

## **H<sub>2</sub> Binding and Reactivity on Transition Metal Complexes Underlying Biomimetic H<sub>2</sub> Production and New Materials for H<sub>2</sub> Storage**

Gregory J. Kubas

*Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM 87545*

*Email: [Kubas@lanl.gov](mailto:Kubas@lanl.gov)*

The H<sub>2</sub> molecule is held together by a very strong two-electron H–H bond but is only useful chemically when the two H's are split apart in controlled fashion. The reverse of this process is formation of H<sub>2</sub> from for example protons and electrons as performed elegantly and efficiently in Nature by hydrogenase enzymes. Both splitting of H<sub>2</sub> and formation of H<sub>2</sub> occurs on transition metal complexes via binding of molecular H<sub>2</sub> to the metal center, often observed as stable solids. Splitting of H<sub>2</sub> occurs by both homolytic (dihydride formation) and heterolytic (formation of metal hydride plus proton) pathways depending on the nature of the metal complex. The molecular chemistry and spectroscopic features of dihydrogen complexes will be the major topic of this talk. We are engaged in synthesizing catalysts for biomimetic photocatalytic hydrogen production consisting of first-row metals such as iron capable of binding and splitting/forming H<sub>2</sub>. Hydrogen binds reversibly to a surprisingly large variety of both metal and main-group atoms, especially at low temperatures, and we are also studying such H<sub>2</sub> complexes for hydrogen storage.