PAPER

Pressure-induced isostructural electronic topological transitions in 2H-$MoTe_2$: x-ray diffraction and first-principles study

Abstract

Synchrotron x-ray diffraction measurements on powder 2H-$MoTe_2$ ($P6_3/mmc$) up to ~46 GPa have been performed along with first-principles based density functional theoretical analysis to probe the isostructural transition in low pressure regime and two electronic topological transitions (ETT) of Lifshitz-type in high pressure regime. The low pressure isostructural transition at ~7 GPa is associated with the lattice parameter ratio c/a anomaly and the change in the compressibility of individual layers. The pressure dependence of the volume by linearizing the Birch–Murnaghan equation of state as a function of Eulerian strain shows a clear change of the bulk modulus at the ETT pressure of ~20 GPa. The minimum of c/a ratio around 32 GPa is associated with the change in topology of electron pockets marked as second ETT of Lifshitz-type. We do not observe any structural transition up to the maximum applied pressure of ~46 GPa under quasi-hydrostatic condition.