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Wednesday, February 16th, 2022 at 4:00pm EST
Virtual Meeting: Zoom

Dr. Gina Noh



Assistant Professor
Chemical Engineering
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Structure-function relationships for acid strength effects

Structure-function relations are a key part of developing active, selective, and stable catalysts. The effects of acid strength in bifunctional catalysis will be examined for: (1) alkane isomerization and β -scission on physical mixtures of Pt/SiO₂ with zeolites and zeotypes and (2) CO₂ hydrogenation to CH₃OH on Cu-based catalysts.

Alkane isomerization and β -scission reactions are mediated by alkene species generated on the metal function. The kinetically relevant step is the skeletal isomerization or C-C bond cleavage of these alkenes, which occurs on Brønsted acid sites. The transition states for these reactions are ion pairs, composed of a carbocation derived from the reactant alkene and the conjugate base of the Brønsted acid. These transition states are therefore stabilized by stronger acid sites, which have more stable conjugate bases. The delocalization of charge throughout skeletal isomerization transition states is similar, resulting in the same intrinsic isomerization product distribution

irrespective of the strength of acid sites. In contrast, the positive charge in β -scission transition state carbocations is localized, resulting in greater stabilization by weak acids of these transition states, compared to those for isomerization. These intrinsic selectivities are challenging to determine experimentally in the case of solid acids composed of a continuous domain of active sites (e.g., zeolites and zeotypes). Instead, measured product selectivities largely reflect the site proximity between acid and metal sites.

For CO₂-to-CH₃OH reactions, Lewis acid sites that are sufficiently proximal to Cu nanoparticles stabilize surface intermediates and promote the formation of CH₃OH. Catalysts composed of Cu nanoparticles dispersed on SiO₂, which has been decorated with isolated group IV and group V metal centers (Ti, Zr, Hf, Nb, Ta), were synthesized using a surface organometallic chemistry approach and tailored molecular precursors. As a result of this synthetic strategy, these catalysts are nearly identical, with only the identity of the group IV or group V metal center being varied. Enthalpies of adsorption for pyridine were used as a functional measure of Lewis acid strength of these dispersed d⁰ metal centers, and CH₃OH formation rates increase as Lewis acid sites become stronger. Spectroscopic characterization indicates that formate and methoxy intermediates are stabilized by these acid sites. In fact, the ¹³C chemical shifts for methoxy intermediates in nuclear magnetic resonance spectroscopy experiments are sensitive to the strength of the Lewis acid sites of the catalyst, reflecting the energy of the empty d-orbital and its ability to accept lone pairs from the methoxy species. The same Lewis acid sites that stabilize these surface intermediates likely stabilize transition states to form CH₃OH, resulting in the promotion of their formation rates.

Speaker Bio

Dr. Noh is an assistant professor of chemical engineering at Penn State University, where her research group focuses on developing structure-function relations for atom-efficient chemical conversions. She was previously a postdoctoral research fellow in inorganic chemistry in the research group of Prof. Christophe Copéret at ETH Zurich in Switzerland, where she designed and synthesized catalysts for CO₂ hydrogenation to methanol and higher alcohols. She received her BS in chemical engineering from the Massachusetts Institute of Technology and her PhD in chemical engineering from the University of California, Berkeley, in the research group of Prof. Enrique Iglesia. At Berkeley, Gina was awarded a Chevron graduate research fellowship in support of her work. She has published her research in several high-impact chemistry and catalysis journals, and she has presented her work at national and international conferences. Gina's other interests include baking, running, mountaineering, and climbing.

Please refer to email announcement for login details.

Presentation 4:00 PM Annual Membership Dues \$35 (*Students = \$15*)

Deadline for reservations is 4:00PM Monday, February 14th, 2022

To make your reservation, fill out the [online form](#).
