The Catalysis Club of Philadelphia

(In Person) Thursday, February 15th, 2024

Brandywine Plaza Hotel
630 Naamans Road, Claymont, DE 19703

Ethylene Oxide Catalyst and Process Innovations: A Successful Journey Towards a Sustainable Industrial Process

Speaker: Dr. Madan M. Bhasin

Innovative Catalytic Solutions, LLC
MATRIC (Mid-Atlantic Technology, Research & Innovation Center)

The Role of Site Flexibility in the Activity of Fe-N-C catalysts

Student Speaker: Piaoping Yang

University of Delaware

Meeting Agenda:

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

Meeting Registration:

Members: $45.00
Non-Members: $55.00
Stud. & Retired Members: $35.00

Please register online for this In-person meeting by ***Thursday, February 8th*** at CCP website.

Meal Selection (Included):

Please make one selection for your dinner (included in registration) when you sign-up for the meeting from the following options:

1. Maryland Crab Cakes. Dessert: chocolate hazelnut cake.
2. Chicken Champagne. Dessert: chocolate hazelnut cake.
3. Eggplant parmesan (vegetarian). Dessert: chocolate hazelnut cake.
4. Roasted Vegetables (vegan). Dessert: fruit cup.

Salad comes with any option: Caesar Salad

Membership Registration:

Membership dues for CCP 2023-24 meeting 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). Please sign-up membership (Link) for more benefits on meeting registrations and net-working events!

Please contact our Treasurer Steve Hardwick (sjh.wilm.de@gmail.com) or Chair Angela Zheng (angela.zheng@matthey.com) if you need any assistance.

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Dr. Madan M. Bhasin

Ethylene Oxide Catalyst and Process Innovations: A Successful Journey Towards a Sustainable Industrial Process

Chief Scientific Advisor, Mid-Atlantic Technology Research and Innovation Center

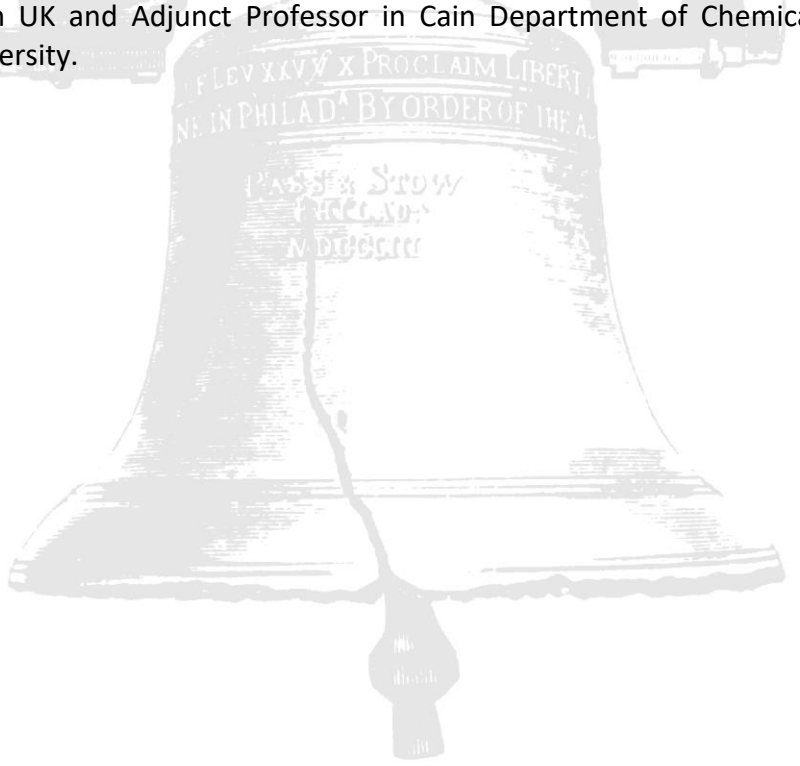
Owner, Innovative Catalytic Solutions, LLC

Abstract: Ethylene oxide (and ethylene glycol) are very large volume, commodity chemicals and building blocks for a large numbers of other derived chemicals-with annual production exceeding 50 Billion pounds per year. These commodity chemicals have been growing globally at the rate of 5-6%/year for the last 3-4 decades. Improving catalyst selectivity and hence reducing carbon dioxide emissions has been very intense competitive activity amongst the major competitors; Union Carbide/Dow Chemical, Shell/Criterion and Scientific Design for the last 50 years. The key catalyst inventions leading to innovations of successively improved generations of ethylene oxide catalysts from about 70% to 90%, over the last three/four decades, will be presented. In addition, the process evolutions from the old multi-reactors in series for Air based and then the multiple parallel reactor based oxygen based processes leading to the current designs of a single reactor to produce 500-1000 MM lbs/year in a single plant, will be presented. In addition, these innovations have resulted in a much simpler process design having lower capital & operating costs along with process simplicity and enhanced process safety. Most importantly, from sustainability standpoint, Carbon dioxide emissions have been reduced enormously, from about 30% to 10%, even though the worldwide capacity has nearly doubled in the last 15 years. Importantly, even more reductions in carbon dioxide emissions and improvement in selectivity are possible in the coming years.

Speaker Bio:

Dr. Madan Bhasin is the Chief Scientific Advisor at Mid-Atlantic Technology Research and Innovation Center (MATRIC) and owner of Innovative Catalytic Solutions, LLC. Dr. Bhasin holds a PhD in Physical Chemistry from the University of Notre Dame and has over 45 years of experience in the chemical industry, primarily with Union Carbide and Dow Chemical. His primary area of expertise is heterogeneous catalysis, with a strong emphasis on surface science and the analytical techniques involved in catalyst characterization. He participated in the discovery, development, and commercialization of eleven generations of improved high efficiency ethylene epoxidation catalysts that have contributed to Union Carbide's and Dow's technology leadership position in this area. Dr. Bhasin received the highest prestigious Hebert DOW Gold medal and the first DOW Chemical President's award.

Dr. Bhasin is a member of the National Academy of Engineering, Fellow of the National Academy of Inventors, ACS Fellow and AIChE Fellow. Dr. Bhasin is the recipient of numerous awards including Eugene Houdry Award of the North American Catalysis Society, Industrial Chemistry Award from ACS, and the Chemical Engineering Practice from AIChE. Dr. Bhasin has 25 U.S. patents and 24 publications in peer-reviewed journals. He was Visiting Honorary Professor at Cardiff University in UK and Adjunct Professor in Cain Department of Chemical Engineering, Louisiana State University.



The Role of Site Flexibility in the Activity of Fe-N-C catalysts

Piaoping Yang

Advisor: Prof. Dion Vlachos, University of Delaware

Abstract: Nitrogen-doped, carbon-supported transition metal catalysts are excellent for several reactions. Structural engineering of M-N_x sites to boost catalytic activity is rarely studied. Here, we demonstrate that the structural flexibility of Fe-N_x site is vital for tuning the electronic structure of Fe atoms and regulating the catalytic transfer hydrogenation (CTH) activity. By introducing carbon defects, we construct Fe-N_3 sites with varying Fe N bond lengths distinguishable by X-ray absorption spectroscopy. We investigate the CTH activity by density-functional theory and microkinetic calculations and reveal that the vertical displacement of the Fe atom out of the plane of the support, induced by the Fe-N_3 distortion, raises the Fe $3dz^2$ orbital and strengthens binding. We propose that the activity is controlled by the relaxation of the reconstructed site, which is further affected by Fe-N bond length, an excellent activity descriptor. We elucidate the origin of the CTH activity and principles for high-performing Fe-N-C catalysts by defect engineering.

Speaker Bio: Piaoping Yang is a fifth-year Ph.D. student at the University of Delaware working with Prof. Dion Vlachos. Piaoping received her Bachelor's degree at Nanjing Tech University and Master's degree in Chemical Technology at Tianjin University in China. Her research interests have been the theoretical heterogeneous catalysis. Her current research focuses on investigating the structure-activity relationship of carbon materials for biomass upgrading through multiscale modeling and simulation.