



Inorganic Chemistry Seminar Series

Thursday, February 23, 2017, 12:30 pm

Seaver Science Library, Room 150

SSC Auditorium next to the library

Professor Michael Rose

Department of Chemistry

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Moving Hydrides with Iron and Electrons through Metal Oxides: Biomimetic and Solar Fuels Approaches for H₂ Utilization and Generation

Abstract:

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 CO₂ fixation. One such enzyme, mono-[Fe] hydrogenase, uses a unique array of non-proteinaceous ligands to activate H₂ and perform hydride transfer to the CO₂-carrier substrate, H₄MPT⁺. 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 H₂ activation and hydride transfer will be discussed.

Second, a key component of solar energy storage is H₂ 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 H₂ generation. We have used both molecular catalysts (PNP-Ni; Re-bpy) and Pt/Au nanoparticles for H₂ generation and CO₂ reduction. We are also investigating the use of embedded molecular wires in metal oxides (Al₂O₃, TiO₂, ZnO) to enhance electron transport across these insulating oxide materials.

Hosted by Professor Smaranda Marinescu

The scientific community is invited

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