Catalysis Club of Philadelphia

Thursday, February 21st, 2018
Crowne Plaza Wilmington North
630 Naamans Road, Claymont, DE 19703

Speaker: Prof. Bingjun Xu

Zeolite Encapsulated Metal Nanoparticles for Selective Tandem Catalysis

University of Delaware

Post-Doc Speaker: Dr. Konstantinos Alexopoulos

Probing the state of single atom catalysts via microkinetic analysis of low temperature CO oxidation

University of Delaware

Meeting Schedule:

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

Meeting Fees:

Members: $40.00
Non-Members: $45.00
Stud. & Retired Members: $25.00

Menu

A broiled Maryland crab cake appetizer, served with a spinach side salad, Tiramisu and your choice of 3 entrees:

1) Roasted Pork Loin – *Complimented by apple cider demi glaze and golden raisins*
2) Cajun Seared Salmon – *Rubbed with Cajun spices and topped with creole cream sauce*
3) Vegan Pasta Dish – *Cavatappi pasta, oven roasted seasonal vegatables, and marinara sauce*

Meal reservations – Please register online by ***Friday, February 15th*** at http://catalysisclubphilly.org/ or notify your company representative or our Treasurer Lifeng Wang (Lifeng.Wang@pqcorp.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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Prof. Bingjun Xu

Zeolite Encapsulated Metal Nanoparticles for Selective Tandem Catalysis

Department of Chemical & biomolecular Engineering University of Delaware

Abstract: Heterogeneous catalysis is one of the pillars of the energy and chemical industries, and a central science in driving the accelerating transition to a carbon neutral future.

Understanding catalytic processes mediated by solid surfaces on the molecular level holds the key to catalyst design, but is challenging due to the complexity of the local environment in which chemical transformations occur. In this lecture, encapsulation of metal nanoparticles in zeolite crystals as an effective catalyst architecture to mediate selective tandem upgrading of biomass derived feedstocks is discussed in the context of two case studies. The sequence to which substrates are exposed to different active sites and the distribution of metal and acid sites in zeolite crystals are shown to play decisive roles in determining selectivity and stability of catalysts.

Speaker Details: Bingjun Xu is currently an Assistant Professor in the Department of Chemical and Biomolecular Engineering at University of Delaware. Dr. Xu received his Ph.D. in Physical Chemistry, advised by Profs. Friend and Madix, from Harvard University in 2011. His thesis established a general mechanistic framework for oxidative coupling reactions on the Au surface through surface science studies. Dr. Xu worked with Prof. Davis at Caltech on the development of a low temperature, manganese oxide based thermochemical cycle for water splitting. Upon finishing his postdoc, he joined the Department of Chemical & Biomolecular Engineering at University of Delaware in 2013. The current research interest of the Xu lab spans heterogeneous catalysis, electrocatalysis and in-situ/operando spectroscopies. Dr. Xu is an awardee of NSF Early Career Award (2017), the Air Force Office of Scientific Research Young Investigator Award (2016), ACS Petroleum Research Fund Doctoral New Investigator Award (2015), and recently selected as one of the I&EC Class 2018 Influential Researchers.

Dr. Konstantinos Alexopoulos

Probing the state of single atom catalysts via microkinetic analysis of low temperature CO oxidation

Vlachos Group, Department of Chemical and Biomolecular Engineering, University of Delaware, USA

Abstract: Single atom catalysts receive extensive attention for reducing noble metal utilization and potential elimination of side reactions. Yet, their active sites remain highly debated and fundamental insights are limited due to experimental challenges. Here we introduce first-principles microkinetic modeling, with CO oxidation over Pd atoms on γ-alumina as a testcase, to provide insights into single atom catalysis. Although CO oxidation has been previously suggested to occur on doped Pd single atoms in alumina, experimental turnover frequencies and reaction orders are well reproduced only if the reaction proceeds on adsorbed Pd single atoms. This finding shows that microkinetic analysis can be essential for understanding the performance of different catalytic materials and for potentially discriminating mechanisms and active sites. Importantly, we show for the first time that the well-established ab initio thermodynamics approach fails to describe the coverages and the correct oxidation state of a catalyst, at least in the single atom or small cluster limit. Instead, a fully kinetic modeling approach is required to expose simultaneously kinetics, adsorbate coverages, and the catalyst oxidation state. These findings have important ramifications well beyond the specific system studied herein for closing the gap between models with kinetic and operando spectroscopic experimental studies.

***Acknowledgments**:* This work is performed in the framework of the PARTIAL-PGMs project – funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No 686086.

Speaker Details: Dr. Konstantinos Alexopoulos is a postdoctoral researcher at the Vlachos Research Group at the University of Delaware. His postdoctoral research focuses on the computational investigation of atomically dispersed catalysts for emission control and chemical production technologies. He received his Chemical Engineering degree in Greece from the National Technical University of Athens. He then moved to Belgium to earn his PhD degree in Chemical Engineering at Ghent University under the supervision of Prof. Guy Marin and Prof. Marie-Françoise Reyniers. After completing his PhD studies, he was offered a non-tenure track assistant professor position in the Chemical Engineering Department of Ghent University. During this time, he developed multiscale modeling approaches for zeolite-catalyzed bio-alcohol conversion processes and visited the Institute for Integrated Catalysis at PNNL to study the effect of dynamics on alcohol adsorption in zeolites. As a result of his research activities and collaborations, he has co-authored 20 publications in high-ranking scientific journals.