Cr doped topological insulator $\text{Bi}_2\text{Se}_3$ under external electric field: A first-principle study

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Abstract. In this paper, we investigated the magnetic topological insulator (MTI) Cr-doped $\text{Bi}_2\text{Se}_3$ film using first principles calculations based on the density functional theory (DFT). The band structure of Cr doped 3QL-$\text{Bi}_2\text{Se}_3$ film was calculated comparing with pure $\text{Bi}_2\text{Se}_3$ film. Our results demonstrate that the doping of Cr atom changes the degenerate surface state of pure $\text{Bi}_2\text{Se}_3$, inducing the ferromagnetism. Under the external electric field, the band gap of pure $\text{Bi}_2\text{Se}_3$ films is determined by the charge transfer and the effect of spin-orbital coupling (SOC). For the MTI, the electric field will redistribute the electrons and enhance the magnetism. Our results will further promote the development of the electronic and spintronic applications of topological insulator.

1. Introduction

Topological insulators (TIs) have become a research hotspot due to its gapless state in the surface and energy gap in the bulk [1-6]. Specifically, the prediction and implementation of three dimensions TIs make it is of great interesting [7-8]. The intricate interplay between the topological order and the ferromagnetic order is promising to induce a series of unconventional spintronic effects which will drive the new device paradigms growth [9-12]. As the magnetism introduced, TI is expected to realize the long-sought quantized anomalous Hall effect (QAHE) [13,14]. It has been revealed that Cr atom can be doped into $\text{Bi}_2\text{Se}_3$ with both the ferromagnetic and insulating properties [15]. In Cr doped $\text{Bi}_2\text{Se}_3$, the Curie temperature has an estimated value of 76K under the doping level of 7.4% [16].

Therefore, the approach to control the band gap of TIs, such as inducing the external electric field, is significant for the application of TIs. Recent study revealed that the pure $\text{Bi}_2\text{Se}_3$ film becomes gapless under the external electric field due to the redistribution of the electron [17]. However, the mechanism for MTIs under the electric field, such as Cr doped $\text{Bi}_2\text{Se}_3$ films, is still not clear.

In this paper, we study the property of 3QL-$\text{Bi}_2\text{Se}_3$ film with one Cr atom doped under the external electric field comparing with the pure case. The total magnetic moment of the system and the band structure are studied using first-principles calculations based on the density functional theory. The result demonstrates that the doped case can be spontaneous stable. In particular, the electric field will slightly enhance the magnetic moment, which has been revealed to break the time reversal
symmetry (TRS), and hence open a band gap. Furthermore, the electron transfer induced by the electric field can also increase the band gap.

2. Method and Model
We perform the first-principle density functional theory calculation using Vienna ab initio simulation package (VASP) [18,19]. We use the projected augmented wave (PAW) potentials [20] describing the interaction of ion-electron with the Perdew-Burke-Ernzerhof generalized gradient approximation (GGA-PBE) [21,22]. GGA+U calculations that U=3 eV and J=0.87 eV are performed to describe the strong electron-electron correlation. Spin-orbital coupling (SOC) is considered. Figure 1 shows the crystal structure for Cr doped 3QL-Bi$_2$Se$_3$ film in our VASP calculation. A Cr atom is replaced for the Bi atom in the upper surface. The experimental lattice constants $a=4.138$ Å and $c=28.64$ Å is used for Bi$_2$Se$_3$. We set the cutoff energy at 300eV. The Brillouin zone for the 3QL-Bi$_2$Se$_3$ is sampled by a gamma-centered $11\times11\times1$ mesh. We use a vacuum layer of 20Å and define the positive direction of the electric field from the doping surface to the un-doping surface.

![Figure 1. Crystal structure illustration of one Cr atom doped in the 3QL-Bi$_2$Se$_3$ surface.](image)

3. Results and Discussions

3.1. Electronic property without the external electric field
We calculated band structure for pure Bi$_2$Se$_3$ and Cr doped Bi$_2$Se$_3$, respectively, as show in Fig. 2. We find that the pure Bi$_2$Se$_3$ has a band gap with the value of 0.111 eV. The gap is induced by the coupling between two surfaces. But for the Cr doped Bi$_2$Se$_3$ film, the gap only 0.099 eV can be obtained because of the nondegenerate band after doping. The result indicates that the magnetic atoms of Cr can be effectively doped in the Bi$_2$Se$_3$ film with the ferromagnetic order and the insulativity, rendering it is promising for realizing quantized anomalous Hall effect.
3.2. Electronic property of the pure Bi$_2$Se$_3$ film under the electric field

Under the electric field, there are two major reasons can change the energy band gap: the magnetic moment of system and the redistribution of electrons. In the former case, it has been revealed that the gap in surface states of a TI can be opened up by the magnetic perturbation [23]. On the other hand, it is also been demonstrated that external electric field can control the magnetism, but also redistribute the electrons to move in the opposite direction of it that induces an internal electric field and make the charge redistribute again.

Figure 3 shows the density of states of 3QLs-Bi$_2$Se$_3$ film under the electrical field of 0 and 0.02 V/Å. We find the partial densities of states of the upper (red) and the lower (green) QLs are almost overlapping, because of its symmetrical structure. With the increase of electric field, the degenerate
state is removed. And the gap of pure Bi$_2$Se$_3$ film decrease gradually, as shown in Fig. 4. It suggests that electric field causes the electron transfer and hence to change the gap.

![Figure 4](image)

**Figure 4.** The band structure of 3QLs-Bi$_2$Se$_3$ film under the electrical field of 0 and 0.02 V/Å

3.3. Electronic property of the Cr doped Bi$_2$Se$_3$ film under the electric field

Comparing with the pure Bi$_2$Se$_3$ film, we study the Cr doped Bi$_2$Se$_3$ film under the electrical field. For the Cr doped Bi$_2$Se$_3$ film, the band gap gradually enlarges as the external electric field increases. While, when $E_{\text{ext}} = 0.02$ V/Å, the band gap is slightly increase by 0.002 eV. From Fig. 6, we can see the gap rises to 0.144 eV for $E_{\text{ext}} = 0.1$ V/Å, from the value of 0.099 eV under the zero fields. This result is different with the pure case. The inevitable reason is that the two surface states are nondegenerate, and the contribution at the top of valence band belongs to the upper surface, which is containing Cr atom, as shown in Fig. 5.

To discuss the magnetic properties of the Cr doped Bi$_2$Se$_3$ film, we calculate the ferromagnetic moment under increasing electric fields. With the field increasing from 0 to 0.1 V/Å, the magnetic moment rise from 2.979 $\mu_B$ to 2.985 $\mu_B$. It suggests the increasing of electric field enhances the magnetic moment, enlarging the band gap. This result indicates that the external electric field plays an important role on the magnetic and electric properties of magnetic topological insulators (MTIs).
Figure 5. Total densities of states (black) for Cr doped Bi$_2$Se$_3$ 3QL film and the partial densities of states calculated for QL1 (red), QL2 (blue) and QL3 (green) under the electric field of 0 and 0.1 V/Å.

Figure 6. The band structure of Cr doped Bi$_2$Se$_3$ 3QL film under the electrical field of 0 and 0.1 V/Å

4. Conclusion
In summary, we have studied for the magnetic atom Cr doped Bi$_2$Se$_3$ films under external electric field using first-principles calculations based on DFT. We found that the pure Bi$_2$Se$_3$ film is more sensitive to the electric field than the Cr doped Bi$_2$Se$_3$ film. Our calculated band structure indicates that substitution of Cr makes system become nondegenerate, resulting in a smaller gap. With the increase of electric fields, the charge transfer and magnetism of system will enhance, resulting the band gap of Cr doped Bi$_2$Se$_3$ enlarged. Our result indicates that Cr doped Bi$_2$Se$_3$ film is electrically tunable, providing significant guidelines towards the study of MTIs.

Reference
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