Engineering a topological phase transition in $\beta$-InSe via strain

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Abstract. We report that $\beta$-InSe endowed with external strain realizes a novel three dimensional topological insulator (TI) by ab initio calculations. We predicate that the promising topological non-trivial state can be observed in an accessible temperature regime in $\beta$-InSe for its large spin–orbital band gap up to 121 meV. Specifically, unlike in previous literature where the band inversion (BI) in TIs is induced using heavy elements that have strong spin–orbital coupling (SOC), we provide a remarkable blueprint for stabilizing BI solely by mechanical deformation so that $\beta$-InSe could display BI even without considering SOC. Nevertheless, SOC is still needed to create a band gap at the crossing point by breaking the incompatibility symmetry of the inverted bands.

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1. Introduction

Recently, the subject of time-reversal-invariant topological insulators (TIs) has attracted great interest in condensed matter physics due to their novel quantum state based on the quantum spin Hall effect and hence the potential application in quantum computation and spintronics [1–6]. Typical TIs differ from normal insulators in that they exhibit gapless boundary states inside a bulk energy gap. These materials support an odd number of surface states with linear dispersion, which can be viewed as a sea of massless Dirac cones, with a single Dirac cone being the simplest case. The conducting surface states in TIs are protected by time-reversal symmetry and are immune to scattering by non-magnetic impurities, thus opening new ways for backscattering-free transport. The existence of an odd number of Dirac cones on the surface is ensured by the $Z_2$ topological invariant of the bulk [7–9]. In TIs, the TI properties can be understood from a simple mechanism of band inversion (BI) caused by the spin–orbital coupling (SOC). Such inversion must occur at the time-reversal-invariant momentum (TRIM) points of the Brillouin zone [7, 10, 11]. The guiding principle to identify TIs is that the conduction and valence bands have the opposite parity, and a BI occurs when the strength of some parameter, say SOC, is tuned [12]. The family of known TIs has grown steadily in recent years; the search for new TIs is under way [13–18]. For example, in a recent study, it was proposed that Pb-based ternary chalcogenides PbBi$_2$Se$_{n+3}$ and PbSb$_2$Te$_{n+3}$ could be new candidates for TIs [19]. In another work, Kim et al and Sa et al predicted the structure-related topological insulating behavior in Ge$_2$Sb$_2$Te$_5$ alloys [3, 20]. Another class is thallium-based ternary III–V–VI$_2$ chalcogenides, which were proposed theoretically [21, 22] and then verified experimentally [23–25]. Nearly all new reported TIs are relatively uncommonly materials; however, a few TIs which could be fully integrated in the current electronic technology have been reported thus far.

Indium selenide (InSe) and other III–VI layered semiconductors have received extensive attention due to the unusual nature of the electronic interaction and also because of their applications in solar energy conversion, nonlinear optics, terahertz generation and memory devices [26–31]. At a more fundamental level, the band structure of InSe presents some specific features that are related to the strong anisotropy of its electronic structure [28]. InSe presents an anisotropic crystalline structure with layers formed by two deformed sublayers of hexagonal symmetry held together by strong covalent bonds. The weaker bonding between the layers is of the van der Waals type and leads to the existence of different polytypes. Among them, the $\beta$-type lattice is the most studied structure [26–31]. The space symmetry group of $\beta$-InSe is $D_{6h}$. This structure consists of covalently bonded Se–In–In–Se tetra-layer sheets (figure 1(a)), with the sheets held to each other by van der Waals forces.

In this work, we theoretically demonstrate that $\beta$-InSe could enter into a topologically non-trivial state at a reasonable biaxial lattice expansion. Specifically, different from the current accepted view that the BI in three dimensional TIs is induced by heavy elements that have strong SOC, we demonstrate that the BI in $\beta$-InSe could be created solely by external strain, even without considering the SOC. SOC plays a vital role in creating a gap at the crossing points originating from the BI; for example, at 6% strain, the SOC yields a gap on the order of 121 meV, which approaches room temperature. These properties offer interesting alternatives for engineering devices for spintronics, ultra-low-dissipation electronics and quantum information processing.
2. Calculation methods

In this study, the first-principles calculations are based on the density functional theory (DFT) in conjunction with projector augmented wave potentials, which is implemented in the Vienna *ab initio* simulation package [32, 33]. For the exchange–correlation functional, the generalized gradient approximations (GGA) [34] of Perdew–Burke–Ernzerhof [35] are used. Pseudopotentials with 4s²4p² and 5s²5p¹ valence electron configurations, respectively, for Se and In atoms are used. The experimental lattice parameters of β-InSe: \( a = b = 4.050 \, \text{Å} \), \( c = 16.930 \, \text{Å} \) are used for the calculations [36]. Strain is simulated by varying \( a \) for a constant cell volume. The isotropic strain is defined as \( \epsilon = \Delta a / a \), where the lattice constant of the strained unit cell is equal to \( \Delta a + a \). A unit cell is used for all the calculations; test calculations with a supercell ensure that unit cell calculations are sufficient. The Brillouin zone is represented by a Monkhorst–Pack special \( k \)-point mesh [37] of \( 13 \times 13 \times 3 \), both geometry optimizations and the static total energy calculations. The relaxation convergences for ions and electrons are \( 1 \times 10^{-3} \) and \( 1 \times 10^{-6} \, \text{eV} \), respectively. A cutoff energy of 450 eV is used for the plane wave expansion of the wave function to converge the relevant quantities. The positions of all the atoms in the supercell are fully relaxed. The electron spin–orbit interaction is introduced with

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Figure 2. Band structures of $\beta$-InSe, with the upper row corresponding to unstrained $\beta$-InSe (a) without SOC and (b) with SOC; the lower row corresponds to band-inverted $\beta$-InSe ($\varepsilon = 6\%$) (c) without SOC and (d) with SOC. The horizontal dashed red lines indicate the Fermi level. The inset in (d) is a magnified view near the Fermi level.

time-reversal inversion SOC calculations [38]. Although the post-DFT calculations [39, 40] may provide relative precise electronic structures, previous theoretical studies [3–5, 11, 16] on TIs have confirmed that the GGA method is valuable to investigate the electronic structures of TIs. In addition, almost all of the previous theoretical studies [3–5, 11, 16] on TIs were based on the GGA method. Thus, for a convenient comparison with previous works, all calculations in this work are also performed using the same method.

3. Results and discussion

The band structures without and with SOC for $\beta$-InSe without strain are plotted in figures 2(a) and (b). They show that $\beta$-InSe is a narrowed band gap semiconductor with a direct band gap at the $\Gamma$ point without SOC. The conduction band minimum (CBM) at the $\Gamma$ point is dominated by Se s, Se p$_z$ and In s states; the valence band maximum (VBM) at the $\Gamma$ point mainly consists
The energy gap $E_{\Gamma}$ with and without SOC under different strain conditions. (b) The main projection of the LCB and the HVB at $\Gamma$ point without SOC under different strain conditions. (c) The main projection of the LCB and the HVB at $\Gamma$ point with SOC under different strain conditions. The positive and negative values in (b) and (c) correspond to $s$ and $p_z$ states, respectively.

By introducing SOC, the band structure of $\beta$-InSe displays a very small change; no BI characterizations of the CBM and VBM were observed. Note that there are two ways to change the band order [11, 41]: (i) if the SOC strength is increased, the necessary BI could occur; (ii) besides varying the SOC strength, which is an intrinsic property of the material and is hard to modulate, the band order can also be changed by varying the coupling potentials. Increasing the strain can lead to a decrease of the coupling potentials, which could reduce the energy difference, $E_k = E_{cb} - E_{vb}$, between the conduction band, $E_{cb}$, and the valence band, $E_{vb}$, at the TRIM points. At a sufficiently large mechanical deformation, even materials with relatively weaker SOC could display BI. In what follows, we apply strain ranging from 0 to 12% to examine the effect of strain on the band properties of $\beta$-InSe. The corresponding band energy difference $E_{\Gamma}$ ($E_k$ calculated at the $\Gamma \in$ TRIM points), is illustrated in figure 3(a). It is seen that with increasing strain, the CBM lowers in energy, thus resulting in a significant decrease of the energy gap $E_{\Gamma}$. Remarkably, in passing from a critical strain of 1.4%, $E_{\Gamma}$ is rapidly quenched to zero and then is incremental with negative values; two bands with $\Gamma^{3+}$ and $\Gamma^{4-}$ symmetries around the Fermi level are inverted, which thus indicates BI characterizations.
The three-dimensional band structure of $\beta$-InSe under this critical strain point is shown in figure 1(d). From this figure, we can clearly see that the BI characterization appears at the $\Gamma$ point yielded by the lowering of the lowest unoccupied band at the $\Gamma$ point. The argument can be confirmed by the direct calculation of the protections of the lowest-conduction band (LCB) and the highest-valence band (HVB) of $\beta$-InSe at the $\Gamma$ point versus the strain variation. The corresponding results are plotted in figure 3(c). Knowing that the positive and negative values correspond to $s$ and $p_z$ states, respectively, one can rapidly find that, below the critical strain of $1.4\%$, the main projections of the LCB and the HVB of $\beta$-InSe at the $\Gamma$ point are predominated by the $s$ and $p_z$ orbitals, respectively. When the strain passes from the critical point, the main projections of the LCB and the HVB of $\beta$-InSe at the $\Gamma$ point are a contribution from the $p_z$ and $s$ orbitals, respectively, meaning that BI at the $\Gamma$ point takes place upon the critical strain point. Taking $\beta$-InSe with $\varepsilon = 6\%$ as an example, as shown in figure 2(d), an insulating phase with a band gap of 121 meV is established. Further calculations reveal that it is indeed a fully gapped insulator. Thus it can be concluded that the $\beta$-InSe could transform from an ordinary semiconductor to a TI by engineering strain. Furthermore, the gap magnitude is significantly larger than $k_B T$ (about 26 meV) at room temperature, suggesting that the TI character could be supported at room temperature. This gap with SOC is very close to the newly discovered actinide TIs [42].

It is known that the most general and direct approach to understand a TI with inversion symmetry is to analyze the $Z_2$ topological invariants $\nu_i$: $(\nu_1\nu_2\nu_3)$. One can interpret non-zero topological invariants as an obstruction to make the wave functions smoothly defined over half of the entire Brillouin zone under a certain gauge of the time-reversal constraint. According to the $Z_2$ classification, $Z_2 = 0$ means a trivial band topology while $Z_2 = 1$ characterizes a non-trivial band topology. Since all the investigated configurations possess inversion symmetry, a parity analysis can be used to identify the $Z_2$ topological invariants $\nu_i$: $(\nu_1\nu_2\nu_3)$. As shown in figure 1(c), there are eight time-invariant points in the Brillouin zone, but only four points ($\Gamma$, $Z$, $M$ and $L$) are inequivalent. Here, following the method proposed by Fu and Kane [7], we calculate the product of the parities of the Bloch wavefunction for the filled bands at all TRIM points in the Brillouin zone. As figure 1(c) illustrates, eight TRIM points are labeled as $\Gamma$, $Z$, $M_{1,2,3}$ and $L_{1,2,3}$. The product of parity eigenvalues of the valence band at TRIM point, $\delta_i$, is $-1$ if an odd number of BIs occur at the corresponding TRIM point; while $\delta_i$ is $+1$ if an even number of BIs occur at the corresponding TRIM point. From our calculation, we find that at the $\Gamma$ point, the parity of one occupied band changes after BI induced by strain, whereas the parity remains unchanged for all occupied bands at the other momenta $Z$, $M_{1,2,3}$ and $L_{1,2,3}$. Therefore, the strained $\beta$-InSe with BI has $\delta_\Gamma = -1$ and $\delta_Z = \delta_{1,2,3} = \delta_{1,2,3} = +1$. Whereas, for unstrained $\beta$-InSe, the parity remains unchanged for occupied bands at the all momenta $\Gamma$, $Z$, $M_{1,2,3}$ and $L_{1,2,3}$. Consequently, the unstrained $\beta$-InSe without BI has $\delta_\Gamma = \delta_Z = \delta_{1,2,3} = \delta_{1,2,3} = +1$. The topological indexes $\nu_0$, $\nu_1$, $\nu_2$ and $\nu_3$ of $Z_2$ $\nu_0$: $(\nu_1\nu_2\nu_3)$ are established by

$$
\begin{align*}
(-1)^{\nu_0} &= \prod_i \delta_i, \\
(-1)^{\nu_1} &= \delta_M \delta_M \delta_L \delta_L, \\
(-1)^{\nu_2} &= \delta_M \delta_M \delta_L \delta_L, \\
(-1)^{\nu_3} &= \delta_Z \delta_L \delta_L \delta_L,
\end{align*}
$$

In other words, $\nu_0$ corresponds to all eight TRIM points, while $\nu_1$, $\nu_2$ and $\nu_3$ correspond to four TRIM points belonging to the parallelepiped constructed by these eight TRIM points.

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Before BI, the calculated $Z_2$ topological invariants $\nu_0; (\nu_1 \nu_2 \nu_3)$ are $0; (000)$, indicating a topologically trivial feature. After BI, the calculated $Z_2$ topological invariants $\nu_0; (\nu_1 \nu_2 \nu_3)$ are $1; (000)$, which confirms the topological non-trivial state.

From previous studies [11, 12], the likelihood of incorporating BI in materials is determined by their SOC strength, it follows that it is more probable to find the TIs among heavier compounds (with stronger SOC). Alternatively, they have proven that if the system is not a TI under equilibrium conditions, it can be made so by applying appropriate strain. Yet, they have also demonstrated that BI in materials would not occur even with sufficient mechanical deformation if it were not for the protection received from the SOC. It is quite a paradox that this holds for all the TIs. Now a question arises: since the driving force for the BI is taken for granted to be SOC according to the existing literature, what is the role related to strain in this procedure? To answer this question, we investigate the evolution of the energy level near the Fermi level at $\Gamma$ point without SOC as a function of strains for $\beta$-InSe; the corresponding results are presented in figure 3(a). It is seen that with the increasing strain, the energy difference $E_{\Gamma}$ decreases and finally becomes zero at $\varepsilon = 1.5\%$. Most excitingly, by further increasing the strains, two bands with $\Gamma^{3+}$ and $\Gamma^{4-}$ symmetries around the Fermi level are inverted. Then the value of $E_{\Gamma}$ is incremental with the increasing strain, indicating that strain will result in the anti-crossing band behavior (as addressed in figure 2(c)), which changes the sign of the parity at $\Gamma$ point at a strain higher than $\varepsilon = 1.5\%$. It is also noted from figure 3(b), at below critical strain $\varepsilon = 1.5\%$, those are the contribution from the $p_z$ and $s$ orbitals, respectively. Herein, in contrast to previous studies, BI characterization at the $\Gamma$ point could be realized by mechanical deformation solely, even without SOC. With the advancement in experimental techniques, we expect that the corresponding experiments will soon be carried out. The experimental data available can then be compared with our interesting theoretical prediction.

Now, since the strain is known to support BI characterization in $\beta$-InSe, to explore the role of SOC we focus here on the contrast between the results with and without SOC. As figure 3(a) displays, the difference between the values of energy gap $E_{\Gamma}$ with and without SOC under different strain conditions are less than 23 and 16 meV for $\beta$-InSe at below and above the strain $\varepsilon = 4\%$, respectively. By comparing with the absolute value of the energy gap $E_{\Gamma}$, these values of the differences are negligible. These results are in good agreement with those addressed in figures 3(b) and (c). Figures 3(b) and (c) display that the critical BI points without and with SOC are slightly different, except the critical point with SOC is smaller than that without SOC in strain by 0.1\%. Quite naturally, it seems that the role of SOC in this proceeding can be ignored. To further uncover the effect of SOC, we additionally compare the bands around the Fermi level with and without SOC. As mentioned above, the changes of band structures by introducing SOC before the BI can be ignored. Here, we focus on introducing SOC after BI and take $\beta$-InSe with $\varepsilon = 6\%$ as an example. In figure 2(c), the band structure of $\beta$-InSe with $\varepsilon = 6\%$ is calculated without SOC. It follows that $\beta$-InSe with $\varepsilon = 6\%$ is semimetal with the band crossing at the Fermi level along the $\Gamma-M$ and $\Gamma-K$ directions if SOC is omitted. By breaking it, i.e. inclusion of SOC, the band gap could be opened at the Fermi level at the crossing points, leading to a typical dip in the band structure for $\beta$-InSe with $\varepsilon = 6\%$. By comparing the two figure parts, one can rapidly obtain that any gap opening at the crossing points must originate from the SOC. It thus can be concluded that although the SOC does not exchange the characteristics of VBM.
Figure 4. (a), (b) The energy difference labeled in (c) versus different strain conditions. For (a), strain I is simulated by varying $c$ for constant $a$ and the slab thickness. For (b), strain II is simulated by varying $a$ for constant $c$. (c) Band structure of $\beta$-InSe without SOC. The horizontal dashed red lines indicate the Fermi level.

and CBM and the corresponding role of SOC in previous literatures can be replaced by strain, the SOC being there to support gap opening at the crossing points of the inverted bands is indispensable for realizing the topologically non-trivial taste of the $\beta$-InSe.

Based on the discussion above, the variation of the BI characterization as a function of strain is the result of a significant change of $E_{\Gamma}$ induced by mechanical deformation. To understand this result more precisely, let us examine the electronic band structure of $\beta$-InSe in detail (figure 4(c)). The direct gap occurs between the bands $\zeta 2$ and $\eta 1$ at $\Gamma$ point of the Brillouin zone. On the other hand, the maximum of band $\zeta 2$ and minimum of band $\eta 1$ are located at point A and degenerate with $\zeta 1$ and $\eta 2$ into bands $\zeta$ and $\eta$, respectively; they form a large gap at point A ($E_A(\zeta - \eta)$, as denoted in figure 4(c)). From the projection analysis, these bands are derived from the $s$-states and $p_z$-states. In detail, the valence bands $\eta, \eta 1$ and $\eta 2$ are predominantly derived from the Se $p_z$ orbitals; while the conduction bands $\zeta, \zeta 1$ and $\zeta 2$ originate from mostly Se $s$ and In $s$ orbitals with weak contribution of the Se $p_z$ orbitals. Notice that the bands $\zeta 1, \zeta 2$ and $\eta 1, \eta 2$ are split from the bands $\zeta$ and $\eta$, respectively, whereas the last two remain degenerate at point A. After this splitting, the energy levels close to Fermi energy turn out to be bands $\zeta 2$ and $\eta 1$. In this case, the energy gap $E_{\Gamma}$ is related to bands $\zeta, \zeta 1, \zeta 2, \eta, \eta 1$ and $\eta 2$, i.e. $E_A(\zeta - \eta), E_{\Gamma}(\zeta 1 - \zeta 2)$ and $E_{\Gamma}(\eta 1 - \eta 2)$ (as labeled
in figure 4(c). As figure 4(c) denotes, $E_A(\xi - \eta)$, $E_\Gamma(\xi 1 - \xi 2)$ and $E_\Gamma(\eta 1 - \eta 2)$ are related to bands $(\xi, \eta)$, $(\xi 1, \xi 2)$ and $(\eta 1, \eta 2)$ respectively; combined with the projection analysis, the formation of $E_A(\xi - \eta)$, $E_\Gamma(\xi 1 - \xi 2)$ and $E_\Gamma(\eta 1 - \eta 2)$ is determined by the s-p$_z$, s-s and p$_z$-p$_z$ interactions, respectively. However, we stress that detecting whether these interactions are intraslab or interslab interactions is challenging. To further uncover the mechanism of this strain induced topological insulting behavior, we consider two types of lattice expansion. In the first case, strain is simulated by the variation of the lattice along the $c$-axis for constant $a$ and the slab thickness (denoted as strain I, as illustrated in figure 4(a)). For the second case, we consider the biaxial lattice expansion, where the crystal structure is expanded in the $ab$ plane and fixed in the $c$-axis (denoted as strain II, as illustrated in figure 4(b)). These situations are more about academic interest rather than for practical applications. As figure 4(a) addresses, on application of strain I, $E_\Gamma(\xi 1 - \xi 2)$ and $E_\Gamma(\eta 1 - \eta 2)$ decrease monotonically and dramatically in energy down to zero. On the other hand, with increasing strain I, the interslab interaction between adjacent slabs (i.e., a weak van der Waals interaction) is substantially quenched due to the remarkable decrease of the distance between the two slabs. Evidently, the $E_\Gamma(\xi 1 - \xi 2)$ and $E_\Gamma(\eta 1 - \eta 2)$ are determined by the interslab s-s and p$_z$-p$_z$ interactions. It is also concluded that the band splitting $(\xi - \xi 1$ and $\xi 2, \eta - \eta 1$ and $\eta 2)$ arises from the effect of interslab coupling. However, $E_A(\xi - \eta)$ is almost independent of strain. Furthermore, the interslab interaction cannot induce large variations of $E_\Gamma$ and thus the BI could not occur. Thus the change of the interslab interaction can nevertheless induce the topological phase transition. We explicitly confirm these conclusions in the strain II situation, to which we now turn. As figure 4(b) illustrates, the $E_\Gamma(\xi 1 - \xi 2)$ and $E_\Gamma(\eta 1 - \eta 2)$ are found to be almost unaltered with strain, except for a slight change. That is because, with increasing strain II, the interslab interaction between adjacent slabs is almost insusceptible, while the intraslab interaction is weakened. It is important to note that, different from strain I situation, strain II reduces the values of $E_A(\xi - \eta)$ significantly. In this case, the $E_A(\xi - \eta)$ is related to the intraslab s-p$_z$ interactions. Additionally, as displayed in figure 4(b), with increasing strain II, the $E_\Gamma$ is rapidly quenched to zero and then is incremental with negative values, meaning an obvious BI characterization. It is therefore worth highlighting that the BI originates predominately from strain II with a weak contribution of strain I. With this result in hand, one can then establish that the topological insulting nature of $\beta$-InSe can be tuned effortlessly by external control parameters, such as the electric field. This can be achieved by growing $\beta$-InSe on the top of a piezoelectric substrate, whose lattice can then be changed by applying an electric field.

4. Conclusion

In conclusion, we have explored the strain tuning of topological band order in $\beta$-InSe by DFT calculations. We have predicated that $\beta$-InSe is a promising TI candidate for its large energy gap up to 121 meV. These results are confirmed by the direct calculations of the topological $Z_2$ invariants. In particular, unlike previous literature, only strain is capable of stabilizing a robust BI in $\beta$-InSe even without considering SOC. However, SOC is indispensable for breaking the incompatibility symmetry of the inverted bands to yield a band gap at the crossing points. Additionally, our detailed calculations have shown that the BI originates predominately from strain II, with a weak contribution of strain I. Our work provides a fascinating guiding principle for tuning the topological order by other controllable external parameters instead of
the immutable intrinsic SOC. All of these make $\beta$-InSe cornucopias of fundamental interest with promising applications.

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