The Catalysis Club of Philadelphia

Webinar: 7 PM, Thursday, February 24th, 2022
Zoom link shared after registration

CCP Award Lecture

Speaker: Prof. Alan M. Allgeier

University of Kansas

CatBioCat: Harnessing the Strengths of Heterogeneous Catalysis and Enzyme Catalysis in Biomass Valorization

Student Speaker: Kewei Yu

Meeting Schedule:

6:30 PM EST: Welcome
7:00 PM: Talk by Kewei Yu
7:25 PM: Talk by Prof. Allgeier
8:30 PM: Meeting adjourns

Meeting Fees:

Free to all who register

Meeting Etiquette:

Please remember to mute your microphone and arrive early to solve any technical issues. Camera sharing prior to the talks is encouraged.

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Online Registration – Please register online by Wednesday, February 23rd at http://catalysisclubphilly.org/webinar-registration/ or Arrangements Chair, hrenjing@seas.upenn.edu.

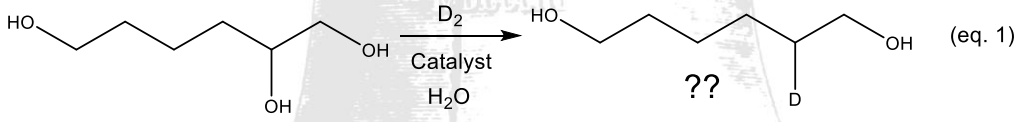
A Zoom meeting invite will be provided through the confirmation email. If you do not receive a confirmation email immediately after registration, please contact Renjing Huang, hrenjing@seas.upenn.edu.

Membership – Dues for the 2021-22 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).

CatBioCat: Harnessing the Strengths of Heterogeneous Catalysis and Enzyme Catalysis in Biomass Valorization

ALAN M. ALLGEIER, PH. D.
University of Kansas
Chemical and Petroleum Engineering
Center for Environmentally Beneficial Catalysis

Abstract: A long-term vision of sustainable chemical production demands utilization of biogenic carbon. In the Center for Environmentally Beneficial Catalysis numerous projects support this long-term vision. The underlying motivation in the Allgeier Group is elucidating catalysis mechanisms at a molecular level and we leverage multiple modalities of catalysis (heterogeneous, homogeneous and enzyme) in our pursuits. This presentation will describe the importance of isotopic labeling studies in differentiating potential mechanisms for the hydrodeoxygenation of aliphatic alcohols derived from cellulose. Using a combination of kinetic isotope effects and regioselective isotope incorporation, we conclude that the hydrodeoxygenation of 1,2,6-hexanetriol over $PtWOx/TiO_2$ is effected by the cooperative interaction of Bronsted sites and hydrogen activation sites, eq 1. Simultaneously we eliminate the potential of the reverse Mars-van Krevelen mechanism and the direct scission of the C-O bond.



In complementary work, we are developing enzyme catalysis using alcohol dehydrogenase enzymes derived from *Saccharomyces cerevisiae* (Sc-ADH) to generate bio-renewable processes to aldehydes. Sc-ADH requires the cocatalyst, nicotinamide adenine dinucleotide (NAD+) to mediate electron and proton transfer at the active zinc catalytic site. Such cocatalysts are prohibitively expensive as stoichiometric agents and we are developing cascade processes to reoxidize the cocatalyst. The performance of one option using reduction of fructose to mannitol via a mannitol dehydrogenase will be described, along with modeling efforts exploring the relevant equilibrium relationships.

Bio: Dr. Alan Allgeier is Associate Professor of Chemical and Petroleum Engineering at the University of Kansas and Associate Director of the Center for Environmentally Beneficial Catalysis. He grew up in the beautiful rural environs surrounding Erie, PA and defended his Ph.D. in Inorganic Chemistry in 1996 at Northwestern University under the guidance of Prof.

Chad A. Mirkin. Dr. Allgeier conducted research in industry for two decades split between pharmaceuticals (Amgen) and chemicals (DuPont), garnering significant expertise in catalysis and process chemistry, as well as, material science. He is a former Arrangements Chair, Treasurer, Director, Chair and Program Chair of the Catalysis Club of Philadelphia and loved every minute he spent in the Club. In 2017 he moved from the Corporate Center for Analytical Sciences of DuPont Central Research to the University of Kansas, building a laboratory for Sustainable Catalysis and Porous Materials. He was also pleased to be one of the founders of the Great Plains Catalysis Society. Dr. Allgeier has been honored with the Amgen Green Chemistry Award (2011), the Russell Malz Award for Service in Catalysis (2014), and the Catalysis Club of Philadelphia Award (2021).

Ethane Non-oxidative Dehydrogenation over Co/SiO2 — Pretreatment and Regeneration

Kewei Yu

Department of Chemical and Biomolecular Engineering, University of Delaware

Abstract:

Light olefins such as ethylene and propylene are important building blocks for modern chemical industries. With the increasing demand over the past decades and recent shale gas revolution, direct dehydrogenation of alkanes to olefins has become an economically viable choice to produce light olefins1. Co/SiO2 is a highly active and selective catalyst for light olefin dehydrogenation, which is also low-cost and environmentally friendly2–4. However, the catalyst activity requires further improvement, active site structure and reaction mechanism remain unclear.

In this study, we synthesized Co/SiO2 with a facile electrostatic adsorption method and optimized the catalyst performance by varying cobalt loadings and pretreatment conditions. A facile high temperature pretreatment method was found to increase the initial activity of the catalyst up to 4 times. Extensive characterizations were conducted to investigate the structure-function correlations of Co/SiO2. Post characterization indicates that hydrogen generated by the reaction plays a key role in catalyst deactivation. Therefore, an effective procedure is also developed for catalyst regeneration.

(1) Sattler, J. J. H. B.; Ruiz-Martinez, J.; Santillan-Jimenez, E.; Weckhuysen, B. M. Catalytic Dehydrogenation of Light Alkanes on Metals and Metal Oxides. Chem. Rev. 2014, 114 (20), 10613–10653.
(2) Hu, B.; “Bean” Getsoian, A.; Schweitzer, N. M.; Das, U.; Kim, H.; Niklas, J.; Poluektov, O.; Curtiss, L. A.; Stair, P. C.; Miller, J. T.; Hock, A. S. Selective Propane Dehydrogenation with Single-Site CoII on SiO2 by a Non-Redox Mechanism. Journal of Catalysis 2015, 322, 24–37.
(3) Huang; Cheng; Ji; Gorte. Atomic Layer Deposition for Preparing Isolated Co Sites on SiO2 for Ethane Dehydrogenation Catalysis. Nanomaterials 2020, 10 (2), 244.
(4) Estes, D. P.; Siddiqi, G.; Allouche, F.; Kovtunov, K. V.; Safonova, O. V.; Trigub, A. L.; Koptyug, I. V.; Copéret, C. C–H Activation on Co,O Sites: Isolated Surface Sites versus Molecular Analogs. J. Am. Chem. Soc. 2016, 138 (45), 14987–14997.

Bio:
Kewei Yu is a third-year Ph.D. student at the University of Delaware working with Prof. Dion Vlachos. Kewei received his bachelor’s degree from Nanjing Tech University in Materials Science and Engineering. His current research interest lies in heterogeneous catalysis for light hydrocarbon conversion, such as alkane dehydrogenation reaction, and electrification including Joule heating reactor design and materials synthesis/characterization.