“Insights into Active Site Structures for Bimetallic Heterogeneous Catalysts”

Virtual Seminar
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Abstract

As the world population continues to grow, catalytic reactions play a vital role in the production of fuels and chemicals necessary to meet global demands. Thus, there exists a need to improve the efficiency and overall sustainability of current chemical transformation processes. Simultaneously, there is a need for the development of new processes for the conversion of next generation feedstocks, including CO_2, biomass, and waste materials. These desired chemical conversions can be facilitated by the development of improved catalytic materials. A grand challenge in the design of better performing catalysts is the identification of the desired active site structure. Many conventionally prepared catalysts contain a broad distribution of structures, each of which contributes differently to catalytic performance. As a result, the desired active site is unknown, hindering the rational design of catalysts. To address this problem, I have synthesized well-controlled bimetallic catalyst surfaces, such that a narrow distribution of well-characterized structures exists. Thus, the catalytic activity over these materials can be readily correlated with these well-defined structures. The resulting structure-performance relationships then are used in the design of improved catalysts.

I will describe three examples investigating the use of bimetallic catalysts for reaction systems of industrial relevance and explore the origins of their improved performance. Investigation of Pd-based bimetallic catalysts for the selective hydrogenation of acetylene and for hydrodechlorination of 1,2-dichloroethane will be explored. Additionally, Pt-based bimetallic catalysts for the hydrogenation of a model α,β-unsaturated aldehyde, citral, will be described. These reaction systems serve as examples of (i) improving existing reaction processes, (ii) producing valuable products from waste streams, and (iii) developing more environmentally friendly routes to producing existing products, demonstrating the variety of ways in which improved catalysts can impact the chemical industry. The insights into active site structures for bimetallic catalysts developed in this work are an example of how structure-performance relationships can enable the development of improved catalytic materials. As a result, such catalysts can be used in industrial processes to reduce use of toxic and costly chemicals and solvents as well as decrease energy requirements, moving forward towards a more sustainable future.

Bio

Madelyn Ball received a B.S. in Chemical Engineering from the University of New Hampshire and a Ph.D. in Chemical Engineering from the University of Wisconsin – Madison under the supervision of James Dumesic. Her Ph.D. research focused on the synthesis and characterization of well controlled bimetallic catalysts with the goal of developing fundamental structure-activity relationships for a range of systems. She is currently an Eckert Postdoctoral Research Fellow at Georgia Institute of Technology in the group of Christopher Jones. Her current studies involve the use of synthetic materials chemistry to develop materials for both catalytic and adsorption applications.

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