325g Study of Spherosiloxane Adsorption on Metal Surfaces

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Metal-metal oxide interfaces are important features of devices prevalent throughout the electronics and semiconductor industry as well as in the field of catalysis. Unfortunately, these interfaces are generally not well understood since they are typically buried beneath a metal particle or film and cannot be accessed through usual surface science techniques. Catalytic activity, as well as the stability of catalyst particles over time, is known to be dependent on the metal-support interfacial chemistry. However, detailed knowledge as to how the nature of the metal/insulator interface affects catalysis is lacking. Indeed, there is almost no fundamental understanding of the bonding interactions between metal and insulator films, or of how those interactions vary with material properties.

Characterizing the adsorption sites at the metal-insulator interface has been difficult experimentally, because (1) the interface has a highly irregular structure, and (2) the interface is buried beneath a metal film, which limits the usefulness of surface science techniques. To overcome these limitations we are preparing a series of model interface structures composed of a layer of silica-like $H_xO_{1.5x}Si_x$ molecules (known as silsesquioxanes or spherosiloxanes) to be deposited on a single-crystal metal surface. These types of molecules have been used to model Si-SiO_2 interfaces in the past. Using this model system in both computational and experimental studies will allow probing of the metal surface while spherosiloxanes are bonded to it.

This model system offers a methodology for studying chemically diverse interfacial structures and their effects on interfacial physics and chemistry. Calculations utilizing density functional theory suggest that spherosiloxanes can form stable adsorption structures on a variety of catalytic metal surfaces, including Ni, Pd, Pt, Cu, Ag, and Au. Experimental studies of this model system are ongoing. In these studies we seek to determine how the metal structure and composition, spherosiloxane size and composition, and partial coverage of oxygen affect spherosiloxane adsorption chemistry. These studies will ultimately aid in elucidating structure-property relationships for metal-SiO_2 interfaces.