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CHEMICAL AND BIOLOGICAL ENGINEERING
SEMINAR ANNOUNCEMENT

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The Pennsylvania State University*

*“Combined Computational and Experimental Study of
Selective Hydrogenation over Bimetallic Heterogeneous
Catalysts”*

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12:00PM

SCITECH ROOM 136

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The catalytic semi-hydrogenation of acetylene to produce ethylene is a common method for the removal of trace acetylene (~1%) in ethylene feed streams destined for ethylene polymerization. An effective catalyst for this reaction converts all of the acetylene to ethylene without further conversion of ethylene to ethane such that there is a net increase in the amount of ethylene. Pd-Ag alloys, and more recently, intermetallic Pd-Ga compounds, demonstrate high selectivity towards ethylene and long-term stability. Improved selectivity is a result of isolation of active Pd hydrogenation sites which reduces over-hydrogenation to form ethane, oligomerization products, and coke formation on the catalyst surface. Replacing Pd-based catalysts with base metal Ni-based catalysts would be highly beneficial in terms of cost and environmental impact. Bulk intermetallic catalysts contain little structural and compositional variance, a property that is not easily attainable with supported catalysts. We report on the catalytic selectivity of unsupported bulk intermetallic Ni-Zn and Pd-Zn catalysts for acetylene semi-hydrogenation. We demonstrate the addition of Ni to Zn improves selectivity to ethylene due to a reduction in acetylene oligomerization products rather than ethane over-hydrogenation. The most selective catalysts had the lowest Ni content with a γ -brass bulk structure. Structural investigation by neutron diffraction demonstrated the presence of well-defined Ni (or Pd) trimers in the γ -brass structure with the number of these trimers increasing with Ni (or Pd) content. The Ni alloys are active for H₂-D₂ exchange, but all surfaces (i.e, different Ni content) are indistinguishable with respect to their catalytic behavior. In the case of Pd-Zn alloys with the γ -brass structure, there are apparent differences in the H₂-D₂ rates and ethylene hydrogenation as the Pd content (and therefore number of Pd trimers) increases. While the Ni and Pd trimers are stable in the bulk structure, the differences in the surface stability of these trimers in the Zn matrix and the corresponding percentage of the trimer-containing surface present in a Wulff reconstruction explain the disparate catalytic results in the seemingly related systems. We demonstrate bulk intermetallics are useful systems to screen compositional and structural (from site-isolated to well-defined 2D clusters) variance on catalytic behavior. Transforming the bulk intermetallic structure into its nanoscale analog still remains a critical challenge for catalyst synthesis.