

modulated structures, thin films and zeo-type materials. No doubt that combining PEDT data and “dynamical refinements” will allow to solve and refine an increasing number of structures on materials inaccessible by other diffraction techniques.

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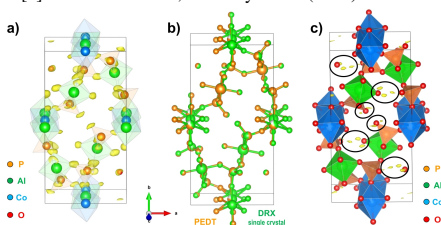


Figure 1. Co-AlPO zeo-type material: a) density map from PEDT data, b) structure from single crystal XRD (green) and PEDT “dynamical” (orange), c) residues in the Fourier difference map after dynamical refinement of PEDT data. Residues inside black circles would correspond to hydrogens.

Keywords: dynamical refinement, incommensurate modulated structures, thin films, zeo-type materials

MS28-O2 MicroED: Three Dimensional Electron Diffraction of Microscopic Crystals

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My laboratory studies the structures of membrane proteins that are important in maintaining homeostasis in the brain. Understanding structure (and hence function) requires scientists to build an atomic resolution map of every atom in the protein of interest, that is, an atomic structural model of the protein of interest captured in various functional states. In 2013 we unveiled the method MicroED, electron diffraction of microscopic crystals, and demonstrated that it is feasible to determine high-resolution protein structures by electron crystallography of three-dimensional crystals in an electron cryo-microscope (CryoEM). The CryoEM is used in diffraction mode for structural analysis of proteins of interest using vanishingly small crystals. The crystals are often a billion times smaller in volume than what is normally used for other structural biology methods like x-ray crystallography. In this seminar I will describe the basics of this method, from concept to data collection, analysis and structure determination, and illustrate how samples that were previously unattainable can now be studied by MicroED. I will conclude by highlighting how this new method is helping us understand major brain diseases like Parkinson’s disease.

Keywords: MicroED; CryoEM; Electron Diffraction; Crystallography; nanocrystals