

The Department of Chemical Engineering Presents:

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ABSTRACT: This presentation will highlight the opportunities for using C₁-based feedstock for producing fuels and chemicals to meet future energy demands and in this context illustrate applications of catalysis for direct non-oxidative conversion of methane and for the conversion of methanol, a chemical platform molecule, to olefins and aromatics.

Methane, the primary component of natural gas, is chemically inert and its conversion involves the removal of hydrogen. The direct conversion of methane by endothermic pyrolysis reactions at high temperatures (950 K) is limited by equilibrium to about 10% yield of benzene. These thermodynamic limitations can be avoided by removing surface hydrogen intermediates formed in C-H bond activation steps. In our proposed strategy, methane dehydrogenation is coupled with transient absorptive removal to develop a catalytic process for the synthesis of hydrocarbon fuels. We illustrate the efficacy of polyfunctional strategies for upgrading of C_1 sources with accelerated rates and enhanced yields based on the systematic assessment of mechanisms and site requirements involved in the non-oxidative conversion of methane.

The indirect C₁ route for this conversion via methanol as a platform chemical is feedstock agnostic and offers a high degree of flexibility in the choice of products. The implementation of methanol-to-olefins (MTO) technology on a commercial scale in China has brought renewed interest in the pathways mediating propagation and termination sequences in in methanol conversion on solid acid catalysts. The *hydrocarbon pool* mechanism involving dual aromatic and olefins-based methylation/cracking cycles has provided over the past decade a context for rationalizing structure-function relationships in this chemistry. This description however, is devoid of mechanistic guidance on pathways that mediate catalyst deactivation. We combine parametric investigations of catalyst lifetime pursuant to changes in methanol space velocity and inlet methanol pressure and interpret trends of cumulative and transient selectivities to implicate formaldehyde as the key intermediate in transforming active olefin- and aromatic- chain carriers to inactive polycyclic intermediates in MTO catalysis.

BIO: Aditya Bhan received his Bachelor of Technology (B. Tech.) in Chemical Engineering from IIT Kanpur in 2000 and his PhD in Chemical Engineering from Purdue University in 2005. From January 2005 to August 2007, he was a postdoctoral scholar at the University of California at Berkeley and since then he has been on the Chemical Engineering and Materials Science faculty at the University of Minnesota where he currently serves as the Shell Chair Professor in Chemical Engineering. He leads a research group that focuses on mechanistic characterization of catalysts useful in energy conversion and petrochemical synthesis. In the recent past, his group at the University of Minnesota has been recognized with the Young Researcher Award from the Acid-Base Catalysis Society and the Ipatieff Prize from the American Chemical Society. He serves as Associate Editor for Journal of Catalysis and as Chair-Elect of the ACS Catalysis Division.

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