MS24 3D electron diffraction

MS24-03
Single-Crystal Analysis of Nanocrystalline Materials: Revealing Details at Atomic Levels
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Abstract
Porous crystalline materials, such as zeolites, metal-organic frameworks (MOFs), and covalent organic frameworks (COFs), have been widely used as absorbents, ion-exchangers, selective catalysts, etc. The unique properties of such materials are associated with their well-defined pores and channels of molecular dimensions. As three-dimensional (3D) arrangement of atoms, their chemical nature and connectivities determine the physical and chemical properties of a material. Knowing the precise structural information at an atomic level will not only help us fundamentally understand a material, but also predict its properties and guide the further development of new materials and technologies.
X-ray diffraction is the predominant technique used for structural determination of crystalline materials. However, challenges are remaining on the structural analysis of nanocrystalline materials which are too small to be studied by single crystal X-ray diffraction. Three-dimensional electron diffraction (3DED) has been developed to tackle the challenges. By taking advantage of the strong interaction between electrons and matter, 3DED allows single crystal structural analysis even when the crystal sizes are down to the range of nanometres[1]. This turns a polycrystalline powder into millions of analytes of single crystals. Moreover, with a short data collection time of 2-5 minutes per crystal, it is possible to analyze individual crystals in a high throughput manner and determine the structure of each tiny crystal.
Here, I give an example of using 3DED technique in high-throughput discovery of a new MOF material among a phase mixture[2]. The new MOF, ZIF-EC1, was discovered with a trace amount in a ZIF-CO3-1 material. Interestingly, the structure of ZIF-EC1 is rather dense, which is built by mono- and binuclear Zn clusters. This offers a high density of N and Zn, which are active sites for electrocatalysis. Furthermore, I will present our recent development by using 3DED to probe molecular motions in MOF nanocrystals, where different degrees of motions can be identified[3]. Last but not least, I will present using 3DED to directly locate guest molecules in open framework materials, where different configurations of the guest molecule can be identified ab initio and atom-by-atom. We believe that 3DED can be used as a powerful analytical tool for discovering new materials and revealing unique atomic properties, which could easily be extended to other crystalline materials.

References
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