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Catalysis Club of Philadelphia

Webinar: 7 pm, Thursday, November 11th, 2021

Zoom link shared after registration

Speaker: Prof. Bruce Gates

*Department of Chemical Engineering
University of California, Davis*

**Atomically Dispersed Supported Platinum
Catalysts: Synthesis, Characterization, Structure,
Stabilization, and Catalysis of Reactions including CO
Oxidation and Propane Dehydrogenation**

Student Speaker: Brandon Vance

Meeting Schedule:

6:30 PM EST: Welcome

7:00 PM: Talk by Brandon Vance

7:25 PM: Talk by Prof. Gates

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,
November 10th 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).

Atomically Dispersed Supported Platinum Catalysts:

Synthesis, Characterization, Structure, Stabilization, and Catalysis of Reactions including CO Oxidation and Propane Dehydrogenation

Bruce C. Gates

*Department of Chemical Engineering
University of California, Davis*

Atomically dispersed noble metals catalysts have drawn wide attention as candidates to replace supported metal clusters and metal nanoparticles. Atomic dispersion offer unique properties as well as maximum utilization of the expensive metals. We report such a catalyst for CO oxidation, Pt/MgO, with the crystalline MgO support chosen for its stable, well-defined structure to host platinum in subsurface bonding sites. The catalyst has been characterized by atomic-resolution imaging, IR spectroscopy of adsorbed CO, EXAFS spectroscopy, and HERFD-XANES spectroscopy, including in-operando characterization. High-throughput density functional theory calculations for assessing all the potentially stable MgO binding sites for platinum combined with automated EXAFS analysis lead to unbiased identification of isolated, subsurface-enveloped platinum cations as the catalytic species, in agreement with experiment. This new theory-guided workflow leads to rigorously determined structural models and provides a more detailed picture of catalytic sites than what is currently possible with conventional EXAFS analysis. As this approach is efficient and agnostic to the metal, support, and catalytic reaction, we posit that it will be of broad interest to the catalysis community.

Addition of a second metal has been found to help reduce the size of platinum ensembles in bimetallic clusters, but the stabilization of isolated platinum atoms in small nests of non-precious metal atoms is challenging. We now report the synthesis, and characterization of a dealuminated zeolite Beta-supported platinum catalyst made so that platinum atoms are stably bonded within nests of zinc atoms located within the nanoscale pores of the zeolite. The catalyst is stable in long-term operation in propane dehydrogenation, exhibiting high activity and high selectivity to propylene. Atomic resolution images, bolstered by X-ray absorption spectra, demonstrate predominantly atomic dispersion of the platinum in the nests, and, with complementary infrared and nuclear magnetic resonance spectra, determine a structural model of the nested platinum.

Bio



Bruce Gates studied chemical engineering at Berkeley and the University of Washington and was a Fulbright postdoctoral scholar in 1966-67 with G.-M. Schwab at the Ludwig Maximilians University of Munich. He was a research engineer at Chevron for a couple of years and then joined the faculty of the University of Delaware and was a member of the Philadelphia Catalysis Club, serving as program director and president. He co-founded and directed the University of Delaware Center for Catalytic Science and Technology. In 1992 he became a professor at the University of California, Davis. He has served on DOE's Basic Energy Sciences Advisory Committee and the SSRL and NSLS-II Scientific Advisory Committees. He edited *Advances in Catalysis* for some years and co-

authored the textbook "Chemistry of Catalytic Processes" with Jim Katzer and George Schuit and authored "Catalytic Chemistry." His research group works on catalysis by atomically dispersed supported metals; supported metal clusters; catalysis by zeolites and MOFs; and techniques for spectroscopic characterization of working catalysts, especially with synchrotron methods.

Bridging the Gap Between Model Alkanes and Polyolefin Hydrocracking

Brandon Vance, Pavel Kots, Cong Wang, Zachary Hinton, Caitlin Quinn, Thomas Epps, III, LaShanda Korley, Dionisios Vlachos

Hydrocracking is an attractive route for the deconstruction of polyolefin (PO) plastics waste. Platinum tungstated zirconia (Pt-WZr) was used in a batch reactor at 250 °C and 30 bar H₂ pressure for 1 – 24 h to study the deconstruction of low-density polyethylene (LDPE, M_w ~ 76 kDa). LDPE hydrocracking over Pt-WZr bifunctional catalysts generates branched fuel- and lubricant-ranged alkanes. The Pt-WZr metal-to-acid site molar ratio (MAB) was altered by varying the Pt and W loadings. Increasing MABs shift the product distribution to larger cracked products and increases the isomerization degree in the residual polymer. We identify the MAB as a catalyst descriptor and propose a new macromolecular hydrocracking mechanism that diverges from model alkane hydrocracking. The details of this mechanism and the role of the MAB in LDPE hydrocracking are discussed.

Bio

Brandon Vance earned his bachelor's degree in chemical engineering from Iowa State University (ISU). While at ISU, he worked on designing heterogeneous catalysts for the CO₂ methanation reaction under the advisement of Prof. Jean-Philippe Tessonier as a Ronald E.

McNair Scholar and Iowa Space Grant Consortium Undergraduate Research Fellow. Currently, Brandon is an NSF Graduate Research Fellow and a 3rd year PhD graduate student under the advisement of Prof. Dionisios Vlachos in the Department of Chemical and Biomolecular Engineering at the University of Delaware. His research interests include plastics waste deconstruction via hydrocracking and hydrogenolysis catalysis and catalyst design.

