Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Spin texture of topological surface states of side-surfaces in Bi_2Se_3 from first principles[1] JOHN VILLANOVA, KYUNGWHA PARK, Virginia Tech - Blacksburg — Topological insulators have recently drawn a lot of attention because of topologically protected surface states with Dirac dispersion and spin-momentum locking induced by time-reversal symmetry and strong spin-orbit coupling, respectively. Recent experiments report interesting transport properties of Bi_2Se_3 nanowires and nanoribbons with growth directions normal to the (111) surface. However, most of the studies of Bi_2Se_3 are focused on the (111) surface. Additionally, surfaces other than the (111) surface would facilitate hole doping with adatoms since both Bi and Se atoms are present at these other surfaces. We investigate the spin texture and electronic structure of topologically protected surface states of two representative side-surfaces of Bi_2Se_3 by using density-functional theory (DFT). In particular, we consider two surfaces normal to the (111) surface, such as $(1\bar{1}0)$ and $(11\bar{2})$, where the former has twofold symmetry and the latter has mirror symmetry. We present our calculated spin textures of the surface states of these side surfaces that qualitatively differ from typical Rashba-like features and from the prediction based on the bulk model Hamiltonian by keeping up to quadratic terms in momentum.

[1]Funding from NSF DMR-1206354 and Computer resources from SDSC Trestles under DMR060009N and VT ARC. Grateful to B. Partoens and C. De Beule for discussion at the early stage of this work.

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Date submitted: 05 Nov 2015 Electronic form version 1.4