

Catalysis in the production of molecules and materials



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In this presentation, we will describe advances in cross-coupling chemistry that have dramatically broadened the ability to prepare chiral compounds. In particular, we will describe enantiospecific cross couplings for the preparation of complex chiral molecules of interest to the pharmaceutical industry and the ability to cross-couple seemingly identical boron substituents with different aryl iodides. The development of novel electrophiles for Suzuki-Miyaura cross coupling chemistry based on organosulfur chemistry for the preparation of bioactive molecules will also be presented.

The use of N-heterocyclic carbenes (NHCs) to modify homogeneous metal catalysts is widespread since the high metal-NHC bond strength renders high oxidative and chemical stability to NHC-ligated metal complexes. Despite this fact, the use of NHCs to modify metal *surfaces* is virtually unprecedented.

In this presentation, we will describe the use of NHCs to modify metal surfaces, including Au(111), Au nanoparticles, Au nanoclusters and the surfaces of other metals including Cu, Ag, Pt and Ni. Films prepared by the deposition of NHCs show molecular ordering on the surface and remarkable stability. They show no decomposition upon heating for 24 hrs in THF, in boiling in water for 24hrs or upon treatment with acid (pH 2) or base (pH 12). Incredibly, they even survive largely after 24 hr exposure to hydrogen peroxide. This remarkable increase in stability relative to thiol-based SAMs will greatly increase the number of reagents and conditions to which the SAMs can be exposed.

The use of NHCs to modify more catalytically relevant surfaces such as nanoparticles and clusters will also be presented. Bidentate NHCs were examined for their ability to protect gold nanoparticles. In addition, NHCs have been shown to be highly useful ligands for the preparation of stable, non-sulfur-containing magic number nanoclusters. The catalytic activity of these species in reactions of key environmental importance, such as the electrocatalytic reduction of CO₂ to CO, will be presented.

