Amgen Seminar Series in Chemical Engineering

in

Cherry Auditorium, Kirk Hall, 1 PM

Presents on February 18, 2016

Drive the Discovery of Green Catalysts for Biomass Conversion using Inverse Molecular Design

By

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Designing efficient catalysts is the key for the development of next-generation technologies of converting biomass into value-added chemicals such as liquid fuels. However, designing biomass catalysts based on earth-abundant metals that can work under mild conditions (e.g., low pressure, low temperature, and with green solvents) remains a challenge. In this talk, I will present the recent research effort in our laboratory on developing new inverse design methods to drive the discovery of novel green catalysts for biomass conversion.

First, we explored the theoretical limits of reaction conditions for the hydrogenation and hydrogenolysis of biomass model compounds, using quantum chemistry calculations based on density function theory. Our results showed that thermodynamically it is indeed possible to design green hydrogenation catalysts that can work at the mildest conditions for converting biomass molecules into value-added chemicals. The thermodynamic study also helped us to understand the selectivity of an existing Cu-doped hydrotalciate catalyst in experiments. Second, we developed a new inverse molecular design method based on tight-binding electronic structure theory to search for novel hydrogenation catalysts. Our approach of inverse design aims at searching for optimum points on the hypersurfaces defining the property-structure relationships for catalysts, and then mapping out the catalyst structures at the optimum points, leading to enhanced success rate of catalysts discovery. Our new inverse design method showed to be effective on searching for novel hydrogenation catalysts with higher activity.

Biography

Dequan Xiao conducted his postdoctoral work at Yale University from 2009 to 2013. He has a PhD degree in theoretical and computational chemistry from Duke University in 2009, and a BS degree in chemistry from Sichuan University (Chengdu, China) in 1996. In August of 2013, he started his career as an assistant professor at the University of New Haven, and established the Laboratory for Integrative Materials Discovery. His research interests focus on developing new theoretical and computational chemistry methods to drive the discovery of new materials, such as green catalysts for biomass conversion and molecular drugs for cancer therapeutics. He published 32 peer-reviewed articles, obtained 4 patents, and wrote two book chapters on “Inverse Molecular Design for Materials Discovery” and “Green Catalysts for Producing Liquid Fuels from Lignocellulosic Biomass”, respectively.

This series at the University of Rhode Island is made possible through the generosity of Amgen, West Greenwich, R.I.

Refreshments provided by the Joseph Estrin Endowment.