Near-Surface Alloys for Improved Water-Gas-Shift Catalysis

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Abstract:

The primary route to hydrogen production from fossil fuels involves the water-gas shift (WGS) reaction ($CO+H_2O \rightarrow CO_2+H_2$), and an improvement of the efficiency of WGS catalysts could therefore imply a major leap forward towards the realization of hydrogen economy. From an interplay of high-resolution scanning tunneling microscopy (STM), x-ray photoelectron spectroscopy (XPS), and density functional theory (DFT) calculations we suggest the existence of a new thermodynamically stable Cu/Pt near-surface alloy (NSA). Temperature-programmed desorption (TPD) and DFT reveal that this Cu/Pt NSA binds CO significantly weaker than Pt, thereby implying a considerable reduction in the potential for CO poisoning of the Cu/Pt NSA surface as compared to pure Pt. In addition, DFT calculations show that this Cu/Pt NSA is able to activate H_2O, which is the rate-determining step for the WGS on several metal surfaces, easily and, at the same time, to bind the products of that reaction and formate intermediates rather weakly, thus avoiding possible poisoning of the catalyst surface. The Cu/Pt NSA is thus a promising candidate for an improved WGS catalyst.

List of Published Journal Articles:

1. **"A Cu/Pt Near-Surface Alloy for improved water-gas shift catalysis",** J. Knudsen, A. U. Nilekar, R. T. Vang, J. Schnadt, E. Kunkes, J. A. Dumesic, M. Mavrikakis, and F. Besenbacher, *Journal of the American Chemical Society* (in press).

Awards/Distinctions for the PI:

1. **Samuel C. Johnson Distinguished Fellowship**.
2. **Visiting Professor,** Department of Chemical Engineering, Technical University of Denmark, Lyngby, Denmark (Fall 2006).
3. Featured in NERSC News (March 2007): http://www.nersc.gov/news/nerscnews/NERSCNews_2007_03.pdf
4. Member of the **Advising Board** for the Center for Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, Lyngby, Denmark (1/07-).

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