Poster Presentations

[MS24-P18] Geometry Controlled Mechanics in Metal–Organic Frameworks.

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Metal–organic frameworks (MOFs) are a class of porous polymeric materials, composed of metal ions or clusters coordinated to organic bridging ligands. Their mechanics are often found to be unusual: many MOFs display negative thermal expansion (NTE), and negative linear compressibility (NLC). These are interesting properties for applications in thermal-expansion-adjustable composites [1] and sensitive high-pressure sensors [2]. Recent studies show that the mechanical properties of these frameworks can be tuned by changing the chemical composition [3], and the topology [4-6]. Yet the enormous structural diversity found in MOFs offers an attractive opportunity to explore not just the roles of chemistry and topology, but also the way in which the geometry of the framework effects mechanical response.

Here we present a way in which we can use geometry analysis to understand and tune the observed mechanics in some MOF families. As an example, we characterise the expansions of two quartz-like MOFs: zinc isonicotinate, and hydrogen indium terephthalate, using variable-temperature powder diffraction. The geometric differences in these MOFs are actually sufficient to invert the thermal responses observed. Moreover, this behaviour can be rationalised in terms of a simple geometric formalism, which can be applied to many other MOF families. This structure-property relationship allows us to identify candidate MOFs that are likely to show attractive anomalous mechanics, such as negative area responses.

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