# Catalysis Club of Philadelphia

**Thursday, September 12th, 2019**
Crowne Plaza Wilmington North
630 Naamans Road, Claymont, DE 19703

## Speaker: Prof. Fabio H. Ribeiro

***Catalysis Club of Philadelphia Award Lecture***
*Purdue University*

## The role of kinetics in the search for the active site in heterogeneous catalysis

## Graduate Student Speaker: Pierre Desir

*University of Delaware – Vlachos Group*

**Reactive Extraction of Biomass Intermediates in Liquid-Liquid Microreactors**

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

**Meeting Fees:**
*Members:* $40.00
*Non-Members:* $45.00
*Stud. & Retired Members:* $25.00

**Menu**

*A broiled Maryland crab cake appetizer, served with Crowne salad, Tiramisu and your choice of 3 entrees:*

1) Chicken Champagne – *Sautéed chicken with a delicate champagne cream sauce*
2) Sliced Roast Sirloin – *Thinly sliced and served with wild mushroom bordelaise*
3) Vegan Pasta Dish – *Cavatappi pasta, oven roasted seasonal vegatables, and marinara sauce*

**Meal reservations** – Please register online by ***Friday, September 6th*** at http://catalysisclubphilly.org/ or notify your company representative or our Treasurer Josh Pacheco (Josh.Pacheco@pqcorp.com) or Chair Jacob Dickinson (Jacob.G.Dickinson@dupont.com)

**Membership** - Dues for the 2019-20 season will be $25.00 ($5.00 for the local chapter and $20.00 for the national club). Dues for students, post-docs and retirees will be $10.00 ($5.00 for local club and $5.00 for national club).

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## Prof. Fabio H. Ribeiro

## The role of kinetics in the search for the active site in heterogeneous catalysis

*Davidson School of Chemical Engineering, Purdue University*

**Abstract:** The identification of the active site plays an important role in the quest for the design of catalysts. Once the site is identified, the goal is then to define the rate constants for all elementary steps in the catalytic cycle. Achieving this goal, fortunately, is usually not necessary in the design of catalysts and a much simpler kinetic description is effective. We will illustrate from examples in the water-gas shift (WGS) reaction, oxidation of NO, and the selective catalytic reduction (SCR) of NOx with ammonia, how the combination of kinetics, spectroscopy, theory and designed materials were used to propose the active site. For the WGS reaction, we will concentrate on the catalysis by Au and show that the active site appears to be metallic, under-coordinated Au. For the oxidation of NO to $NO_2$ on Pt, the active site appears to be a Pt surface with the proper oxygen coverage. Finally, and most interestingly, the sites for ammonia SCR of NOx on copper-zeolites are mobilized copper ions.

**Speaker Details:** Fabio H. Ribeiro is currently the R. Norris and Eleanor Shreve Professor of Chemical Engineering and Director of the National Science Foundation Engineering Research Center on the Innovative and Strategic Transformation of Alkane Resources (CISTAR) at the Davidson School of Chemical Engineering, Purdue University. He received his Ph.D. degree from Stanford University in 1989, worked for Catalytica, Inc. in Mountain View, California, held a post-doctoral fellowship at the University of California – Berkeley, and was on the Worcester Polytechnic Institute faculty before joining Purdue University in August 2003. His research interests are centered on the kinetics of heterogeneous catalytic reactions and catalyst characterization under reaction conditions. He has over 140 publications in scholarly journals. He was Chair for the American Institute of Chemical Engineer's Catalysis and Reaction Engineering Division (2010) and editor for Journal of Catalysis (2010-2018). His honors include the NSF CAREER award (1997-2002), the Excellence in Catalysis Award from the Catalysis Society of Metropolitan New York (2005), the Henry J. Albert Award from the International Precious Metals Institute (2012), the Purdue College of Engineering Faculty Award of Excellence on Research (2014), Herman Pines Award from The Chicago Catalysis Club (2015), Giuseppe Parravano Memorial Award for Excellence in Catalysis Research from the Michigan Catalysis Society (2019), Catalysis Club of Philadelphia Award (2019).

## Pierre Desir

# Reactive Extraction of Biomass Intermediates in Liquid-Liquid Microreactors

Pierre Desir*, Basudeb Saha, and Dionisios G. Vlachos

*Department of Chemical and Biomolecular Engineering, University of Delaware, 150 Academy Street, Newark, Delaware 19716, United States*

**Abstract:** As an alternative to depleting fossil fuel resources, lignocellulosic biomass has been shown to be the only renewable source of energy and carbon to potentially substitute petroleum-based fuels and chemicals. In particular, biomass derived carbohydrates can undergo acid-catalyzed dehydration reactions in water to produce intermediate furanic compounds such as 5-hydroxymethylfurfural (HMF), which is considered as a platform chemical for the production of fuels, fuel additives, renewable plastics, and advanced materials. The process involves many side reactions that require the addition of an organic solvent in order to extract HMF from the aqueous phase and prevent its further degradation. Biphasic batch reactors require frequent recycling of the organic phase, are limited by heat and mass transfer, and are unsuitable for large scale production. Continuous flow microreactors enable process intensification by the formation of tunable, two-phase flow patterns with large specific interfacial areas that provide mass transfer rates that are 2 – 3 orders of magnitude greater than their batch counterparts for rapid extraction of HMF with improved yield, selectivity, and process economics. In this study, we design an ethyl acetate/water capillary biphasic microreactor for the reactive extraction of HMF from HCl-catalyzed fructose dehydration. Firstly, we investigate the fluid mechanics of the two-phase flow patterns inside the microreactor. Secondly, we conduct extraction studies of HMF from the aqueous phase to the organic phase to evaluate the mass transfer characteristics of the flow patterns. Thirdly, we perform reactive extraction experiments in the biphasic microreactor and assess the reactor performance by modeling the two-step process to determine optimal reaction conditions maximizing the HMF yield.

**Speaker Details:** Pierre Desir is a 5th-year Ph.D. student in Prof. Dionisios G. Vlachos' group at the University of Delaware. He earned his B.S. degree in Chemical Engineering with a concentration in Nuclear Engineering from the City College of New York in 2015. At the City College of New York, his undergraduate research work aimed at designing and synthesizing lipid-coated microbubbles with bound surface active peptides for drug delivery applications. As a Ph.D. candidate in the Chemical Engineering Department at the University of Delaware, his research focuses on tackling global energy challenges and reducing petroleum-based emissions by designing, building, modeling, and optimizing continuous flow microreactors as portable technologies that improve energy efficiency and reduce processing times by 1000-fold during the chemical conversion of carbohydrates derived from non-edible plant matter (lignocellulosic biomass) into intermediate platform chemicals such as 5-hydroxymethylfurfural (HMF) for the production of renewable fuels, fuel additives, and advanced materials.