Ab-initio study of structural and electronic properties of thin film and bulk forms of Bi$_2$Q$_3$ (Q= Se, Te) as topological insulators

AHMAD RANJBARDIZAJ, HIROSHI MIZUSEKI, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku University, Sendai 980-8577 — Bi$_2$Q$_3$ (Q=Se, Te) are the best-known bulk thermoelectric materials, which have been demonstrated to be topological insulators (TI). TI’s are insulators with conductive surface states consisting of a single Dirac cones. These materials have layered structures consisting of stacked quintuple layers (QL), with relatively weak coupling between the QL’s. Therefore, it might be easy to prepare the Bi$_2$Q$_3$ in the form of thin films with particular thicknesses using the available experimental techniques. In this study, the electronic and structural properties of bulk Bi$_2$Se$_3$ are investigated using density functional theory. Our results show that the Bi$_2$Se$_3$ is an indirect semiconductor with energy gap of $\approx$ 0.27 eV. Additionally, the electronic structure dependence of Bi$_2$Se$_3$ to the thicknesses of thin films (n-QL’s with n=1,2...9) is considered. It is observed that the electronic structure of this kind of thin films depends on the number of QL’s. For n-QL’s with n larger than three, the thin film has a bulk band gap and has protected conducting states on its surface. Moreover, the effect of number of layers (n) on band-gap energy is studied. Similar calculations and discussions are carried out for Bi$_2$Te$_3$ and the results are compared to the Bi$_2$Se$_3$ case and also the available theoretical and experimental results.