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Probing ground and excited state charge transfer in Metal Organic Frameworks through X-ray Spectroscopy

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Abstract: Metal organic frameworks (MOFs) are hybrid solid state materials composed of metal ions or clusters connected by organic molecules to form crystalline microporous networks. Their diversity in chemical makeup and tunable, permanent porosity make MOFs attractive candidates for traditional adsorption-based applications such as chemical separation and storage. Efforts to engender redox or photoredox properties offer new opportunities for applications that rely on MOF conductivity, stable electron transfer and/or long-lived charge separation such as resistive sensors, electrochromic devices, and single site electro- or photocatalysis. Synthetic strides in developing frameworks with these properties have, however, far outpaced the progress in advancing the fundamental understanding of their electronic structure and photophysics. Consequently, there are often significant ambiguities in the structure/function relationships that give rise to their utility. In our research, we use a targeted set of spectroscopy methods to make those connections by producing molecular level understanding of observed MOF behavior. Specifically, the talk will focus on two types of redox active MOF systems. In the first part, photoredox active frameworks will be introduced and our efforts to elucidate the nature and dynamics of their charge separated excited states using X-ray transient absorption spectroscopy will be presented. In the second part of the talk, we will focus on ground state charge transfer and explore the nature of framework host-redox active guest species interactions in a conductive MOF system using conventional and high-resolution X-ray absorption spectroscopy.

Host: Dugan Hayes (dugan@uri.edu, 401-874-5516)