Can 3D Electron Diffraction Provide Accurate Atomic Structures of Metal-Organic Frameworks?

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Many framework materials such as metal-organic frameworks (MOF) or porous coordination polymers (PCPs) are synthesized as polycrystalline powders, which are too small for structure determination by single crystal X-ray diffraction (SCXRD). Here, we show that a three-dimensional (3D) electron diffraction method, namely continuous rotation electron diffraction (cRED), can be used for ab initio structure determination of such materials. As an example, we present a complete structural analysis of a biocomposite, denoted BSA@ZIF-CO3-1, where Bovin Serum Albumin (BSA) was encapsulated in a zeolitic imidazolate framework (ZIF). Low electron dose was combined with ultrafast cRED data collection to minimize electron beam damage of the sample. We demonstrate that the atomic structure obtained by cRED is as reliable and accurate as that obtained by single crystal X-ray diffraction. The high accuracy and fast data collection open new opportunities for investigation of cooperative phenomena in framework structures at atomic level.