Chemical and Petroleum Engineering

SEMINAR NOTICE

Bin Liu

Associate Professor
Tim Taylor Department of Chemical Engineering
Kansas State University

Dr. Bin Liu is the Associate Professor of Chemical Engineering at Kansas State University. He received his B.S. in Chemical Engineering from Dalian University of Technology in China in 2003, and Ph.D degree in Chemical Engineering from Colorado School of Mines in 2008. Before joining the Tim Taylor Department of Chemical Engineering at Kansas State University in 2013, he worked as a postdoctoral researcher at the Center for Nanoscale Materials at Argonne National Laboratory.

His research focuses on molecular modeling of various catalytic processes related to sustainable chemicals and fuels production, using Density Functional Theory. A main portion of his work has been sponsored by National Science Foundation, and US Department of Energy Basic Energy Science Office. He has received the Outstanding Tenure-Track Assistant Professor Award in 2016, the Wayne Harms Keystone Research Scholar in 2019, and William Honstead Professorship in Chemical Engineering in 2020.

How Will Molecular Modeling Aid Sustainable Chemicals Production?

Abstract

One of the most urgent, contemporary issues in chemical industry is to mitigate or even negate the impact on environment during chemicals production. In this regard, effective, innovative catalysis is at the heart of chemical engineering.

Density Functional Theory (DFT) has established itself as a mainstream tool as an integral part of catalysis science and engineering. In this talk, I will discuss two case studies based on our recent work, i.e., ammonia synthesis and dry reforming of methane (DRM), both of which are conventionally energy intensive processes. First, ammonia synthesis adopting the chemical looping strategy will be introduced. The theoretical approach, a combined DFT calculation and kinetic modeling, helped advance the composition and functionality manipulations in order to boost the extraction of lattice N species and NH3 formation. For DRM, the ternary Co3Mo3N, which is shown to be both active and coke resistant, was considered as a novel material. Both the reactivity and coke prohibition were investigated using DFT, which also resulted in a microkinetic model to account for the distinct catalytic functionalities versus transition metal DRM catalysts.

Tuesday, March 23rd | 1:00 – 1:45PM

Zoom Meeting: 998 8566 6254 | Passcode: 560824