Catalysis Club of Philadelphia

Webinar: 6:30pm EST, Thursday, January 14th, 2020

Webinar link shared after registration

Speaker : Dr. Hai-Ying Chen

Johnson Matthey, Wayne, PA 19087, USA

From Atoms to Automobiles: Exhaust Emission Control Catalysts

Graduate Student Speaker: Sai Praneet Batchu

Department of Chemical and Biomolecular Engineering, University of Delaware

Role of Ga in non-oxidative dehydrogenation of ethane on Ga/Al_2O_3 catalyst

Meeting Schedule:

6:30 PM: Networking Time
7:00 PM: Student Speaker
7:20 PM: Main Speaker

Meeting Fees:

Free to CCP Members

Meeting Etiquette:

Please remember to mute your microphone and arrive early to solve any technical issues.

Webinar Registration:

Please register online by **Wednesday, *January 13th*** using this **LINK** or notify Arrangements Chair Jian Chang (CJ).

A webinar meeting invite will be provided on January 14th to all those who register.

Membership:

Dues for the 2020-21 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 local club and $5 for national club). Use this **LINK** for membership registration.

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From Atoms to Automobiles: Exhaust Emission Control Catalysts

Hai-Ying Chen

Johnson Matthey, Wayne, PA 19087, USA.

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Abstract:

Since the first installation on automobiles in 1974, exhaust emission control catalysts have represented one of the great achievements in the history of catalysis. Nearly all new automobiles produced today around the world are equipped with emission control catalysts to reduce the harmful CO/HC/NOx/PM pollutants from the engine exhausts. It is estimated that emission control catalysts have reduced air pollutants, worldwide, by more than 10 billion tons.

Depending on the applications, a wide range of catalyst technologies have been developed. Even within a given emission control system, multiple catalytic components, typically supported on monolith honeycombs, are integrated to achieve the high conversion efficiencies for each pollutant in order to meet the stringent environmental regulations. These catalytic components can be materials with isolated single atoms that perform the required catalytic functions, or zeolites with microporous framework structures that provide both catalytic centers and molecular sieve effects, or mesoporous oxide supports that not only provide surfaces to disperse and maintain metal nano-particles but may also function as active constituents drastically promoting the catalytic functions of the metal nano-particles.

This presentation will give examples of developing various exhaust emission control catalysts from isolated single atoms to fully formulated monolith honeycombs, covering a length scale of ~ 0.1 nm to ~1 m, or about 10 orders of magnitude.

Speaker's Biography:

Dr. Hai-Ying Chen is a Global Technology Fellow at Johnson Matthey. His expertise is in the development of advanced emission control catalysts and technologies to enable gasoline and diesel vehicles to meet stringent environmental regulations. Hai-Ying received his Ph.D. in Chemistry from Fudan University, China. Hai-Ying has published more than 60 technical papers and holds more than 380 granted patents in various jurisdictions around the world. In 2017, Hai-Ying was elected as a Fellow of the Society of Automotive Engineers. He received numerous awards, including the Catalysis Club of Philadelphia Award in 2014, Eugene J. Houdry Award in Applied Catalysis by the North American Catalysis Society in 2019.

Role of Ga in non-oxidative dehydrogenation of ethane on Ga/Al_2O_3 catalyst

Sai Praneet Batchu

Department of Chemical and Biomolecular Engineering, University of Delaware

Abstract:

The catalytic dehydrogenation of ethane to ethene is a challenging reaction of increasing importance owing to the growing demand for ethene, a commodity chemical central to the chemical industry worldwide. Ga_2O_3-based catalysts have garnered interest as potential catalysts for alkane dehydrogenation and a potential alternative to the currently used costly Pt-based catalysts and toxic Cr based catalysts. Especially, Al_2O_3-supported Ga catalysts have shown promising selectivity towards ethylene product. Although it is believed and hypothesized that synergy between Ga and support-Al sites is responsible for the higher activity of Ga/Al_2O_3 when compared to Al_2O_3, the nature of active sites and the roles of Ga and Al are unknown.

In this work, we employ density-functional theory (DFT) calculations and microkinetic analysis to investigate the efficacy of Ga-modified γ- Al_2O_3 for the catalytic dehydrogenation of ethane and the synergy between Ga and Al sites. We model modified surfaces either by grafting or by doping at varying Ga loading. Also, we validate the results of the microkinetic models by comparing them with experimental kinetic results. We synthesize different Ga-loadings on Al_2O_3 and evaluate the corresponding rates, apparent activation energies, reaction orders, and compare them with those on pristine-Al_2O_3.

Our experiments indicate that the dehydrogenation rates are significantly higher, and the apparent activation energies are significantly lower on Ga-doped Al_2O_3 catalysts compared to pristine- Al_2O_3. Our simulations underscore that grafted Ga sites are catalytically inactive and that only doped sites can enhance the activity of γ- Al_2O_3(110). We demonstrate that trace amounts of water and surface hydroxyl groups preferentially block Al_{III} sites, and that supported-Ga sites become vital to the catalytic dehydrogenation of ethane. Inclusion of water explains the experimentally observed apparent activation energies and changes the most active site.

Speaker Biography:

Sai Praneet Batchu is a 4th year Ph.D. student in the Vlachos group at the University of Delaware. He pursued his undergraduate studies in chemical engineering at the Indian Institute of Technology Madras (IIT Madras), India. His research interest lies in computational catalysis and works on investigating the reaction mechanisms and kinetics of various important heterogeneous catalytic reactions such as ethane dehydrogenation and conversion of biomass-platform chemicals to dienes.