**Principal Investigator: Jenny Lockard**

Title: Spectroscopic explorations of redox active metal-organic frameworks
Funding agency: NSF – DMR

NON-TECHNICAL SUMMARY:
This project involves the investigation of a class of porous materials called metal-organic frameworks that have potential applications ranging from fuel cell technology to industrial chemical production to solar energy conversion. While significant progress has been made in developing novel frameworks for these purposes, basic insight on how these materials work is severely lacking. The research activities in this project, which rely on several X-ray and optical characterization methods, meet this need by targeting a fundamental understanding of the properties and processes behind the applications, including how charges move and are distributed in these materials. The outcome of this work is crucial for facilitating the rational design of the next generation of these materials with improved performances and therefore has far reaching implications for a broad range of energy and environmental sustainability applications. Furthermore, as part of a broader mission to integrate research in education, the outreach component of the project will provide not only hands-on research experiences for high school science teachers in the Newark region, but a mechanism for translating those experiences into meaningful high school science curricula that meet the specific needs of the students in this urban community. This outreach initiative stands to have a large impact on the students in these schools since it targets the educators that teach them.

TECHNICAL SUMMARY:
The research focuses on understanding fundamental structure/function relationships in redox and photoredox active metal organic frameworks (MOFs), an emerging class of hybrid materials composed of metal ions or clusters connected by organic molecules to form crystalline microporous networks. Their intrinsic porosity and tunable architecture allow electronic structure (bandgap-like) manipulation, selective guest species interaction and the incorporation of redox active components and other synergistic characteristics. Furthermore, these multicomponent framework functionalities inevitably lead to increasingly complicated structure-function relationships, involving subtle structural rearrangements, electronic delocalization and cooperative interactions of the framework host and guest species. Redox active MOFs therefore not only engender emerging technological interest but serve as a unique and fascinating platform for fundamental studies of host-guest chemistry, electron transfer and organometallic photophysics in 3D coordination space. The proposed research focuses on MOF systems that exhibit redox activity in the ground state, excited state and/or associated with donor-acceptor host-guest interaction. The principal objectives in studying these systems are to expose the prevalence and role of electronic delocalization and pertinent electronic and molecular level structural changes associated with their redox or photoredox processes. To accomplish these goals, a targeted set of vibrational, optical, and X-ray spectroscopy methods are employed in combinations of steady state, *in situ*, and in some cases time-resolved studies of MOF systems to garner real time information on their electronics, host-guest interactions and molecular level structure changes. These insights will help elucidate the mechanisms behind their redox behavior. Ultimately the trends afforded by this study will facilitate the rational design of the next generation of MOF materials with improved performance for redox-based applications.