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The Catalysis Club of Philadelphia

(In Person) Thursday, Sep 19th, 2024

Brandywine Plaza Hotel
630 Naamans Road, Claymont, DE 19703

Navigating the Boundaries between Fundamental and Applied Research in Zeolite Catalysis

Speaker: Prof. Jeffrey Rimer

University of Houston

Magnesiothermic Reduction of Carbon Dioxide in a Porous Monolith for Carbon Dioxide-Derived Composite Materials

Student Speaker: Hadas Elazar-Mittelman

Johns Hopkins University

Meeting Agenda:

Social Hour .... 5:30 PM
Dinner .... 6:30 PM
Meeting .... 7:30 PM

Meeting Registration:

Members: $45.00
Non-Members: $55.00
Stud. & Retired Members: $35.00

Please register online for this In-person meeting by ***Thursday, September 12th*** at CCP website.

Meal Selection (Included):

Please make one selection for your dinner (included in registration) when you sign-up for the meeting from the following options:

1. Sliced Roast Sirloin. Dessert: Cheesecake.
2. Chicken Champagne. Dessert: Cheesecake.
3. Seared Salmon. Dessert: Cheesecake.
4. Cavatappi Pasta (vegan). Dessert: fruit cup.

Salad comes with any option: Caesar Salad

Membership Registration:

Membership dues for CCP 2023-24 meeting season will be $25 ($5 for the local chapter and $20 for the national club). Dues for students, post-docs and retirees will be $10 ($5 for the local club and $5 for the national club). Please sign-up membership (Link) for more benefits on meeting registrations and net-working events!

Please contact our Treasurer Steve Hardwick (sjh.wilm.de@gmail.com) or Chair Zhuonan (Nick) Song (zsong@wlgore.com) or Program Chair Brandon Bukowski (bbukows1@jhu.edu) if you need any assistance.

The Catalysis Club of Philadelphia

Thursday, September 19th, 2024

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630 Naamans Road, Claymont, DE 19703

Prof. Jeffrey D. Rimer

Navigating the Boundaries between Fundamental and Applied Research in Zeolite Catalysis

University of Houston

Abstract: The diverse network of confined pores in zeolites have been widely used for shape-selective catalysis in the (petro)chemical industry and in applications related to energy transition and the evolving environmental landscape. This talk will focus on recent progress made in our group on the design and characterization of zeolite catalysts where our work lies at the boundary between fundamental and applied research. The complex pathways of zeolite crystallization make it difficult to control their physicochemical properties;[1] however, we have made significant progress in understanding zeolite nucleation and growth mechanisms using a combination of experimental and computational approaches that include the first high-temperature in situ scanning probe microscopy measurements of zeolite surface growth.[2, 3] Our long-term objective is to apply this knowledge to the development of state-of-the-art catalysts where we seek to improve the physicochemical properties of materials, including one of the most common obstacles in zeolite crystal engineering: overcoming the inherent mass transport limitations of nanopores. In this talk, I will highlight several methods to tailor zeolite crystal size, morphology, and composition in ways that reduce diffusion limitations and/or control acid siting, thereby enabling the design of catalysts with superior performance compared to materials obtained by conventional synthesis routes.[4, 5] Our research has explored methods of structure direction employing organics, inorganics, and combinations thereof to reduce synthesis times and tailor physicochemical properties. Additional studies of zeolite synthesis have shown how heteroatoms can be integrated in both conventional and hierarchical zeolites to enhance catalyst performance.[6] Among the hierarchical zeolites we have recently synthesized are self-pillared

pentasils that exhibit four-fold increases in both catalyst lifetime and total turnovers; and a new class of catalysts, referred to as *finned zeolites*, which are prepared by seeded growth to introduce fin-like protrusions with identical crystallographic registry as the interior crystal.[7] Examples of 1-, 2-, and 3-dimensional zeolites will be discussed using methanol to hydrocarbons (MTH) and olefin cracking as benchmark reactions, as well as advanced characterization techniques such as high-resolution electron tomography, operando spectroscopy, novel acid titration methods, and molecular modeling to correlate structural features of hierarchical zeolites and their diffusion properties with enhanced catalyst performance.

1. Mallette, A.J., K. Shilpa, and J.D. Rimer, *The Current Understanding of Mechanistic Pathways in Zeolite Crystallization.* Chemical Reviews, 2024. **124**(6): p. 3416-3493.
2. Choudhary, M.K., R. Jain, and J.D. Rimer, *In situ imaging of two-dimensional surface growth reveals the prevalence and role of defects in zeolite crystallization.* Proceedings of the National Academy of Sciences of the United States of America, 2020. **117**(46): p. 28632-28639.
3. Lupulescu, A.I. and J.D. Rimer, *In Situ Imaging of Silicalite-1 Surface Growth Reveals the Mechanism of Crystallization.* Science, 2014. **344**(6185): p. 729-732.
4. Le, T.T., W. Qin, A. Agarwal, N. Nikolopoulos, D.L. Fu, M.D. Patton, C. Weiland, S.R. Bare, J.C. Palmer, B.M. Weckhuysen, and J.D. Rimer, *Elemental zoning enhances mass transport in zeolite catalysts for methanol to hydrocarbons.* Nature Catalysis, 2023. **6**(3): p. 254-+.
5. Le, T.T., K. Shilpa, C.S. Lee, S.M. Han, C. Weiland, S.R. Bare, P.J. Dauenhauer, and J.D. Rimer, *Core-shell and egg-shell zeolite catalysts for enhanced hydrocarbon processing.* Journal of Catalysis, 2022. **405**: p. 664-675.
6. Abutalib, A., D. Parmar, J. Kim, and J.D. Rimer, *Pairing Ga/Al-Zeolites with tailored acidity as tandem catalysts for the conversion of alcohols to olefins.* Journal of Catalysis, 2024. **433**.
7. Dai, H., Y.F. Shen, T.M. Yang, C.S. Lee, D.L. Fu, A. Agarwal, T.T. Le, M. Tsapatsis, J.C. Palmer, B.M. Weckhuysen, P.J. Dauenhauer, X.D. Zou, and J.D. Rimer, *Finned zeolite catalysts.* Nature Materials, 2020. **19**(10): p. 1074-+.

Speaker Bio:

Jeff Rimer is the Abraham E. Dukler Endowed Chair and Professor of Chemical Engineering at the University of Houston. Jeff received B.S. degrees in Chemical Engineering and Chemistry from Washington University in St. Louis and Allegheny College, respectively. He received his Ph.D. in Chemical Engineering from the University of Delaware where he was an active member of the Philadelphia Catalysis Club. He then spent two years as a postdoctoral fellow at New York University's Molecular Design Institute prior to joining the University of Houston (UH) in 2009. Jeff's research in the area of crystal engineering focuses on the rational design of materials with specific applications in the synthesis of microporous catalysts and adsorbents, and the development of therapeutics to inhibit crystal formation in pathological diseases. Jeff is a Senior Member of the National Academy of Inventors and has received numerous awards that include the NSF CAREER Award, the 2016 Owens Corning Early Career Award and 2017 FRI/John G. Kunesh Award from AIChE, and the inaugural 2016 Mellichamp Emerging Leader Lecturer at the University of California at Santa Barbara. In 2018 he received the Norman Hackerman Award in Chemical Research from The Welch Foundation, and in 2020 the Edith and Peter O'Donnell Award in Engineering from TAMEST. He has also received several research, teaching, and mentoring awards at both the University and College levels. He is a former chair of the Southwest Catalysis Society, an executive committee member for the International Zeolite Association, and has chaired two Gordon Research Conferences on Crystal Growth & Assembly and Nanoporous Materials & Their Applications. He currently serves as the Director of Graduate Studies at UH and as the Program Director for the Welch Center for Advanced Bioactive Materials Crystallization. Jeff is also an Associate Editor of *Crystal Growth & Design* and serves on the advisory boards for the *AIChE Journal*, *Molecular Systems Design & Engineering*, *Reaction Chemistry & Engineering*, and *Green Carbon*.

Hadas Elazar-Mittelman

Magnesiothermic Reduction of Carbon Dioxide in a Porous Monolith for Carbon Dioxide-Derived Composite Materials

Co-Advised: Prof. Jonah Erlebacher and Prof. Michael Tsapatsis, Johns Hopkins University

Abstract:

Gigaton-scale permanent sinks for anthropogenic carbon dioxide (CO2) in industries such as construction, agriculture, and manufacturing are crucial to meet climate goals, yet the chemical stability of CO2 presents a significant challenge. Most existing approaches to CO2 transformation involve partial reductions to fuels or polymer precursors like ethylene, or its capture as carbonates. However, direct reduction of CO2 to create nanomaterials, while explored, has yet to be effectively scaled for large industrial applications. Discussed herein is a novel method for producing structural carbon composites using a chemical vapor infiltration (CVI) process, where CO2 acts as the reactive infiltrating gas and is reduced by magnesium (Mg) vapor. The process yields a dense carbon-MgO composite through a controlled, layer-by-layer growth mode under reaction diffusion-controlled conditions within three-dimensional scaffolds. This innovative approach not only provides a pathway for the sustainable manufacture of materials with promise for use in structural applications, but also contributes to the permanent sequestration of CO2 and inspires further exploration of alternative routes for building sustainable infrastructure.

Speaker Bio:

Hadas Elazar-Mittelman is a doctoral candidate in the Materials Science and Engineering department at Johns Hopkins University. She is co-advised by Prof. Jonah Erlebacher and Prof. Michael Tsapatsis on projects focused on reaction engineering and the conversion and utilization of CO2. She currently holds a bachelors and master's degree in Materials Science and Engineering from University of Maryland, College Park and Johns Hopkins University, respectively. Her research is supported by the Ralph O'Conner Sustainable Energy Institute, where she also serves as a graduate student representative. She is the founder and student liaison for the Hopkins Catalysis Club, the co-President of the Materials Graduate Society, and maintains an appointment at the Johns Hopkins University Applied Physics Laboratory as an Associate Research Scientist.