22AG002, 22BU007 BL-7

Investigating the possibility of creating a "pure" p-type Bi_2Se_3

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Keywords: Topological insulator, Bi_2Se_3, ARPES, QSGW calculation

Three-dimensional topological insulators (TIs), which hold spin-polarized Dirac cone type metallic bands on the surface while the bulk is insulating, are promising materials to realize next-generation spintronics devices. For example, controlling the Fermi level by, *e.g.,* charge doping, and making both n-type and p-type from a single TI sample will allow to create p-n topological junction [1-4], a device that has a great possibility to solve the problem of processing the explosive volume of information, which cannot be solved by the existing electronics technology based solely on the charge degrees of freedom. Bi_2Se_3 is a typical n-type TI whose bulk valence band maxima (BVBM) was predicted to located close to the Dirac point (DP) both theoretically and experimentally [5-8]. This means that even by doping the sample and tuning the Fermi level below the DP, it is impossible to create a "pure" p-type Bi_2Se_3, because the bulk band crosses the Fermi level simultaneously. This situation makes the spin-polarized surface electrons diffusing into the bulk, and therefore difficult to generate a highly efficient spin current in practical applications.

In this study, we performed state-of-the-art ARPES measurements and DFT calculations to obtain precise information on the bulk band behavior to have a proper understanding on the electronic structure of Bi_2Se_3, and to discuss the feasibility of this TI for spintronics devices. ARPES measurements were performed at the beamline BL-7 of HiSOR. The bulk band along the $\bar{\Gamma}-\bar{\mathrm{M}}$ direction, the direction where the BVBM was predicted to be above the DP, was measured using photon energies ($h\nu$) from 33 eV to 89 eV. This $h\nu$ range covers more than a single Brillouin zone along the $k_\perp$ direction. Fig. 1(a) shows the band structure obtained at $k_\perp = 4.10\ \text{Å}^{-1}$ and Figs. 1(b)-(d) are the $k_\perp$-dependent EDCs measured at different $k_\parallel$. The band structure in Fig. 1(a) shows that the BVBM is located at the $\bar{\Gamma}$ point and below the DP, and a saddle-like-valence band (SVB) to be present along the $\bar{\Gamma}-\bar{\mathrm{M}}$ direction. Furthermore, the EDCs in Figs. 1(b)-(d) show that the BVMBs are located below the DP throughout the entire 3D Brillouin zone, and the SVB to show a $k_\perp$ dependence. In order to confirm these experimental results, we have performed DFT calculations using the Quasiparticle Self Consistent GW (QSGW) [9-11], a method that has the property of showing the band gap more accurately than the DFT calculations used in former studies. Two types of projected bulk band are shown in Fig. 2 (a) and(b). The theoretically obtained results using QSGW indicates the BVBM to be located at the Γ point, and therefore strongly support our experimental results. The present results also suggest that it is possible to make a "pure" p-type Bi_2Se_3 by hole-doping, and therefore the possibility of using this TI as a material to realize novel spintronics devices.

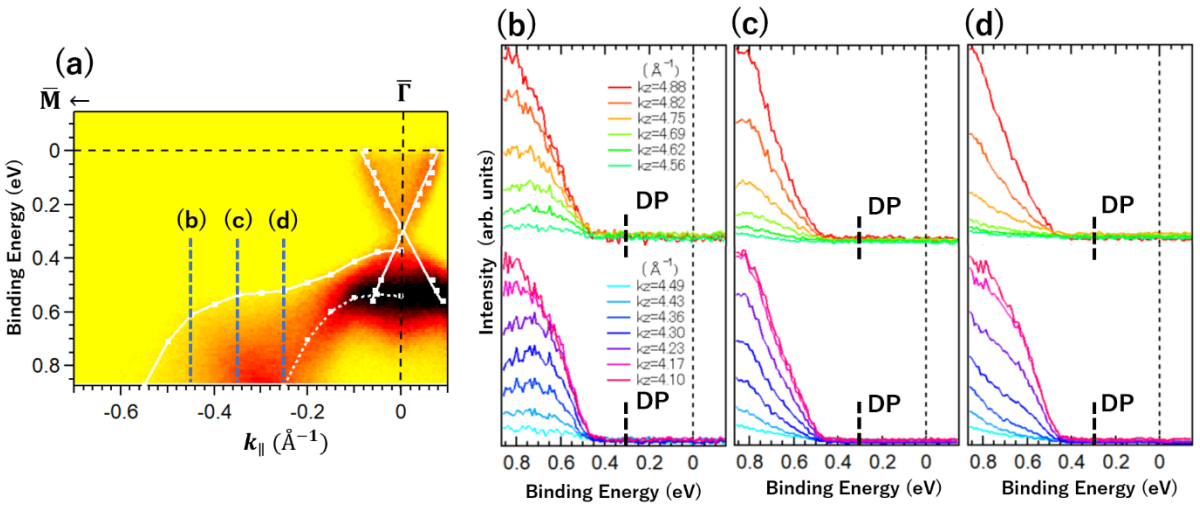

Figure 1. (a) Band structure of Bi_2Se_3 along $\bar{\Gamma} - \bar{M}$ at $k_\perp = 4.10$ Å^{-1}, and (b)-(d) $k_\perp$-dependent EDCs at different $k_\parallel$. $k_\perp = -0.45$ Å^{-1} in (b), -0.35 Å^{-1} in (c), and -0.25 Å^{-1} in (d). The range of $k_\perp$ is larger than that of single Brillouin zone.

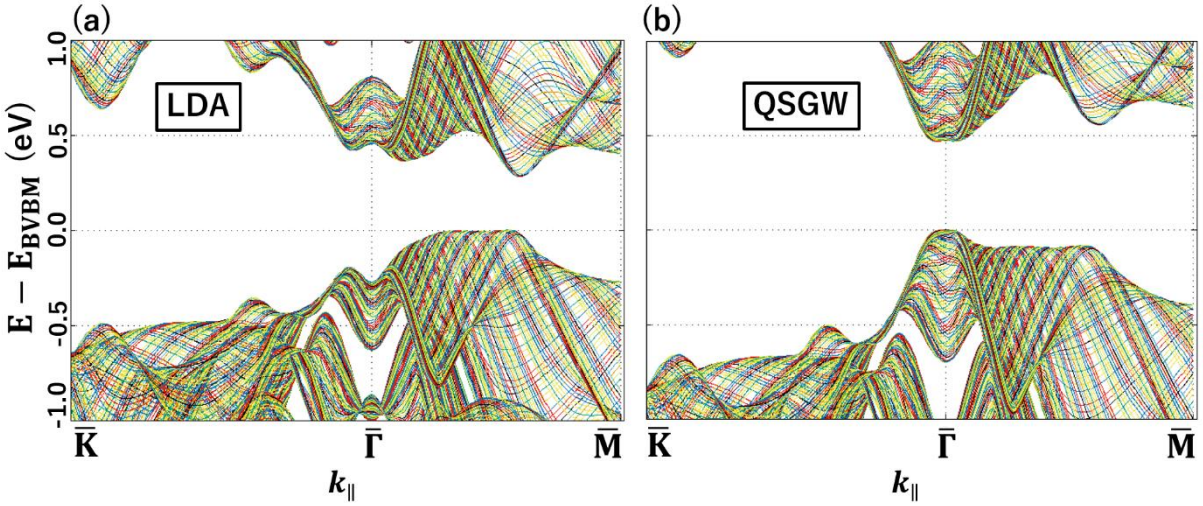

Figure 2. Theoretical projected bulk band structure along the $\bar{K} - \bar{\Gamma} - \bar{M}$ direction of the 2D Brillouin zone obtained using (a) LDA and (b) QSGW.

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