Single crystal diffuse scattering — from mesmerizing patterns to new avenues in reticular chemistry and beyond

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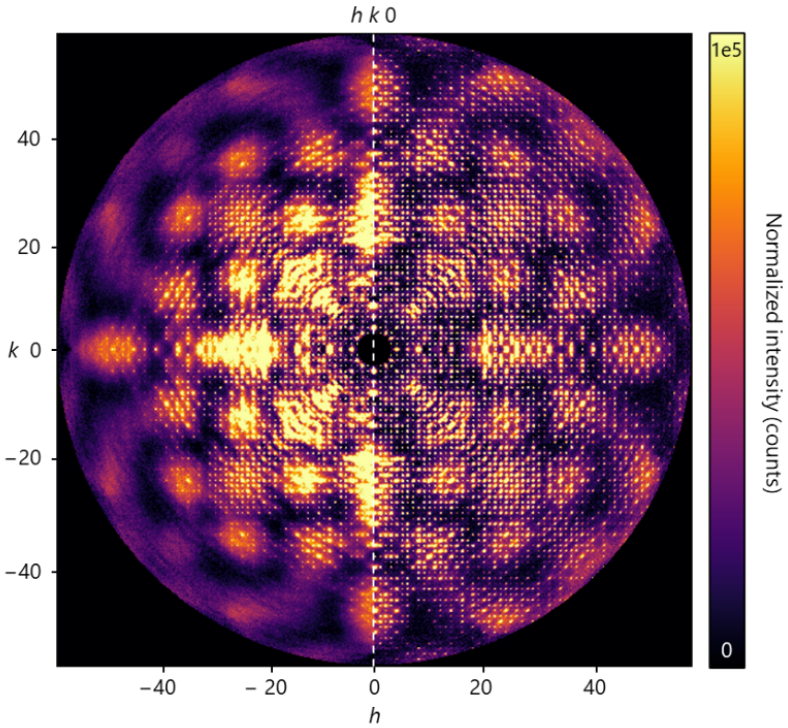
Single crystal diffraction analysis is largely considered the gold standard for atomic structure determination. This is surely due to an ever-advancing automation of methods, software and instruments, but a more fundamental reason is that single crystals provide 3D-resolved data, where structural information along different crystallographic directions is not averaged out by a broad distribution of crystallite orientations. If, on the one hand, crystal structures can be reliably determined by using appropriately indexed powder XRD profiles, real structure features such as defects, disorder and their local arrangement produce broader diffuse scattering signals, whose 3D features can only be analyzed using single crystal data. While the presence of such intensities in single crystal diffraction data has been known since the early days of crystallography, it is only recently that methods for extracting real structure information from them became available. In this contribution I will show how single crystal (3D) diffuse scattering analysis can be currently used to decipher real disordered structures even in relatively complex materials such as metal–organic frameworks (MOFs) [1,2]. In this context, I will introduce this technique and present recent results that project it to become key enabler in the development of disorder-structure engineering practices in the chemistry of MOFs, and potentially any other class of crystalline solids assembled from molecular building blocks.



Total scattering pattern of MOF single crystals synthesized with distinct structural disorder (left vs. right; adapted from ref. 2).

[1] S. Griffin, N Champness et al., *Nature Communications*, **2025**.
[2] C. Koschnick, S. Canossa, B. V. Lotsch, et al., *JACS*, **2024**, *145*(18), 10021–10060.