Scientific Achievements and Activities in Yiying Wu group

Prof. Yiying Wu joined the Department of Chemistry and Biochemistry of OSU in 2005, was promoted to associate professor in 2011 and to full professor in 2014. He received the Cottrell Scholar Award in 2008, the NSF CAREER award in 2010, the CAPA Biomatik Distinguished Faculty Award and the Commissioner's Award in 2014. In 2011, he was ranked #6 worldwide on the Times Higher Education "Top Materials Scientists of the Past Decade." He is also an associate editor for *ACS Applied Materials and Interfaces*.

Wu group has been working at the interface of synthetic molecular chemistry, solid state materials chemistry, and (photo)electrochemistry. Our current focuses are dye-sensitized solar cells, metal-air batteries, and (photo)electrocatalysts for solar fuels. We utilize knowledge, concepts and techniques from chemistry, physics, materials science and engineering to create new materials, explore new sciences, and enable new applications. We welcome students with various backgrounds to join our group.

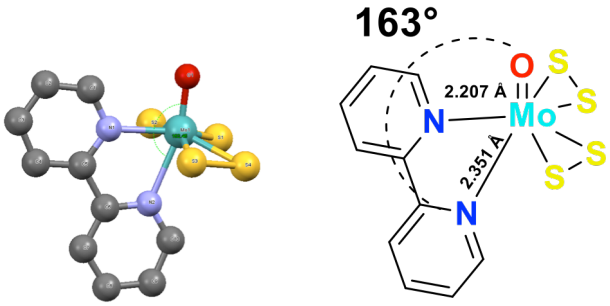

Figure 1. Crystal structure of $MoO(S_2)_2bpy$.

1: Electrocatalysts for hydrogen evolution: This project aims at studying molecular complexes with the structural motif of $MoO(S_2)_2L$ (Fig. 1), in which L is a bidentate ligand such as 2,2'-bipyridine (bpy) and the Mo-S_2^{2-} moieties mimic the MoS_2 edge sites for electrocatalytic hydrogen production. *The fundamental hypothesis is that, through ligand design, the electron-donating (or withdrawing) properties of the ancillary ligand L can tune the electron density of the Mo(VI) center, thereby influencing the Lewis basicity of the disulfido ligands. Therefore, the H-adsorption energy on the disulfuide ligands can be systematically tuned.* Furthermore, tunable ligand design can also provide the local proton source, while controlling the aqueous solubility of the molecular catalysts or their immobilization on electrodes. The catalytic mechanism will also be probed by combining experimental methods such as synchrotron X-ray absorption spectroscopy with computational efforts with density functional theory (DFT) calculations. This systematic and synergistic synthetic and mechanistic study should shed light on the relationship between the structures of the molecular catalysts and their electrocatalytic activity. The mechanistic knowledge will also provide insight into functions of bulk MoS_2 and biological enzymes. This is a collaborative project between the Wu group and Hadad group funded by National Science Foundation.

- Benjamin R. Garrett, Shane M. Polen, Kevin A. Click, Mingfu He, Zhongjie Huang, Christopher M. Hadad, and Yiying Wu*, "Tunable Molecular MoS2 Edge-Site Mimics for Catalytic Hydrogen Production", *Inorg. Chem.*, 2016, 55, 3960−3966 (DOI: 10.1021/acs.inorgchem.6b00206)
- Huang, Z., Luo, W., Ma, L., Yu, M., Ren, X., He, M., Polen, S., Click, K., Garrett, B., Lu, J., Amine, K., Hadad, C., Chen, W., Asthagiri, A. and Wu, Y. , "Dimeric [Mo2S12]2− Cluster: A Molecular Analogue of MoS2 Edges for Superior

Hydrogen-Evolution Electrocatalysis", *Angew. Chem.* 127, no. 50 (2015): 15396-15400.

2: P-type dye-sensitized solar cells (p-DSSCs) and solar fuels: Wu group has made pioneering contribution to p-DSSCs, including (1) designing new dye sensitizers for efficient hole injection into semiconductor supports, (2) synthesizing new nanostructured p-type semiconductors with proper band energies, high visible transparency and high hole mobility, and (3) investigating the fundamental charge transport and transfer processes at the p-semiconductor/dye/electrolyte interfaces. For example, his group designed the first cyclometalated Ru dyes for p-DSCs (Fig. 2). These p-DSSCs hold promise in constructing high-efficiency tandem dye-sensitized solar cells. Moreover, his group has also used the p-DSsCs as a platform for solar-driven reduction of water into hydrogen fuels. This project has been funded by Department of Energy.

- Kevin A. Click, Damian R. Beauchamp, Zhongjie Huang, Weilin Chen, and Yiying Wu, "Membrane Inspired Acidically Stable Dye-Sensitized Photocathode for Solar Fuel Production", Journal of the American Chemical Society, 2016, 138(4), 1174-1179 (highlighted by C&EN).

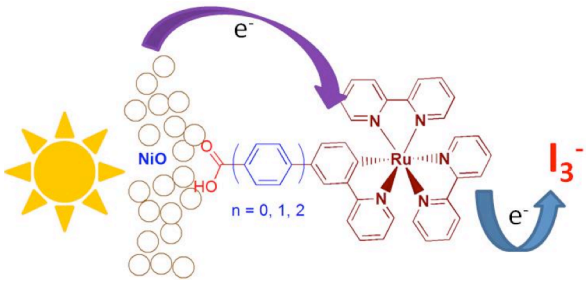

Figure 2: Examples of cyclometalated dyes and the interfacial electron transfer processes in p-DSSCs.

- Z. Ji, M. He, Z. Huang, U. Ozkan, Y. Wu "Photostable p-Type Dye-Sensitized Photoelectrochemical Cells for Water Reduction", *J. Am. Chem. Soc.*, **2013**, *135* (32), pp 11696–11699.

3: K-O2 batteries: Metal-air batteries are the most dense electrochemical power sources and are anticipated to play an important role in electrification of transportation and grid energy storage. A major challenge in metal-air batteries, such as zinc-air and lithium-air batteries, is the overpotentials caused by the multi-electron chemical processes oxygen goes through in order to store and dispense energy. Since expensive catalysts are required to reduce these high overpotentials, these batteries are neither energy- nor cost-efficient. In 2013, Wu group invented K-O_2 battery that is based on the reversible one-electron O_2/KO_2 redox couple, which eliminates the need for these electrocatalysts (Fig. 3). This method has elegantly solved the oxygen reduction and evolution kinetics limit, and brings metal-air batteries closer to practical applications. This invention has received broad attention in the battery community. This project is funded by National Science Foundation

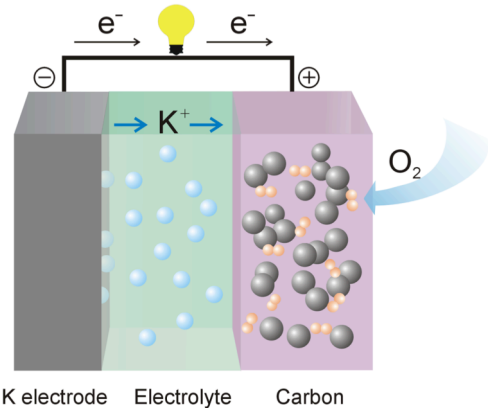

Figure 3. The schematic of a K-O_2 battery

- X. Ren, Y. Wu, "A low-overpotential potassium-oxygen battery based on potassium superoxide**",** *J. Am. Chem. Soc.* **2013**, *135* (8), pp 2923–2926.
- William D. McCulloch, Xiaodi Ren, Mingzhe Yu, Zhongjie Huang, and Yiying Wu, "A Potassium-Ion Oxygen Battery Based on a High Capacity Antimony Anode", *ACS Applied Materials & Interfaces. 7*, no. 47 (2015): 26158-26166.

4: Solar batteries: Wu group's recent breakthrough is in solar batteries based on the idea that photoelectrochemistry could be directly integrated into batteries because both fields use redox couples as the charge-transport shuttles. In 2014, his group demonstrated a solar oxygen battery that uses solar energy to assist the charging process of Li-O_2 batteries. Later the concept was extended to solar flow batteries that use solar energy to assist the charging process of Li-iodine flow batteries. These pioneering works are useful for creating new technology that can directly store the solar energy, which solves the intermittent nature of sunshine. This work has been highlighted by Department of Energy, Columbus Dispatch (front-page story) and NBC4.

- M. Yu, X. Ren, L. Ma, Y. Wu, "Integrating a Redox-Coupled Dye-Sensitized Photoelectrode into a Lithium-Oxygen Battery for Photo-Assisted Charging", *Nature Communications* 5:5111 (2014).
- M. Yu, W. D. McCulloch, D. R. Beauchamp, Z. Huang, X. Ren, Y. Wu, "Aqueous Lithium-Iodine Solar Flow Battery for the Simultaneous Conversion and Storage of Solar Energy", J. Am. Chem. Soc., 2015, **137**, pp8332-8335.