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Electronic structure studies on competing phases of Aurivillius $Bi_4Ti_3O_{12}$ 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 ($Bi_4Ti_3O_{12}$) 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 $Bi_4Ti_3O_{12}$ due to the potential applications in the electronic devices.

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