

The departments of Chemical Engineering, Chemistry & Biochemistry, and the Partnership for International Research in Electron Chemistry and Catalysis at Interfaces are pleased to announce a

SPECIAL SEMINAR

Bulk Composition Dependent H₂ Dissociative Adsorption Energies on Cu_xPd_{1-x} Alloy (111) Surfaces

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The bulk composition dependent dissociative adsorption energy of hydrogen on CuPd alloys has been measured experimentally and modeled using density functional theory. The hydrogen adsorption energy cannot be simply defined by a single reactive site, nor as a composition weighted average of the pure metal components. Detailed modeling of such systems is difficult due to the distribution of active sites with varying composition, site-dependent, and effects such as segregation. We utilized a composition spread alloy film approach to measure the kinetics of hydrogen dissociation on Cu-Pd alloys as a function of composition. We developed a modeling approach that uses a basis of active sites to estimate the bulk composition dependent adsorption energy, weighted by the site probability distribution for a random alloy. With this method we can explain the composition dependent adsorption energy on Cu-rich alloy surfaces with relatively little computational effort. Deviations from predicted trends in the Pd-rich region can also lend insight into the experimental results at an atomistic level. In Pd-rich alloys a Pd-hydride phase forms which results in deviations from adsorption on the metallic alloy surface.