

Catalysis Club of Philadelphia

Thursday, October 11th, 2018

Crowne Plaza Wilmington North

630 Naamans Road, Claymont, DE 19703

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F.G. Ciapetta Award Lecture

Speaker: Dr. Teh C. Ho

Ultra-Deep Diesel Hydrodesulfurization Catalysis and

Process: A Tale of Two Sites

Hydrocarbon Conversion Technologies

Student Speaker: Cong Wang

**Pt-WO_x/C: An Intriguing Catalyst for Selective Conversions of Furfurals
and Cresols**

University of Pennsylvania

Meeting Schedule:

Social Hour5:30 PM

Dinner6:30 PM

Meeting7:30 PM

Meeting Fees:

Members: \$40.00

Non-Members: \$45.00

Stud. & Retired Members: \$25.00

Menu

*A Crab Cake appetizer, served with a
Spinach Side Salad, Crème Brulee
Cheesecake and your choice of 3
entrees:*

- 1) Chicken Champagne –
*Sautéed chicken breast
served with a delicate
champagne cream sauce*
- 2) Slow Roasted Prime Rib –
*Served with Au Jus and
Horseradish*
- 3) Vegan Pasta Dish – *Angel
hair pasta with oven roasted
seasonal vegetables topped
with vegan marinara sauce*

Meal reservations – Please
register online by **Friday,
October 5th** at

<http://catalysisclubphilly.org/>

or notify your company
representative or our
Treasurer Lifeng Wang
(Lifeng.Wang@pqccorp.com)
or Chair Eric Sacia
(Eric.R.Sacia@dupont.com)

Membership - Dues for the
2018-19 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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Dr. Teh C. Ho

F.G. Ciapetta Lectureship Awardee

Ultra-Deep Diesel Hydrodesulfurization Catalysis and Process: A Tale of Two Sites

Hydrocarbon Conversion Technologies, Bridgewater, NJ 08807, USA

Abstract: Hydrodesulfurization catalysts have two types of active sites for hydrogenation and hydrogenolysis reactions. While hydrogenation sites are more active for desulfurizing refractory sulfur species, they are more vulnerable to organonitrogen inhibition than hydrogenolysis sites. In contrast, hydrogenolysis sites are less active for desulfurizing refractory sulfur species but are more resistant to organonitrogen inhibition. This dichotomy is exploited to develop an ultra-deep hydrodesulfurization stacked-bed reactor comprising two catalysts of different characteristics. The performance of this catalyst system can be superior or inferior to that of either catalyst alone. A theory is developed to predict the optimum stacking configuration for maximum synergies between the two catalysts. The best configuration provides the precise environment for the catalysts to reach their full potentials, resulting in the smallest reactor volume and maximum energy saving. Model predictions are consistent with experimental results. A selectivity-activity diagram is developed for guiding the development of stacked-bed catalyst systems.

Speaker Details: Dr. Teh C. Ho worked at Exxon and Exxon Mobil for over thirty years in several capacities, including as Senior Research Associate, Head of the Hydroprocessing Research, Head of Mathematical Modeling, and Task Force Leader for Catalyst Scale-up. His research areas include Hydrodesulfurization, Hydrodenitrogenation, Hydrogenation, Hydrocracking; Residue Upgrading; Fluid Catalytic Cracking; Catalytic Reforming; Delayed Coking; Fouling; Selective Oxidation of Hydrocarbons; Synthesis and Characterization of Sulfide and Oxide Catalytic Materials; Catalyst Technology Transfer and Scale-up; Multiphase Reaction Engineering, Modeling of Large-Scale Reaction Systems. He has over 95 publications and 54 US patents, and has won several prestigious awards, including Lawrence B. Evans Award of the AIChE (2010), Industrial Innovation Award of the ACS (2006), Wilhelm Award of the AIChE, and the F.G. Ciapetta Lectureship of the North American Catalysis Society (2018) for his substantial contributions to industrially significant catalysts and catalytic processes. He was inducted into the National Academy of Engineering in 2016 for his efforts in hydrotreating. Currently, he serves as a consultant to several international energy companies.

Pt-WO_x/C: An Intriguing Catalyst for Selective Conversions of Furfurals and Cresols

Cong Wang

Advisor: Prof. Raymond J. Gorte

Department of Chemical & Biomolecular Engineering, University of Pennsylvania, PA, 19104

Abstract:

In this talk, I will present results showing that WO_x overlayers on Pt/C can promote the activity and selectivity towards desirable ring-opening of tetrahydrofurfural alcohol (THFA) to 1,5-pentanediol (1,5-PeD) and the selective hydrodeoxygenation (HDO) of *m*-cresol to toluene. In the reaction of THFA to 1,5-PeD, Pt paired with WO_x was highly active and selective, even though the individual components were not active or selective. The active form of the catalyst is shown to exist as a sub-monolayer of WO_x species on the Pt surface. This thin film could be formed by Atomic Layer Deposition (ALD) of W(CO)₆ onto the Pt nanocrystals and STEM-EDS mapping demonstrated that ALD deposition occurred selectively on the Pt. When the catalyst was prepared by impregnation of Pt and W salts, the WO_x is shown to be mobile and to anchor on the Pt surface to form the active interface. In the HDO of *m*-cresol to toluene, Pt/C was found to exhibit only modest selectivity and low stability, while Pt-WO_x/C was found to be unusually active and selective to toluene. The Pt-WO_x/C catalyst was more than 94% selective to toluene and exhibited little to no deactivation under a wide range of reaction conditions. Reactivity studies in combination with density functional theory (DFT) calculations indicate that the HDO reaction on Pt-WO_x/C proceeds via a direct hydrogenolysis of the C-O bond in *m*-cresol adsorbed on oxygen vacancy (or redox) sites on WO_x species. The DFT results also indicate that Pt helps stabilize the WO_x film while facilitating oxygen vacancy formation.

Speaker Bio: Cong Wang is a 4th-year Ph.D. student in the Gorte Group at the University of Pennsylvania. He received his M.S. in Chemical and Biomolecular Engineering at the University of Pennsylvania and his B.S. at Tsinghua University, China. His primary research interests are in heterogeneous catalysis, specifically metal/metal-oxide interactions for the selective biomass upgrades. His research projects thus far have mainly focused on the applications of hydrodeoxygenation, hydrogenation/dehydrogenation and acidic catalysts involving WO_x overlayers.