Materials Seminar

Thursday, March 8, 2018 at 12:15 pm
Rm 1315 Chemistry

Prof. Shelley Minteer

University of Utah

"Electrocatalysis for Energy & Electrosynthesis Applications"

Recently there has been an increased interest in the development of small molecule electrooxidation catalysts such as (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO), for use in the anodic compartment of a biofuel cell. Some TEMPO derivatives are capable of electrochemically oxidizing short chain alcohols and various sugars to the corresponding aldehydes and carboxylic acids under physiological aqueous conditions. However, building libraries of such a catalyst is difficult due to the limited number of commercially available TEMPO derivatives and the lack of modular synthetic pathways to more complicated TEMPO structures. A promising alternative to the physical preparation of such libraries is the use of computational modeling to allow for *in silico* catalytic screening of a much wider range of TEMPO compounds. We have recently developed a descriptive model that correlates the electrocatalytic activity of nitroxyl radical catalysts to their redox potentials under aqueous conditions. Fundamental characteristics derived from this model have enabled the design of highly active and promiscuous catalytic materials. In addition, we have incorporated highly active TEMPO derivatives into an artificial protein to impart unusual selectivity onto the nitroxyl radical catalyst.

Hosted by Prof. Shannon Stahl