Prediction of a controllable Weyl semi-metallic phase in inversion-asymmetric BiSb

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Recent experimental realization of long sought Weyl fermions in non-magnetic crystals has greatly motivated condensed matter physicists to search for materials supporting Weyl fermions. Weyl fermions appear to be very promising for future electronics, often referred as Weyltronics. Here, by means of first-principle calculations, we report a stoichiometric crystal structure of BiSb with broken space-inversion symmetry. This structure is insulating in bulk and has non-trivial band topology. We observe a pressure driven Weyl semi-metallic phase transition in this crystal structure. The obtained Weyl semi-metallic phase exists in the 4.0 - 6.0 GPa pressure range. We find that a total 6 pairs of Weyl points, 6 monopoles and 6 antimonopoles, exist in the Brillouin zone. The Weyl points with opposite chirality are located at different energy values yielding separate electron and hole Fermi-surfaces. Additionally, the spin-texture of the bulk BiSb compound appears to be electrically controllable when the interlink between pressure and an electric field is exploited. This produces novel manipulable topological transport properties in this system which are very promising for implementation of this kind of materials in next-generation Weyltronics and spintronic devices.

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Weyl fermions have recently attracted the attention of researchers due to their unique intriguing physical properties such as the presence of discontinuous Fermi-arc.1–4 quantized anomalous Hall effect,5,6 quantum transport,7 anomalous magnetoresistance,8 etc. Weyl fermions are an alternative massless solution of the two-component Dirac equation, which is also known as the Weyl equation.9 These fermions were initially hypothesized by particle physicists to explain the chiral and massless behavior of neutrinos (assuming neutrinos have negligible mass). In condensed matter systems, Weyl fermions can be realized as low-energy excitations near the touching points of two non-degenerate bands at discrete k-points in the momentum space of a bulk system. These gapless band touching points are known as Weyl nodes or Weyl points.2 Close to a Weyl point, bands have linear dispersion in all directions in k-space. In 3D, Weyl points are similar to the well-known Dirac points except for the fact that Weyl points are spin non-degenerate, but Dirac points have spin-degeneracy. By breaking either the time-reversal (TR) symmetry or space-inversion (I) symmetry, one can lift up the spin-degeneracy of the Dirac points in a Dirac semimetal10 and realize a Weyl semimetal (WSM). Hence, the lack of TR-symmetry or I-symmetry is an essential requirement for realization of WSM phase in 3D systems.

Each Weyl point can be characterized by an associated chirality (left handedness or right handedness) or by a monopole and an antimonopole having charge +1 or −1, respectively. Weyl points are always created in pairs via pair-creation of a monopole and an antimonopole.11–13 Similarly, they can disappear only via the pair-annihilation process. Thus, the total charge in k-space is always zero and the total number of Weyl points is always even. In I-symmetric WSMs, opposite Weyl points in a Weyl-pair are located at the same energy while in I-asymmetric WSMs opposite Weyl points are separated both in the momentum space and in energy. This eliminates the possibility of realization of a nodal semimetallic state by tuning the Fermi-level and thus, separate electron and hole Fermi-surfaces exist in the I-asymmetric WSM systems. Such systems are very interesting and possess novel topological transport properties.6,11,14–19

In recent years, many different theoretical proposals have been reported for realization of WSM phase in I-symmetric1,20–22 and I-asymmetric systems.13,23–31 Several experimental groups have recently reported the experimental realization of WSM phase in single crystal compounds.32–35 and in photonic crystals.36 To the best of our knowledge, there is no report of controllable WSM phase in a compound. However, ferroelectric-like polar WSM compounds having large spin-orbit coupling (SOC) could open a new avenue of realization of novel transport properties. When we combine SOC with ferroelectricity, we obtain a class of novel multifunctional materials, called Ferro-Electric Rashba Semiconductors (FERSC).37 Due to the giant Rashba spin-splitting present in FERSCs, the electric-field control of the spin-texture is possible in FERSCs. Recently, S. Picozzi et al. have theoretically demonstrated the possible control and switching of the spin-texture by means of an electric field in GeTe, which is a ferroelectric compound inheriting large SOC.37,38 This prediction was later experimentally corroborated.39 In addition to GeTe compound, a possible control of the spin-texture and spin-valley-tronics via an electric-field has been predicted for tin iodine pervoskites (FA)SnI340 —with FA = (NH2CHNH2)+— and
BiAlO$_3$/BiIrO$_3$ (111)/(111) superlattices.\(^4\) The Bi$_{1-x}$Sb$_x$ alloys are the first generation topological insulator.\(^4\) In 2013, H. J. Kim et al. reported experimental evidence of WSM phase in Bi$_{1-x}$Sb$_x$ alloys for $x = 3\%$ by magnetoresistance measurements.\(^8\) In the present work, we report a stoichiometric crystal structure of BiSb with broken I-symmetry. This structure belongs to the space group 160 ($R3m$) and has non-trivial band topology. By means of first-principle calculations, we observe a pressure-induced WSM phase transition in the present BiSb system in 4.0 - 6.0 GPa pressure range. We have further exploited the coupling between large SOC and ferroelectricity of BiSb to tune the spin-texture of Rashba-like bands by an electric field. Our first-principle calculations show that the chirality of the Weyl points in BiSb can be switched by an electric field. This property of a ferroelectric-like polar WSM is very important and such electric-field control of Weyl points could play a vital role in the next generation Weyltronics and spintronics devices.

Bulk bandstructure is calculated with and without-SOC. Figure 1(a) and 1(b) represent the calculated electronic bandstructure along the high symmetry lines of the hexagonal Brillouin zone. From bands without-SOC (fig. 1a), one can see that BiSb is an indirect bandgap semiconductor with indirect energy gap of 0.16 eV. The direct bandgap is located at the L-point (0.5, 0.0, 0.5) of the Brillouin zone with an energy gap of 0.43 eV. In the presence of SOC, each band of BiSb shows spin-splitting (fig. 1b) and the band-inversion occurs at the L-point. It is worthwhile to note that the spin-degeneracy of bands still exits at the L-point (Kramers’ point), which confims that BiSb breaks the I-symmetry but preserves the TR-symmetry. For TR-symmetric systems, lack of I-symmetry is an essential requirement for realization of WSM phase. Thus, this system fulfills the fundamental requirement to be in the WSM phase. The energy gap between the conduction band bottom (CBB) and valence band top (VBT) decreases due to the presence of SOC, particularly close to the L-point it has more pronounced changes. However, there still exists a small direct energy bandgap at the L-point along with indirect energy gap along the A-L path.

In the $R3m$ space group, BiSb has a layered crystal structure with alternative layers of Bi and Sb atoms oriented along the $c$-axis of the rhombohedral unit-cell (see crystal structure in fig. 4a). Two alternative layers of Bi and Sb form a bilayer, which is repeated along the $c$-crystallographic direction of the unit-cell. Lattice parameters of the fully relaxed unit-cell are: $a = b = 4.51$ Å, $c = 11.92$ Å and the angles are: $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$. Additional details regarding crystal structure are given in the supplemental information. To study the dynamical stability of BiSb, we performed phonon calculations using Density Functional Perturbation Theory (DFPT) as implemented in ABINIT code.\(^43\)–\(^45\) We used different approximations for exchange-correlation functional (LDA, LDA+SOC, PBE and PBE+SOC) to compute phonon modes. We obtained positive phonon frequencies for all four cases, which indicates that $R3m$ phase of BiSb is vibrationally stable at the level of DFPT calculations (supplemental information). However, we see a significant change in the phonon spectra due to the presence of SOC, which is in agreement with similar work reported for pristine Bi and Sb.\(^46\)–\(^48\) Furthermore, we found that phonon frequencies are positive until 10.0 GPa external applied pressure. Beyond 10.0 GPa pressure phonon modes start becoming softer, which is indicative of a structural phase transition at higher pressures. To further ensure the stability of the crystal structure, we have performed calculations to obtain elastic constants.\(^39\),\(^50\) Our calculations yield that BiSb system satisfies the mechanical stability criteria\(^31\),\(^52\) for a rhombohedral cell (details can be found in the supplemental information). Therefore, phonon and elastic constants calculations confirm the vibrational and mechanical stability of the BiSb system. We also find that this structure is robust against the structural and atomic disorders.
ally results in the inversion of the bands at the L-point. The strong SOC of Bi and Sb atoms is responsible for the bands-inversion. The band-inversion process is more evident along H → L direction. Such a band-inversion process yields topologically protected conducting surface states in the bulk insulating system. Thus, the band-structure calculations reveal the non-trivial topological nature of bands in the BiSb system.

In 2014, R. Okugawa and S. Murakami proposed an effective model Hamiltonian to explain the evolution of Fermi-arcs and the WSM phase transition in I-asymmetric systems. In their model, they introduce a control parameter \( m \) in the effective Hamiltonian to tune the bulk bandgap. By slowly varying \( m \), one can close the bulk bandgap and realize gapless Weyl points at discrete points in the Brillouin zone. For I-asymmetric systems, these gapless Weyl points exist for a finite range of the control parameter \( m \). On the other hand, for I-symmetric systems, Weyl points appear at a particular value of \( m \) (say \( m_o \)) via pair-creation of monopoles and antimonopoles. With further increase in \( m \) (\( m > m_o \)), pair-annihilation occurs and the Weyl points disappear. Thus, for I-symmetric systems, the WSM phase lies exactly at the intermediate boundary of two distinct phases of topological insulator or normal insulator.

In the present work, we use isotropic pressure (P) as the control parameter to tune the bulk bandgap. Figure 2(a) shows the evolution in the direct bandgap along H → L direction for different values of applied pressure. The direct bandgap along H → L direction (\( E_g^L \)) decreases as we increase pressure up to 3.0 GPa (fig. 2b). Interestingly, with further increase in pressure, \( E_g^L \) becomes zero at 4.0 GPa pressure and remains zero until 6.0 GPa. In this pressure range, the CBB and the VBT accidentally touch each other along H → L direction (see fig. 2(a) for 5.0 GPa case). The dispersion of the bands close to the band touching point is linear in k and the band touching point is not located at any Kramers' points or along any high-symmetry direction of bulk Brillouin zone. These facts give us signatures of a Weyl semimetallic phase in 4.0 - 6.0 GPa pressure range. When we further increase the external pressure, we observe that the direct bandgap \( E_g^L \) reopens. However, the system becomes semimetallic due to crossing of the Fermi-level by other topologically trivial bands. Thus, a pressure induced non-trivial insulator-WSM-semimetal phase transition takes place in the present BiSb system. A similar pressure induced phase transition has been reported for trigonal Te and Se systems. More details about the Weyl semimetallic phase occurring at 5.0 GPa pressure are given below.

Figure 3(a) shows the projection of spin-components (\( S_x \), \( S_y \), and \( S_z \)) on bands for 5.0 GPa applied pressure. We observe similar behavior of spin-projections on the bands for other values of P. Here, we have chosen the (001) direction as the quantization axis for all spin dependent calculations. Red (Blue) color represents the up (down) spin state. In figure 3(a), we calculate the band structure along two different directions in k-space: H/2 → L → H'/2 and A/2 → L → B/2 (see figure 3(c) for directions). Along the H/2 → L → H'/2 direction, one can clearly notice that two non-degenerate gapless points are present in the vicinity of the L-point. Such gapless points in k-space are called Weyl points or Weyl nodes and unlike Dirac points they are 2-fold degenerate rather than 4-fold. Weyl points (W1) along H/2 → L → H'/2 direction are located near the Fermi-level and are related by TR-symmetry (L-point as Kramers' point). Hence, these two points have the same chirality and topological charge. Bandstructure along A/2 → L → B/2 direction reveals presence of two more spin non-degenerate gapless points located slightly below Fermi-level. These two gapless points represent another set of Weyl points depicted.
by W2. W2 Weyl points are related by TR-symmetry and hence, they share the same chirality and topological charge. To determine the chirality of W1 and W2 Weyl points, we have calculated the Berry flux through a closed surface enclosing only one Weyl point at a time.\textsuperscript{54,55} Our calculations reveal that W1 and W2 have opposite chirality and therefore, they carry opposite topological charges. Consequently, W1 behaves like a monopole and W2 behaves like an antimonopole in k-space. These two opposite Weyl points are located at different energy values. Existence of such opposite Weyl points, located at different energies, is attributed to the broken I-symmetry of the present BiSb system. Since W1 and W2 are separated in momentum space as well as in energy, it is impossible to realize a nodal semimetallic phase by tuning the Fermi-level and there always exists a state with separate electron and hole Fermi-surfaces. Weyl points exist in the system as long as the electron Fermi-surface is separated from the hole Fermi-surface. Such a property of WSM is very interesting as it could yield chiral magnetic effect and novel topological transport properties in the system. In recent years, these properties have attracted much theoretical interest.\textsuperscript{6,11,14–19}

Using the symmetry of the crystal the position and chirality of all other Weyl points can be determined. Figure 3(c) shows the location of all monopoles and antimonopoles present at the $k_z = \frac{\pi}{a}$ surface of the hexagonal Brillouin zone. In reciprocal space, coordinates of the W1 and W2 points are: $(0.494 \frac{2\pi}{a}, -0.012 \frac{2\pi}{a}, 0.500 \frac{2\pi}{c})$ and $(0.494 \frac{2\pi}{a}, 0.012 \frac{2\pi}{a}, 0.500 \frac{2\pi}{c})$, respectively. To further confirm the existence of two Weyl points in the $k_x = 0.494$ plane, we have calculated the band dispersion in the $k_y$-$k_z$ plane (at constant $k_x = 0.494$) near W1 and W2 points (see plane along cut-1 in figure 3c). Two gapless points can be clearly noticed in figure 3(d). One point is located at positive $k_y$ and another point is located at negative $k_y$, but both are located at the same $k_z$. There are three equivalent L-points in the hexagonal Brillouin zone and two Weyl points (W1 and W2) are located near each L-point. We further exploit $M_x$ and $M_y$ mirror symmetry operations to find the pairs of Weyl points located near each L-point. Thus, in total there are 12 Weyl points, 6 monopoles and 6 antimonopoles, in the first Brillouin zone (figure 3c).

Observation of Fermi-arcs connecting two Weyl points is crucial to confirm the prediction of a WSM phase. For this purpose, we have performed the spin-texture calculations at (001) surface of a BiSb-slab.\textsuperscript{56} The slab was constructed from the primitive cell of BiSb. We observe two trivial Fermi-circles along with two open Fermi-curves [Fig. 3(e)]. These open Fermi-curves are reminiscent of the Fermi-arcs connecting opposite Weyl points.\textsuperscript{57}
Having established the existence of WSM phase in BiSb, we will finally comment on the possibility to control the chirality of Weyl points. It is important to note that the experimental control of the spin-related properties stands as one of the key features in future devices and applications. The coupling between electric polarization and SOC in novel class of FERSC materials promises to solve this issue. Furthermore, the recent experimental discovery of ferroelectric-metals has generated huge interest in polar materials. The polar ferroelectric-metals simultaneously exhibit two self-contradicting properties: polarity and metallicity. This particular behavior has been theoretically explained as follows: in ferroelectric-metals the free electrons screen out the long-range electrostatic forces favoring a polar structure with a net dipole moment. The interplay between SOC and polarity could yield exotic quantum phenomena in polar ferroelectric-metals. Our calculations show that BiSb is a narrow-bandgap ferroelectric semiconductor at zero pressure. Also Bi and Sb atoms are known to exhibit strong SOC, as previously reported. Here, we take advantage of the large SOC and ferroelectric polarization to control the spin-related properties in the present BiSb system.

At zero pressure, the BiSb material is a narrow-bandgap semiconductor which exhibits Rashba-like spin-splitting as observed in figure 2. In the $R3m$ phase, Bi and Sb atoms are displaced from the ideal rocksalt sites. The polar displacement of the Bi atoms along the direction of red arrows (see crystal structure shown in figure 4a) yields to a ferroelectric-like polarization in the BiSb system. The calculated unit cell polarization components (denoted as $\mathbf{P}_s$ and obtained by means of the Berry-phase approach) are $P_x$, $P_y$, and $P_z$ with values of -0.95, 1.64, and -5.31 $\mu$C-cm$^{-2}$, respectively. It is worth mentioning that we can switch the polarization by reversing the direction of polar displacement of Bi-atoms (along blue arrows in figure 4b) from the ideal rocksalt sites. We notice that the spin-polarization of all three spin components of Rashba-like bands at 0.0 GPa gets inverted when we switch the direction of the ferroelectric polarization. This, as expected from the ferroelectric and SOC coupling terms in the Rashba Hamiltonian, makes BiSb (in $R3m$ phase) a FERSC material at ambient conditions. After this process, we apply 4.0 GPa isotropic pressure to reach the WSM phase with inverted spin-polarized bands. Figure 4 shows dispersion of bands along W1 and W2 Weyl points for original and inverted polarization cases. The shape of bands and the location of Weyl points in energy and momentum space is exactly the same for both $P_x$ and $P_y$ polarizations. However, after inverting the polarization we do notice a change in the spin-projected bands. We found that the spin-projection on the bands changes in spin-orientation which is depicted by switching of the up and down $S_z$ spin-components (figure 4). We observe similar behavior for $S_y$ and $S_x$ band spin-projections. The band spin-switching happens along both k-directions containing W1 and W2 Weyl points when the polarization is reversed. As a result, the topological charge and chirality of Weyl points attain opposite values after inverting polarization. This points to the possibility of switching of the monopole and antimonopole charges in a WSM via an electric field. This property is very important for designing new generation Weyltronics and spintronics devices. Here, it is important to remark that the WSM-phase will retain the polar-like displacements similar to the case of “ferroelectric-metals”. This analysis demonstrates the coupling between the polarization and the SOC-degree of freedom in the TI- and WSM-phases in this BiSb crystal. In addition to this work, a recent study has also predicted the existence of a WSM phase in ternary hyperferroelectrics by means of chemical doping and alloying.

In summary, we report a stoichiometric layered structure of BiSb which is enthalpically, vibrationally and mechanically stable at the DFT level. This structure has a bulk insulating gap at zero pressure with non-trivial band topology. Pressure dependent electron band structure calculations reveal the existence of a WSM phase in the pressure range 4.0 - 6.0 GPa. We have found 6-pairs of Weyl points at $k_z = \pi/c$ surface of the Brillouin zone. We clearly observe linear dispersion of spin non-degenerate bands near each Weyl point. Surface state calculations further confirm the presence of WSM phase in BiSb. Additionally, the WSM phase of this non-magnetic system relies on the broken inversion symmetry of the crystal rather than the time-reversal asymmetry. This feature makes this material very appealing and interesting to experimentalists. We further discussed the possibility to control the chirality and topological charge of the Weyl points by means of applied pressure and electric field. The existence of a polar-like Weyl semimetallic phase in this BiSb...
compound calls for further studies on the underlying exotic quantum phenomena.\textsuperscript{65}

\section*{Computational Details}

We used the projected augmented wave (PAW) method implemented in the VASP code to perform all DFT-based first principle calculations.\textsuperscript{66,67} We considered fifteen valence electrons of Bi ($5d^{10}6s^26p^3$) and five valence electrons of Sb ($5s^25p^3$) in the PAW pseudo-potential. For exchange-correlation potential, we used exchange-R3m implemented in the VASP code to perform all DFT-based first principle calculations.\textsuperscript{66,67} For ionic relaxations, the cell was relaxed, first in the internal coordinates and then in the volume until the total energy difference criterion was defined as $10^{-8}$ eV. For ionic relaxations, the cell was relaxed, first in the internal coordinates and then in the volume until the total energy difference between two consecutive steps was smaller than $10^{-5}$ eV. Spin-orbit interaction was included for all ionic relaxations. We use ABINIT code to calculate phonon spectra.\textsuperscript{43–45} We have used a q-mesh of size $4 \times 4 \times 4$ for all phonon calculations. Band-structure calculations were done (i) with spin-orbit coupling (SOC) and (ii) without SOC. For all pressure dependent electronic structure calculations, we employ isotropic pressure ranging from 1 GPa to 10 GPa on the original unit cell. To visualize the open Fermi-arcs, we have calculated the spin-texture at (001) surface of a BiSb-slab.\textsuperscript{56} This 55.6 Å thick slab consists 14-bilayers of BiSb and a vacuum layer of 12.0 Å thickness. VESTA,\textsuperscript{71} PyProcar\textsuperscript{66} and MAYAVI\textsuperscript{72} softwares were used to make some figures.

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