

# **CORE-CM SEMINAR**

## **Michigan State University**

**Dr. R. Morris Bullock**

**Center for Molecular Electrocatalysis**  
<https://efrc.pnnl.gov/cme/>  
**Pacific Northwest National Laboratory**  
**Richland, Washington 99352**  
[morris.bullock@pnnl.gov](mailto:morris.bullock@pnnl.gov)

### **Design of Molecular Electrocatalysts for the Production and Oxidation of Hydrogen**

Solar and wind are carbon-neutral, sustainable energy sources, but because they are intermittent, reliable, large scale energy storage is needed. Catalysts that efficiently interconvert between electrical energy and chemical bonds (fuels) are needed for sustainable, secure energy. Electrocatalysts based on inexpensive, earth-abundant metals (“Cheap Metals for Noble Tasks”) are needed. Ni complexes with “P<sub>2</sub>N<sub>2</sub>” ligands have been studied in our lab for production of H<sub>2</sub> by reduction of protons. The “P<sub>2</sub>N<sub>2</sub>” diphosphine ligands have pendant amines that function as proton relays, facilitating *intramolecular* and *intermolecular* proton mobility. The crucial role of controlled structural dynamics is recognized for many enzymes, but is seldom used in synthetic catalysts. Appending long alkyl chains in the outer coordination sphere of the Ni catalyst leads to slower structural dynamics of the ligand, with the turnover frequency increasing by orders of magnitude as the conformational dynamics become slower. Controlling all of the system components reverses the trade-off normally encountered between rates and overpotentials, providing design principles for multi-electron, multi-proton reactions. Iron and manganese complexes are being studied for the opposite reaction, oxidation of H<sub>2</sub>, with some of these complexes exhibiting unusually fast reversible heterolytic cleavage of H<sub>2</sub>.

**Thursday, October 17, 2019**

**12:00 NOON**

**Room 1400 – Biomedical & Physical Sciences**

**Professor Tom Hamann - Host**