PennState College of Engineering | CHEMICAL ENGINEERING

Chemical Engineering Seminar Series

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Tuesday
April 14, 2020

Via Zoom:
https://psu.zoom.us/j/461070254

11:00 - 12:00 pm

First-principles investigation of isolated active sites in heterogeneous catalysis

Abstract

Although site isolation is an important concept in heterogeneous catalysis, the catalytic performance of isolated active sites is not always well understood. To this end, first-principles-based simulations can provide a wealth of insights with unprecedented spatial and temporal resolution. In the first part of my talk, I will illustrate how microkinetic analysis can be essential for discriminating between different active sites and mechanisms in the catalytic oxidation of carbon monoxide. Given that isolated sites anchored on a support can occasionally undergo sintering, the present work underscores the necessity to model simultaneously surface chemistry and catalyst dynamics for the rational design of highly reactive and stable sites. In the second part of my talk, I will use a prominent example of isolated active sites, namely Brønsted acid sites in highly siliceous zeolites, to showcase how mechanistic information for bio-ethanol dehydration can be translated from the atomic level all the way up to the industrial scale. Incorporating this type of information into multiscale models allows to explore a vast decision space, reconcile observations at different reaction conditions and capture effects that go beyond the active site. In addition, multiscale models based on first principles can guide the rational selection of reaction conditions and reactor configuration to achieve the desired product selectivity.

Biosketch

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 shale gas conversion 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. Hydrocarbon oxidation over metal oxide catalysts was the subject of his doctoral research. Upon completion of his PhD studies, he was offered a non-tenure track assistant professor position at 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 more than 20 publications in high-ranking scientific journals.