Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Ab-initio study of structural and electronic properties of thin film and bulk forms of Bi_2Q_3 (Q= Se, Te) as topological insulators AHMAD RANJBARDIZAJ, HIROSHI MIZUSEKI, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku University, Sendai 980-8577 — Bi_2Q_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_2Q_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_2Se_3 are investigated using density functional theory. Our results show that the Bi_2Se_3 is an indirect semiconductor with energy gap of ≈ 0.27 eV. Additionally, the electronic structure dependence of Bi_2Se_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_2Te_3 and the results are compared to the Bi_2Se_3 case and also the available theoretical and experimental results.

Ahmad Ranjbardizaj
Institute for Materials Research, Tohoku University, Sendai 980-8577

Date submitted: 19 Dec 2012 Electronic form version 1.4