Truths between Bragg peaks and the real structure of functionalised MOFs: the case of MIL-53

Structural disorder in metal–organic frameworks (MOFs) is not only a relatively common characteristic, but also a phenomenon capable of hindering or enhancing their functional properties.[1] Perhaps the most common origin of disorder is the use of functionalised linkers, a very established practice to endow these materials with additional functionalities for sensing[2], catalysis[3] or selective gas¬-sorption applications [4]. Importantly, these disordered components often interact with each other and with the framework itself resulting in short-range order domains with substantial impact on the material properties. In the present work we investigated linker disorder in a widely studied MOF, namely MIL-53(Al) [5], by means of total-scattering single-crystal X-ray and electron diffraction. This approach is based on the combined use of Bragg reflections and diffuse intensities from diffraction experiments to provide details regarding the structure and distribution of short-range order domains, thus affording a more reliable description of the MOF real structure. Our results revealed significant gaps in the understanding of nitro- and bromo-functionalised MIL-53, providing the first crystallographic proof of the presence of paracrystalline lattice disorder and variable porosity.

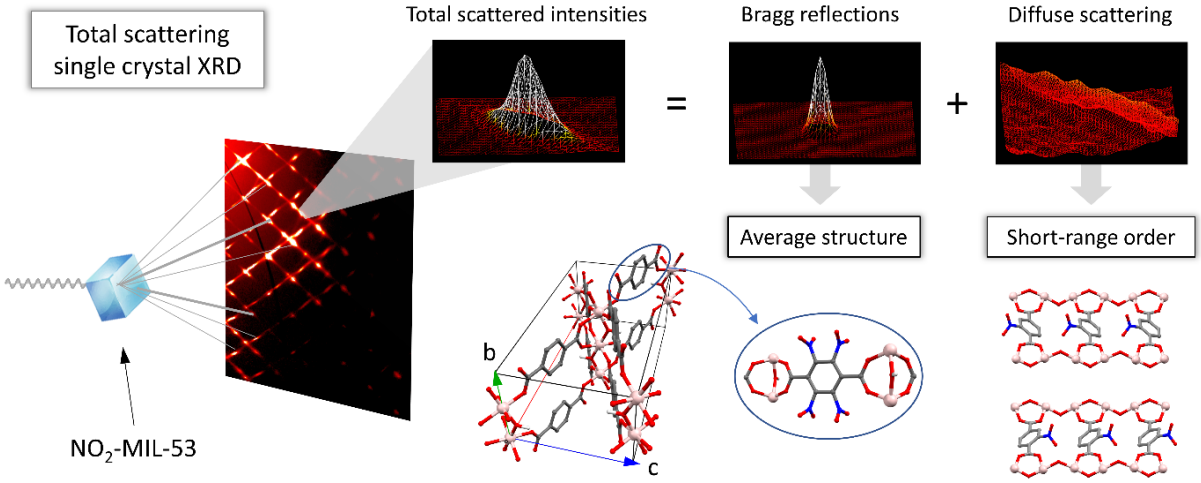

Figure 1. *Schematic representation of the total scattering approach for the study of disorder in single crystals of NO_2-MIL-53(Al).*

References

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