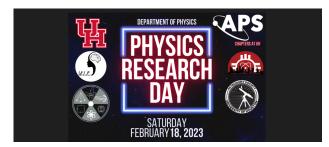Contribution ID: **22**   Type: **Poster**

Investigating the Local Structure of MoTe2 Using Atomic Pair Distribution Function and EXAFS Techniques.

Saturday 18 February 2023 13:10 (5 minutes)

At temperatures below 250K, 1T'MoTe$_2$ undergoes a first-order structural phase transition (SPT) to a non-centrosymmetric orthorhombic T$_d$ phase, marked by the appearance of Weyl points protected by broken inversion symmetry. Despite the similar structures of these two phases and a small energy barrier between them, distortions are evident at both macroscopic and atomic scales. This study investigates the local structure of 1T'MoTe$_2$ at temperatures ranging from 95K to room temperature using more advanced scattering techniques. Results show that lowering the temperature leads to significant changes in interlayer atomic distances, but not in intralayer distances. Using large box modeling approach reveals the effects of stacking faults and layer rotations on interlayer distances, consistent with experimental observations. Understanding the interlayer behavior in MoTe$_2$ through local structure study could help clarify the mechanisms of the SPT and the emergence of Weyl points at low temperatures.

Academic year

5th year and/or beyond

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