties are of importance for the exploration and recovery of coal-bed methane and shale gas. Different computational approaches are known to predict the elasticity of confined fluids. The grand canonical Monte Carlo (GCMC) approach is among the most used methods. However, GCMC simulations are computationally intensive and inefficient for predicting fluid elasticity in large pores.[1,2] To overcome these limitations, we developed a new molecular dynamics simulation method to calculate the elasticity of confined fluids and applied it to methane confined in cylindrical carbon nanopores. The method is based on volume fluctuations in the isothermal-isobaric ensemble (*NPT*),

$$K_T = \frac{k_{\mathrm{B}} T \langle V \rangle}{\langle \delta V^2 \rangle},$$

Where K_T is the bulk modulus, k_B the Boltzmann factor, and the bracketed factors are the mean and variance of the simulation box volume.

Our method is one order of magnitude faster than the Monte Carlo approach, and allows calculations for pore sizes up to 100 nm. Our elasticity predictions are shown in Figure 1.

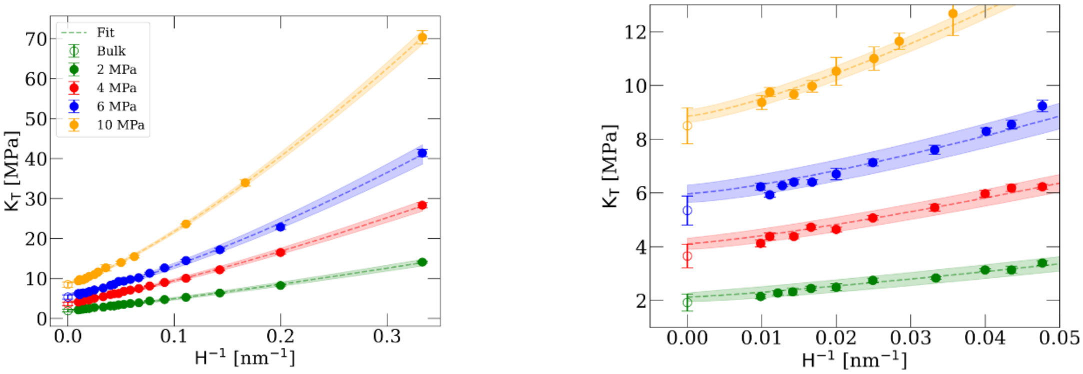


Figure 1: Bulk modulus of methane confined in cylindrical pores (from 3 nm to 100 nm) at 273 K, and pressures ranging from 2 MPa to 10 MPa. The dashed lines are a curve fit, and the shaded areas are the error of the fit.

Our simulations predicted an increase in the fluid bulk modulus by a factor of 7 in 3 nm cylindrical pores and showed a gradual decrease with increasing pore size, so that at 100 nm the deviation from the bulk is negligible. Our results expand our understanding of the mechanical properties of confined fluids, while our developed molecular approach enables elasticity predictions for more complex systems, such as flexible and larger molecules.[3]

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2025-NECZA Poster Abstract
Type: Graduate
Consideration in poster competition: Yes

Data Science shows that Entropy correlates with Accelerated Zeolite Crystallization in Monte Carlo Simulation

Hong, S.,[1] Auerbach, S.[1,2]

[1] *Department of Chemical and Biomolecular Engineering, University of Massachusetts Amherst, 686 North Pleasant Street, Amherst, 01002*

[2] *Department of Chemistry, University of Massachusetts Amherst, 710 North Pleasant Street, Amherst, 01002*

Zeolites are nanoporous aluminosilicate materials with high specific surface area, regular pore sizes, strong acidity, and ion exchange capacity. Zeolites are widely applied in various fields including catalysis, separations, and storage. There is increasing demand for zeolites, including tailor-made zeolite structures, to reach sustainability-related goals such as catalyzing biofuel production and capturing carbon dioxide. Targeting tailor-made zeolites is challenging because of limited atomic-level understanding of how zeolites form in the first place, prompting research into zeolite crystallization mechanisms and rates. Towards this end, we recently reported both Monte Caro simulations and zeolite synthesis experiments showing that using tetramethylammonium (TMA) as a secondary organic structure-directing agent (OSDA) can speed up zeolite formation of all-silica LTA zeolite.[1] However, the fundamental cause of the speed-up in the Monte Carlo simulations remained poorly understood because of the complexity of the simulations. The present study applies data science methods to investigate the cause of the speed-up from including the secondary OSDA, finding that entropy plays a critical role.

The Smooth Overlap of Atomic Positions (SOAP)[2] was used to represent structures from the Monte Carlo simulation snapshots, thereby encoding local environments with translational-, rotational-, and exchange-invariance. Various Machine Learning (ML) tools were used to distinguish the 1OSDA and 2OSDA structures. These ML tools include unsupervised learning via Principal Component Analysis (PCA), which was found to be unable to distinguish 1OSDA and 2OSDA structures; supervised learning via a linear Support Vector Machine (SVM), which successfully classified 1OSDA and 2OSDA structures with high fidelity; and Principal Covariates Regression (PCovR), which reduces dimensionality within the space of the SVM regression exercise. SVM decision functions reveal that the 2OSDA system presents narrow histograms suggesting a lower entropy for the 2OSDA zeolite formation. Inspired by this finding, we computed pair Si-O and Si-Si entropies[3] during the process of zeolite formation, finding that the Si-Si pair entropy difference between 1OSDA and 2OSDA systems quantitatively reproduces the apparent crystallization speed-up of 1.6. Thus, adding a secondary OSDA within fixed volume reduces the configurational entropy of the silica network in the Monte Carlo simulations, which in turn reduces the barrier to crystallization that arises because of the loss of entropy upon reaching an ordered state. Testing the role of entropy in zeolite crystallization rates for systems at fixed volume is challenging, but could be pursued by using pressure as a control variable in zeolite synthesis.

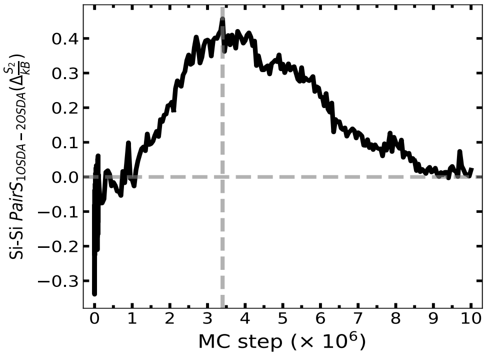

Figure 1. Pair entropy difference between 1OSDA and 2SODA dataset from configuration only Si-Si pair. The horizontal line refers to zero value, and the vertical line is the MC step where the maximum difference is located.

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2025-NECZA Poster Abstract
Type: Industrial
Consideration in poster competition: no

Powder X-Ray Diffraction for Heterogeneous Catalyst Analysis

Nicholas, Collette L.,[1,2] Mowat, J.P.S., [3,*] Nicholas, C.P.[1,2,*]

[1] *Låkril Technologies Corporation, Chicago, IL, USA*

[2] *C2P Sciences L3C, 825 Chicago Ave., Suite 10B, Evanston, IL 60202, USA*

[3] *Structure Forge LTD, Brightside, Ardwell, Stranraer, Scotland, UK DG9 9NZ.*

Despite its importance and ubiquity, the information contained in powder XRD data for materials in catalysts is often neither fully harnessed nor correctly interpreted. With the poster, we aim to provide discussion on some of the most encountered key aspects of powder XRD instrumentation, sample preparation, data collection, and analysis procedures used to characterize both catalyst active phases and the complex technical bodies used in full-scale commercial reactors. We will emphasize characterization of broad classes of materials including zeolites and MOFs, as well as the technical bodies relevant to large scale catalysis where various crystal sizes, shapes, dimensionalities and mixtures of materials including metal oxides and metals are encountered. We hope that researchers across many fields, including those who are new to powder XRD or for whom XRD is not their primary technique, can become familiar with key diagnostics and therefore be better equipped to interpret them in the context of their samples.

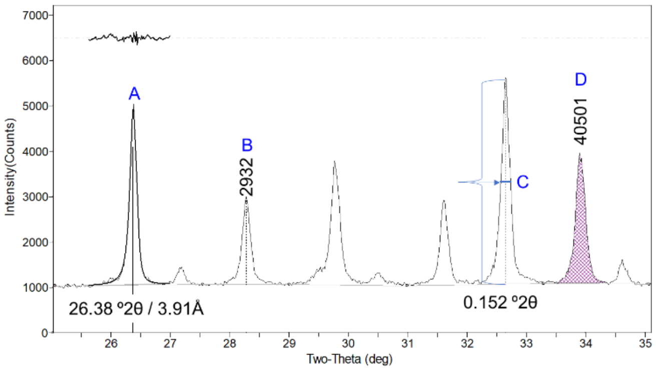

Fig. 1 Typical measurements that can be made on an XRD pattern.

A is peak position

B is peak height in counts which can be used to estimate the relative intensity of a phase.

C is Full Width at Half Max (FWHM) in degrees two theta and must be used with an instrumental broadening curve to determine crystallite size.

D is peak area integration in area counts for relative intensity of the phase

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2025-NECZA Poster Abstract
Type: Postdoc
Consideration in poster competition: No

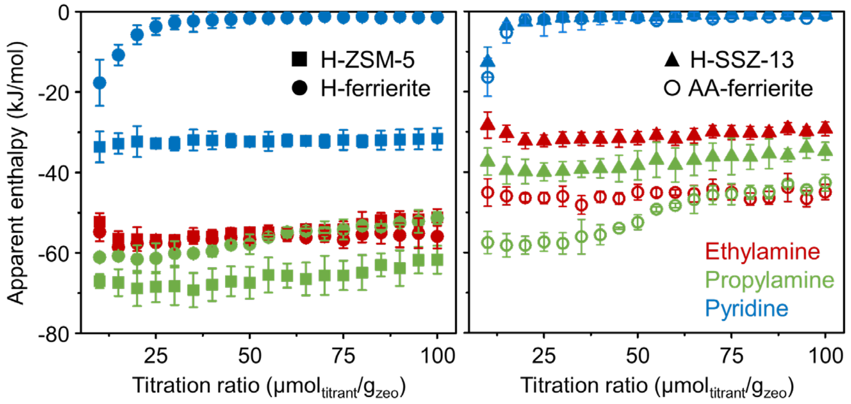
Thermochemical Analysis of Acid-Base Reactions in Solvated Zeolites

Lee, J. H.,[1] Mu, Y.[1], Rioux, R. M.[1,2,*]
[1] *Department of Chemical Engineering, The Pennsylvania State University, University Park, PA 16802*
[2] *Department of Chemistry, The Pennsylvania State University, University Park, PA 16802*

The unique nanoporous architecture and robust stability of zeolites have enabled their widespread use in acid-catalyzed processes, especially within contemporary petroleum refining and petrochemical sectors. The emergence of alternative chemical feedstocks, environmental pressures associated with climate change, and growing requirements for increasingly complex chemical compounds have driven a transition in zeolite catalyst applications toward innovative catalytic transformations involving large and/or intricate molecules in liquid media.[1,2] In liquid-phase systems, solvents serve dual functions: they enhance the transport of reactants and products while stabilizing intermediate species, consequently affecting both reaction kinetics and product distribution.[3,4] Thus, comprehending how solvents influence acid-base interactions is crucial for developing effective liquid-phase catalytic processes.

Isothermal titration calorimetry (ITC) provides direct thermodynamic measurements of chemical interactions in solution by quantifying heat changes, which enables the determination of adsorption enthalpies. By comparing these solution-phase calorimetric data with gas-phase results, a Born-Haber thermodynamic cycle can be constructed to elucidate the influences of water and zeolite pore architecture on acid-base reactivity in zeolites.

The figure presents ITC calorimetric data for acid-base interactions between base molecules and protonated zeolites of various framework topologies in aqueous solution. Although gaseous pyridine is known to access the 10-membered ring (10-MR) pores of ferrierite (FER framework),[5] solvated pyridine cannot reach acid sites within the 10-MR channels of H-ferrierite (0.54 × 0.42 nm), in contrast to H-ZSM-5 (MFI framework) with its 10-MR apertures (0.51 × 0.55 nm ↔ 0.53 × 0.56 nm). The changes in ethylamine adsorption enthalpy observed for acetic acid-dealuminated H-ferrierite likely result from preferential removal of aluminum from the 10-MR channels. Furthermore, the elevated adsorption enthalpies of small amines on acetic acid-treated ferrierite (AA-ferrierite) relative to H-SSZ-13 indicate differing degrees of amine solvation in the ferrierite 8-MR channels versus the *cha* cages. This conclusion is corroborated by Born-Haber cycle analysis combining liquid- and gas-phase adsorption measurements.



Apparent enthalpy for adsorption of bases on H-zeolites with MFI, FER, and CHA topologies in water at 25 ºC. Apparent enthalpy refers to the enthalpy calculated by normalizing the heat evolved by the amount of titrant injected.

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2025-NECZA Poster Abstract
Type: Industry
Consideration in poster competition: (no)

Interzeolite conversion of FER-type zeolite to CHA for NH_3-SCR

Gilleland, D[1]. Spell, L[1]. Turrina, A[2]. Yang, S.
[1]Johnson Matthey Technology Center, Savannah, Georgia 31408 (US)
[2]Johnson Matthey Catalysis Main Stores Chilton Avenue Billingham Cleveland TS23 1LB UK

Zeolites are microporous aluminosilicates valued for their stability, ease of synthesis, and broad catalytic applications. SSZ-13 is one of the most important types of zeolite and has a three-dimensional CHA type framework composed of 6 and 8-membered rings, making it a highly effective catalyst for ethylene-to-propylene conversion, NH_3-SCR, and CO_2 storage[1]. CHA is typically synthesized using N,N,N-trimethyladamantammonium hydroxide and alumina sources such as sodium aluminate or other zeolites via interzeolite conversion. To improve CHA's catalytic performance, especially for NO_x abatement, research has explored cation addition[2], crystal size modification[3], and raw material substitution. Prior literature has demonstrated that interzeolite conversion with alternative parent zeolites can result in improved physical characteristics of the final zeolite product[4-6]. In this study the conversion of FER zeolite into CHA and its catalytic performance in NH_3-SCR was investigated and patented[7].

Figure 1. shows H-form CHA that has been converted from FER zeolite. Both Sample-A and Sample-B are a pure and highly crystalline CHA and has a SAR of 17.3 and 19.2 respectively. Both zeolites have high microporous surface area values and the SEM showed a similar morphology for both but a difference in size and agglomeration. The H-form product was tested in NH_3-SCR and both samples showed strong fresh NOx conversion. However, Sample-B, with its higher SAR demonstrated a stronger hydrothermal stability and consequently had higher activity for aged performance compared to Sample-A across the temperature range as expected.

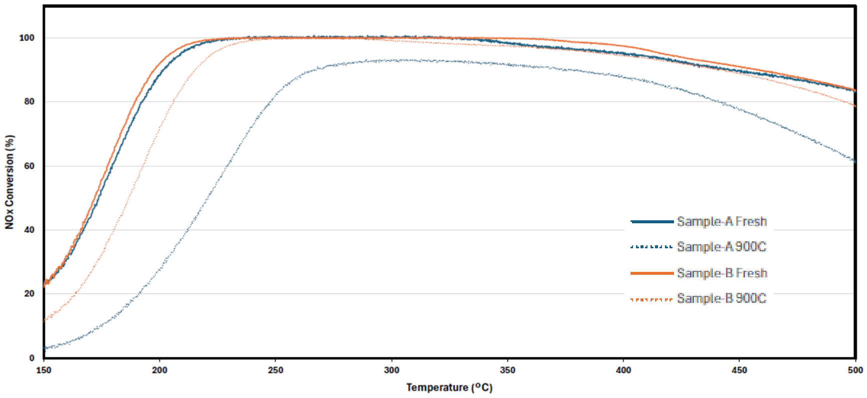

Figure 1. *NH_3-SCR of Sample- A (blue) and Sample-B (orange) both fresh and aged at 900C for 5 hours*

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2025-NECZA Poster Abstract
Type: Graduate
Consideration in poster competition: no

Microkinetic Modeling of Ethylene Formation in Mo/ZSM-5 with Machine Learning Potentials

Yanqi Huang, Xiang Ryan Zhou, Brandon C. Bukowski*
Department of Chemical and Biomolecular Engineering, Johns Hopkins University, 3400 North Charles Street, Baltimore, Maryland 21218, United State

Mo/ZSM-5 catalyzes methane dehydroaromatization (DHA), yet the mechanism and role of entropy on reactive intermediates and transition states remain unresolved. At 1000 K, entropy contributions to the Gibbs free energy of reactive intermediates and transition states are large which can have consequences for predicted reaction kinetics. Here we focus on one section of the overall DHA mechanism, methane dehydrogenation to ethylene on [MoC]2+/ZSM-5 and compare two pathways: a C–C coupling pathway that forms ethylene after sequential dehydrogenation and hydrogen association, and a MoC regeneration pathway that forms ethylene then reconstitutes [MoC]2+. We evaluated the harmonic oscillator approximation and partition function methods that assign hindered translational and rotational motions to low frequency modes to compute entropies at 1000 K. We then applied molecular dynamics using a machine learned potential (MLP) to obtain activation free energies for methane activation and hydrogen association via well-tempered metadynamics. Monte Carlo integration using an MLP was used to explicitly calculate translational and rotational entropy contributions for adsorbed methane. By comparing different entropy models, we demonstrate that translational and rotational modes are necessary for weakly adsorbed intermediates. Mean-field microkinetic modeling was used to quantify reaction orders and apparent activation energies for different entropy approximations. The C–C coupling mechanism was found to be kinetically dominant for direct ethylene formation, and the apparent kinetics depend on the entropy model.