

Advancing in situ Dynamic Single-crystal X-ray Diffraction

Gage Bateman, Dr. Jason Benedict

SUNY Buffalo

In situ X-ray diffraction techniques provide the ability to monitor the change in the structure of crystals, such as Metal-organic Frameworks (MOFs), in response to changes in the local chemical environment surrounding the material. These methods reveal the location and concentration of guest species as well as the reorganization of the host framework as the contents of the void spaces are exchanged. Previous work in our group examined the dehydration of a flexible cobalt-based framework in the single crystalline phase using dry nitrogen gas as well as the exchange of the lattice waters with ethanol. To examine the impact of grain size on the dehydration reaction, recent results from *in situ* powder X-ray diffraction measurements on the CoMOF system will also be presented. Finally, *in situ* single crystal X-ray diffraction measurements performed on an isostructural nickel-based framework resulted in markedly different guest exchange behavior. Possible explanations for this change in reactivity as well as recent improvements to the environmental control cell to enable exciting new experiments will be discussed.