Catalysis Club of Philadelphia

Webinar: 6:30pm EST, Thursday, November 12th, 2020

Webinar link shared after registration

Speaker (2020 CCP Awardee) : Prof. Raul F. Lobo

Department of Chemical and Biomolecular Engineering, University of Delaware

From C5 Sugars to Industrial Chemicals Through Catalysis

Graduate Student Speaker: Yichen Ji

Department of Chemical and Biomolecular Engineering, University of Pennsylvania

Dehydra-decyclization of Tetrahydrofuran to 1,3-butadiene over ZrO_2

Meeting Schedule:
6:30 PM: Networking Time
7:00 PM: Student Speaker
7:20 PM: Main Speaker

Meeting Fees:
Free to CCP Members

Meeting Etiquette:
Please remember to mute your microphone and arrive early to solve any technical issues.

Webinar Registration:
Please register online by **Wednesday, *November 11th*** using this **LINK** or notify Arrangements Chair Jian Chang (CJ).

A webinar meeting invite will be provided on October 15th to all those who register.

Membership:
Dues for the 2020-21 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 local club and $5 for national club). Use this **LINK** for membership registration.

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From C5 Sugars to Industrial Chemicals Through Catalysis

Prof. Raul F. Lobo

Catalysis Center for Energy Innovation and Center for Catalytic Science and Technology

Department of Chemical and Biomolecular Engineering, University of Delaware

Abstract:

Much effort has been devoted to the transformation of glucose, a 6-carbon sugar, into new and known species that can be incorporated in the existing chemical industry infrastructure. All these processes, however, go through the dehydration of glucose to form hydroxymethylfurfural (HMF), a molecule that is unstable under hydrolytic conditions limiting yield and increasing costs. In contrast, an established industry already exists based on the dehydration of 5-carbon sugars into furfural from non-edible biomass precursors such as bagasse and corn stover. More than 300,000 tons of furfural are produced yearly that today mostly go into the production of furfurylalcohol, furoic acid and other C5 derivatives.

As part of the Catalysis Center for Energy Innovation, we have been investigating catalytic processes to produce valuable molecules from these C5 intermediates motivated by their wide availability and relative low cost, and this talk will summarize our efforts in this direction. We use an array of catalytic processes, homogeneous and heterogeneous, to make molecules for which there is already an existing market, such as benzoic acid and □-methylstyrene, from furfural or methylfuran. We also show that furfural can also be a precursor to the production of molecules known to have interesting chemical and physical properties, or that are very difficult to produce from petroleum-based precursors. We will present a summary of our investigations in the synthesis of vinylfurans, bifuran-dicarboxylic acids and a highly selective synthesis of 4,4'-dimethylbiphenyl from C5 sugars, a precursor to polymer precursors with exceptional physical and chemical properties. These results show there is ample room for innovation through the synergy of catalysis and process chemistry to find new and interesting ways to use renewable carbon sources to produce a more sustainable chemical industry.

Speaker Biography:

Raul F. Lobo is the Claire D. LeClaire professor of Chemical and Biomolecular Engineering at the University of Delaware. His research interests span development of catalysts for energy and the environment, development of novel porous materials for catalysis and separations, the chemistry of zeolites, and the scientific aspects of catalyst synthesis. He has published over one hundred eighty refereed reports and he is co-inventor in six US patents. He obtained his undergraduate degree in Chemical Engineering at the University of Costa Rica in 1989 and later moved to California to pursue graduate studies in Chemical Engineering at Caltech with Prof. Mark Davis. He worked for one year at Los Alamos National Laboratory, New Mexico as a postdoctoral fellow and started his academic career at the University of

Delaware in 1995. He was director for the Center for Catalytic Science and Technology from 2012 to 2020.

Prof. Lobo has conducted research in the use of zeolites for nitrogen/oxygen separations, and carbon dioxide separations from flue gases. He has contributed to the fundamentals of zeolite nucleation and crystal growth and to the application of zeolites for a number of catalytic applications. In particular his group research helped understand the mechanisms of reaction and stability of zeolite catalysts used for the removal of NOx gases from combustion exhaust, developed catalytic materials for the transformation of biomass-derived furans into commodity aromatic molecules, and discovered new materials for the selective activation of methane using copper oxide clusters.

Dehydra-decyclization of Tetrahydrofuran to 1,3-butadiene over ZrO_2

Yichen Ji

Department of Chemical and Biomolecular Engineering, University of Pennsylvania

Abstract:

Butadiene, one of the most important conjugated dienes, plays an important role in the rubber industry. Currently, butadiene is produced as a side product of naphtha cracking for production of ethylene in the United States. However, such production of butadiene is considered unsustainable because of the use of fossil sources and inefficient since it is not the main target reaction. Thus, a sustainable and more effective pathway is required. Recent studies have shown that conjugated dienes can be obtained from dehydro-decyclization of cyclic ethers, which can be derived from biomass sources, over Brønsted acidic catalysts through a carbocation pathway. However, most of these reactions are industrially undesirable because of their reaction activities.

In finding a proper catalyst to carry this reaction, zirconia appeared to be a promising catalyst and a series of metal oxides with Lewis acidity were tested to compare with it. While most of the Lewis catalysts showed activity to this reaction at similar temperature, zirconia has shown high selectivity to butadiene (~90%) and promising reaction rate. Near quantitative yields to butadiene could be achieved over tetragonal zirconia (t-ZrO_2) at 673 K and a WHSV of 0.93 g THF $gcat^{-1}$ h^{-1}. Methyl-substituted THF gave only moderate increases in rates and the products showed minimal isomerization of the carbon backbone. The t-ZrO_2 catalyst was found to be relatively stable with time on stream, experiencing alkene products polymerization as a likely source of deactivation. Complete regeneration of the catalyst was demonstrated through calcination alone, allowing for multiple regenerations with no irreversible loss in activity or selectivity. The catalytic activity of zirconia was found to be structure insensitive, with t-ZrO_2 and monoclinic zirconia (m-ZrO_2) exhibiting similar initial activities; however, m-ZrO_2 was observed to deactivate much more rapidly.

Speaker Biography:

Yichen Ji is currently a 5th-year Ph.D. student in the Gorte group at University of Pennsylvania. He received his B.S. degree in the Art and Science of Chemistry from Nanjing University, China, and after that he has been working as a process engineer at LG Chem Ltd. for 3 years. Yichen's primary research interests are in heterogeneous catalytic upgrading of biomass, and his main research projects have been focused on the upgrading of furan related compounds.