Department of Chemistry Seminar Series
Spring 2023

Friday, March 6, 2023, 3:30 PM – **HPA1-O119 (Health Sciences)**

Leveraging zirconia and titania multivariate metal-organic frameworks for the design of crystallographically and chemically complex materials

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Edge-1-transitive metal-organic frameworks (MOFs) are amenable for the homogeneous distribution of multicomponent link mixtures to form multivariates (MTV). From Vegard's law, edge-1-transitive MTV MOFs offer a high degree of predictability and provide a unique avenue to deconvolute structure-property relationships. Using zirconia MOFs that form in predictable topologies, we can reliably access targeted crystallographic parameters by mixing homeomorphic links with varying metrics. This strategy allows for precise control over both functionality and metrics independently. We can use similar strategies toward the design of MOFs with targeted properties like photocatalysis. Since MOFs based on titania secondary building units exhibit exceptional photoredox activity, we use this MTV approach to prepare a new library of photoredox active titania MOFs (UCFMOF-*n*, where *n* = # of phenyl rings in the link). UCFMOFs feature high substrate uptake which, in combination with light harvesting functionalization, results in superior visible light driven oxidation of benzyl alcohol. This work outlines strategies for combining continuous isoreticular expansions with link functionality to systematically study MOFs as complex materials.