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High-Throughput Electron Diffraction Techniques Accelerate the Discovery of New Materials

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Understanding the three-dimensional arrangement of atoms is fundamental to elucidating the properties and functions of molecules and materials. While X-ray crystallography remains the cornerstone of structural analysis, it faces significant limitations when applied to nano- and micro-crystals, as well as complex polycrystalline samples. Despite advances in high-throughput synthesis and data-driven materials design, the structural characterization of polycrystalline powders continues to be a major bottleneck.

Electron crystallography offers unique advantages for studying crystals that are too small, or too complex for X-ray diffraction.[1] I will present several high-throughput electron diffraction (ED) methods developed in my group; continuous rotation electron diffraction (cRED) [2], serial electron diffraction (SerialED) [3], and serial rotation electron diffraction (SerialRED) [4-5]. These techniques have enabled the structural analysis of a broad range of energy materials—from zeolites and metal-organic frameworks (MOFs) [6], to hybrid perovskites—at atomic resolution.

I will demonstrate how high-throughput automated data collection and analysis allow not only the study of extremely beam-sensitive crystals but also phase identification and the detection of minor phases that remain undetectable by conventional X-ray diffraction [7-8]. Moreover, electron diffraction enables the visualization of fine structural features such as hydrogen positions, host–guest interactions, and structural transformations.

We envision that the development of automated pipelines will transform electron diffraction into a fast, reliable, and accessible characterization technique that can be adopted even by researchers without specialized training in TEM or crystallography. The integration of these emerging methods has already begun to reshape the field of crystallography and offers unprecedented opportunities for discovering novel materials, resolving complex structures, and probing structure–property relationships.

References:

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