The Devil is in the Details: Pitfalls and Ambiguities in the Analysis of X-ray powder Diffraction Data of 2D Covalent Organic Frameworks.

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X-ray Powder Diffraction (XRPD) data of Covalent Organic Frameworks (COFs) seem to be simple and apparently do not contain a lot of structural information, as these patterns usually do not show more than 3-5 Bragg peaks. As COFs are inherently complex materials showing a variety of disorder phenomena like stacking faults, layers curving, or disordered solvent molecules populating the pores, the interpretation of the XRPD patterns is far from being trivial. We would like to emphasize the critical need for precision and caution in XRPD data acquisition, refinement and interpretation to avoid common pitfalls and overinterpretations in data analysis. It serves as a comprehensive guide, educating the community on the nuances of refinement processes necessary for advancing COF research with clarity and accuracy.

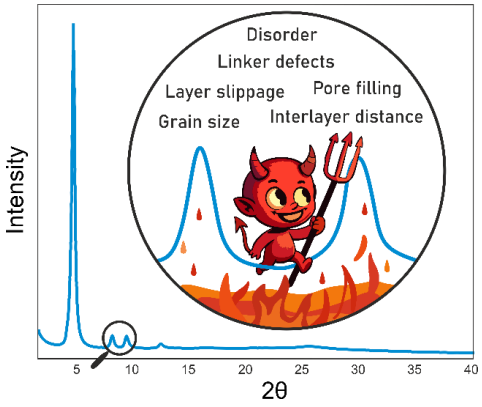

Figure 1: Graphical abstract.