MS17 Total scattering studies and disorder

MS17-05
Correlated linker disorder in a metal-organic framework
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Abstract
Having long focused on the elegant control possible over crystalline metal-organic framework (MOF) structures[1], the field is now increasingly exploiting the presence and nature of disorder in MOFs as an important design tool with which to tune their physical and chemical properties[2]. The objective of this work is to purposely introduce correlated disorder in a MOF structure and characterize the disorder by means of diffuse scattering and Monte Carlo modelling. Ultimately, we want to understand how to control disorder in MOFs, as well as how to systematically characterize disorder and how it can affect MOF properties.
Combining the low symmetry linker 1,3-BDC (BDC = benzene dicarboxylic acid) with a Zn salt resulted in TRUMOF-1. The structure is disordered both orientationally and occupationally (Fig. 1). Monte Carlo simulations confirmed the disorder to be correlated, extracting the local from the average structure. Further DFT studies indicate a correlation between the pore volume and energy, hinting towards the coupling of topological disorder and porosity percolation.
In conclusion, in this work we show how to approach the design of a correlated disordered MOF and successfully analyse its local structure by means of diffuse scattering and Monte Carlo simulations. Ultimately, DFT studies enabled us to show how the disorder directly translates to the pore network and thus porosity.

References
[1] O. M. Yaghi, et al., Nature, 2003, 423, 705–714.
[2] E. G. Meekel and A. L. Goodwin, CrystEngComm., 2021.

Fig. 1: TRUMOF-1 characterisation summary.