



Contribution ID: 93

Type: Poster

Synchrotron X-ray Diffraction studies of Metal Organic Frameworks (MOFs) at high-pressure

Thursday, 8 September 2022 19:35 (1 hour)

Metal-Organic Frameworks (MOFs) are functional materials where the interconnection of inorganic coordination and organic linker chemistries provides a virtually unlimited chemical parameter space to investigate material responsiveness through chemical-structural changes. Their open network structure gives MOFs an extraordinary structural flexibility that often results in a large structural response to pressure (P) as an external stimulus, revealing a variety of material properties of large academic and technological relevance such as negative linear and area compressibility, mechanical energy storage and barocalorics amongst others. Identification of crystal chemistry principles to explain the interrelation between composition, structure and P-responsiveness of a MOF is key for synthesizing MOFs with potentially new and useful P-responses. In parallel, the discovery of electrically conductive MOFs raises fascinating questions of how the conductive pathways are affected by P-induced structural changes –an untouched research area with promising opportunities in applied and academic research.

Following structural changes as a function of hydrostatic P demands the use of high-P powder X-ray diffraction (HPPXRD) cells, which are ideally operated at synchrotron light sources. Such experiments deliver information about the mechanical properties and thermodynamic stabilities of MOFs thereby providing the data basis for the application and optimization of MOFs as barocalorics, or as piezochromatic sensors, to name a few. However, existing HPPXRD cells come with limitations such as difficult and time-consuming sample loading procedures, a poor P-control in the low-pressure range relevant for soft material research, i.e., $P < 1$ GPa, or a restricted maximum achievable P often insufficient to fully reflect the chemical diversity of MOFs. Additionally, simultaneous electrical conductivity measurements at high-P still involve a remarkable experimental challenge. To fully harness the potential of this research area, the development of new experimental techniques tightly coupled to chemical synthesis is key. In this contribution, we will discuss the required features of a prototype HPPXRD setup for further advancing in high-P research of MOFs and soft materials, clarify and improve existing structure-property relations that determine the mechanical properties of MOFs at high-P and provide proof-of-principle studies related to the high-P dependency of charge transport properties in electrically conductive MOFs.

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Session Classification: List of posters presented during the conference