



COLLEGE OF ARTS & SCIENCES  
Department of Chemistry

Brown and Williamson Series

Friday, February 21, 2020  
@12:30 pm  
Chemistry Building, LL-16



## **Qingfeng Ge, Ph.D.**

Professor, University Distinguished Scholar Chair  
Department of Chemistry and Biochemistry  
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Associate Editor, Journal of CO<sub>2</sub> Utilization (Elsevier)

**BIO:** Dr. Qingfeng Ge is University Distinguished Scholar and Professor in the Department of Chemistry and Biochemistry of Southern Illinois University Carbondale. He currently serves as the Chair of the department and is an Associate Editor of Journal of CO<sub>2</sub> Utilization (Elsevier). Dr. Ge received his education in

Chemical Engineering from Tianjin University, China, obtaining B.S., M.S. and Ph.D degrees. He worked as Postdoctoral Research Associate in Copenhagen University, Denmark and Cambridge University, U.K. and as Research Scientist in University of Virginia. He joined SIUC as an Assistant Professor in 2003 and was promoted to Associate Professor in 2007 and to Professor in 2010. He is one of the 70 recipients of the Presidential Hydrogen Fuel Initiative grants in 2005 and the winner of 2018 ACS Midwest award. A main thrust of his research is using modeling/simulation in combination with experimental studies to address materials issues related to energy and environment. Current research projects include CO<sub>2</sub> hydrogenation, electrochemical reduction of CO<sub>2</sub>, CO<sub>2</sub> coupling with methane, and biomass conversion/utilization. His experiences ranged from experimental characterization and kinetics modeling to first principles based simulations of catalytic materials and processes. He authored/coauthored ~ 170 peer-reviewed publications.

## **Simulating Heterogeneous Catalysis for Energy- and Environment-Related Applications**

**ABSTRACT:** Sustainable development of the world requires efficient processes and materials that can convert sustainable resources into fuels and chemicals. The design and development of robust heterogeneous catalysts for practical applications have been hindered by our limited understanding of the underlying physical/chemical processes that govern the catalytic transformations. Recent advances in DFT-based electronic methods, molecular simulations and the availability of computing power provide unprecedented ability to track these molecular transformations and how they proceed at specific sites and within particular environments. Over the past decades, we have the opportunities of applying these methods in studies of catalytic materials and processes related to CO<sub>2</sub> and CH<sub>4</sub> activation and conversion and other application. In this talk, I will present selected results and discuss their implication to practical applications.