Revealing Structural Details with 3D Electron Diffraction/Microcrystal Electron Diffraction

Jungyoun Cho[1], Xiaodong Zou[2]

[1]Stockholm University [2]Stockholm University

jungyoun.cho@mmk.su.se

3D electron diffraction (3D ED), or Microcrystal diffraction (MicroED) can facilitate access to single crystal data from sub micrometer-sized crystals of small organic molecules, pharmaceutical, porous materials, and macromolecules. Recent developments of 3D ED/MicroED techniques have opened new opportunities to answer important fundamental questions across scientific disciplines. Despite the fear of dynamical scattering of electrons that faltered the growth of the discipline for numerous decades, accurate atomic positions can now be acquired within minutes of the 3D ED data collection. The strong interaction between electrons and the samples has brought both challenges and opportunities. Ingenious sample preparation and data collection strategies are being devised to encompass intrinsic sample properties. Serial electron diffraction (SerialED/SerialRED) approach helps to determine and quantify polymorphs of pharmaceutical samples and different porous materials. Guest molecules in porous materials can now be revealed at the atomic resolution. We will demonstrate the use of 3D ED to reveal the smallest structural detail in different crystalline materials. Optimization of the 3D ED method to each specimen is the key to the success.