MS28-P01 | SOLVING THE DISORDERED STRUCTURE OF BETA-Cu_2Se USING THE THREE-DIMENSIONAL DIFFERENCE PAIR DISTRIBUTION FUNCTION

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High-performing thermoelectric materials such as Zn_4Sb_3 and clathrates have atomic disorder as the root to their favorable properties. $Cu_{2-x}Se$ is an intensely studied, cheap and non-toxic high performance thermoelectric material with highly peculiar transport properties, which must be related to the crystal structure. Attempts to solve the crystal structure of the room temperature phase, β-$Cu_{2-x}Se$, have been unsuccessful since 1936. So far, all studies have assumed that β-$Cu_{2-x}Se$ has a three-dimensional periodic structure, but here we show that the structure is ordered only in two dimensions while it is disordered in the third dimension with a near random stacking sequence. Using the three-dimensional difference pair distribution function (3D-ΔPDF) method for diffuse single crystal X-ray scattering, we solve the structure of the two-dimensional ordered layer and show that there are two modes of stacking disorder present, which give rise to an average structure with higher symmetry. The present approach allows for a direct solution of structures with disorder in some dimensions and order in others, and can be tought of as a generalization of the crystallographic Patterson method. The 3D-ΔPDF gives an intuitive method for structural solution of disordered systems without the need for reverse Monte-Carlo simulations or energy minimization calculations. The local and extended structure of a solid determines its properties and $Cu_{2-x}Se$ represents an example of a high-performing thermoelectric material where the local atomic structure differs significantly from the average periodic structure observed from Bragg crystallography.