

# INORGANIC SEMINAR

## Moving Hydrides with Iron and Electrons through Metal Oxides: Biomimetic and Solar Fuels Approach for Hydrogen

The use and generation of hydrogen as a renewable fuel and feedstock is gaining importance as the pressure to diminish our dependence on fossil fuels grows. Nature has developed elegant methods to activate and utilize hydrogen, especially for the purpose of carbon dioxide CO<sub>2</sub> fixation. One such enzyme, mono-[Fe] hydrogenase, uses a unique array of non-proteinaceous ligands to activate H<sub>2</sub> and perform hydride transfer to the CO<sub>2</sub>-carrier substrate, H<sub>4</sub>MPT<sup>+</sup>. The iron center is ligated by a unique organometallic pyridone-acyl cofactor, which along with two carbonyls and a Cys-S stabilizes a low-spin Fe(II) center. We have developed a novel anthracene-scaffold ligand that mimics the biological coordination sphere – in both the identity and crucial facial geometry of the CNS donor set. Studies of H<sub>2</sub> activation and hydride transfer will be discussed.

Second, a key component of solar energy storage is H<sub>2</sub> generation from solar fuels devices. Our work utilizes a combination of silicon photoelectrodes, molecular interfaces and metal oxide passivating layers to achieve stable photoelectrochemical performance. The molecular nature of the interface between the electrode and the passivating metal oxide is critical in controlling electron transfer and, ultimately, the efficiency of H<sub>2</sub> generation. We have used both molecular catalysts (PNP-Ni; Re-bpy) and Pt/Au nanoparticles for H<sub>2</sub> generation and CO<sub>2</sub> reduction. We are also investigating the use of embedded molecular wires in metal oxides (Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, ZnO) to enhance electron transport across these insulating oxide materials.

**Prof. Michael Rose**

**University of Texas, Austin**

**Wednesday, February 14, 2018**

**3:30pm in room 1315 Chemistry**

If you wish more information please call 262-6815.

Refreshments will be available at 3:10 pm in Shain Tower Atrium