Electronic structure studies on competing phases of Aurivillius Bi4Ti3O12 using first-principles calculations FU-CHANG SUN, University of Connecticut, Department of Physics, SANJEEV NAYAK, University of Connecticut, Department of Materials Science Engineering, DEEPAM MAURYA, SHASHANK PRIYA, Virginia Tech, Bio-inspired Materials and Devices Laboratory (BMDL), Center for Energy Harvesting Materials and Systems (CEHMS), S. PAMIR ALPAY, University of Connecticut, Department of Materials Science Engineering — The low temperature ferroelectric to high temperature paraelectric phase transition in bismuth titanate (Bi4Ti3O12) has been experimentally observed at Curie temperature (T_C) around 675 °C. The first-principles calculations using density functional theory as implemented in the Vienna ab initio simulation package (VASP) with generalized gradient approximation (GGA) for the exchange-correlation interaction are performed to investigate this monoclinic (b1a1) to tetragonal (I4/mmm) crystal structural transition. We further, provide discussion of the band structure and the Ti-O orbital hybridization, in addition to the frequency dependent dielectric and optical properties of Bi4Ti3O12 due to the potential applications in the electronic devices.

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