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Orgin of band inversion in topological Bi2Se3

\documentclass[aps,superscriptaddress,floatfix,amsmath,amssymb, amsfonts]{revtex4-1}

\begin{document}

\title{Origin of Band inversion in Topological Bi_2Se_3}

\date{\today}

\begin{abstract}
Topological materials and more so insulators have become ideal candidates for spintronics and other novel applications. These materials portray band inversion which is considered to be a key signature of topology. It is not yet clear what drives band inversion in these materials and the basic inferences when band inversion is observed. We employed a state-of-the-art \textit{ab initio} method to demonstrate band inversion in topological bulk Bi_2Se_3 and subsequently provided a reason explaining why the inversion occurred. From our work, a topological surface state for Bi_2Se_3 was described by a single gap-less Dirac cone at the $\vec{k}$= 0 which was essentially at the Γ point in the surface Brilloiun zone. We realized that band inversion in Bi_2Se_3 was not entirely dependent on spin-orbit coupling as proposed in many studies but also occurred as a result of both scalar relativistic effects and lattice distortions. Spin-orbit coupling was seen to drive gap opening but it was not important in obtaining a band inversion. Our calculations reveal that Bi_2Se_3 has an energy gap of about 0.28 eV, which in principle agrees well with the experimental gap of $\approx$ 0.20-0.30 eV.
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This work contributes to the understanding of the not so common field of spintronics, eventually aiding in the engineering of materials in different phases in a non-volatile manner.
\end{abstract}

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