

Giant Rashba splitting in InBi/SbBi chains on InSb(110): Surface reconstruction as a route to spin-split one-dimensional states

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Bismuth-induced (1×2) and (1×3) surface reconstructions on InSb(110) exhibit a tunable giant Rashba splitting associated with one-dimensional atomic chain structures. Remarkably, the lower Bi-coverage Bi/InSb(110)- (1×3) phase shows a larger Rashba splitting parameter than the (1×2) phase, revealing a counterintuitive dependence of spin splitting on adsorbate concentration. Combining surface-science experiments and density functional theory, we show that the magnitude of band splitting is governed by the interplay between atomic-scale surface corrugation and spin-orbit coupling from Bi. Our calculations further indicate that, while Bi is essential to induce the Rashba effect, the significant contribution arises from the InSb substrate. The Bi/InSb(110) reconstructed surface consists of Bi chains bonded selectively to In or Sb of the substrate. These results establish Bi/InSb(110) as a platform for engineering the strength of spin splitting and for enabling the ordered growth of InBi nanostructures.

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I. INTRODUCTION

Low-dimensional bismuth structures are of increasing interest due to their unique quantum properties, such as topological edge and corner states [1,2], localized trimer states [3], and spin-polarized states [4,5]. In low-dimensional systems, non-Fermi liquid behavior may appear as a result of reduced screening and enhanced fluctuations [6,7]. The Rashba effect—a spin-polarized splitting of electronic bands as a mutual effect of the large spin-orbit interaction and structural inversion asymmetry—is an actively studied phenomenon in one-dimensional (1D) and two-dimensional (2D) systems [8–10]. A quantitative description of the Rashba effect in a parabolic dispersion is given by the Rashba parameter, $\alpha_R = 2 \times \Delta E_R / \Delta k_0$, which evaluates band splitting in energy (ΔE_R) and momentum space (Δk_0). The magnitude is considered giant when α_R is more than $3 \text{ eV \AA}$ [4,8,9,11].

Rashba splitting has been explored by depositing heavy elements such as Bi and Pt on various material surfaces, e.g., Bi/Ag(111) [12], Bi/Ag(110) [13], Pt/Si(110) [14], Bi/InAs(110) [4], and Bi/GaSb(110) [11,15]. While some progress has been made in utilizing the Rashba effect for spin manipulation in semiconductor substrates, achieving high spin-charge conversion efficiency is still challenging [13]. Demonstrating and understanding large spin splitting is the first step towards high spin-charge conversion efficiency in spintronic applications [16]. So far, most of the effort is limited to 2D systems or heterostructures [17], but the Rashba splitting in 1D systems is generally larger than in the 2D systems due to the larger in-plane potential gradients [18]. Bi-induced 1D structures on InAs and GaSb have been investigated for large Rashba splitting [4,8,11,19], utilizing the large spin-orbit coupling of Bi and structural inversion asymmetry in the zinc blende crystal structure of III-V compound semiconductors [20]. However, there is a strong requirement for new spin-polarized electron structures and an improved understanding of the relation between substrate, Bi-induced 1D structures, and the strength of the Rashba splitting.

Among the III-V semiconductors, InSb is particularly notable due to its most significant spin-orbit coupling [21], narrow bandgap, and large electron mobility. Furthermore, compared to the other nonpolar III-V surfaces, Bi/InSb(110) is unique, as it has been reported to induce flexible surface reconstructions with sample annealing, resulting in (1×2) and (1×3) surface reconstructions at low and high annealing temperatures, respectively [22,23]. Like other

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Bi/III-V(110)-(1×2) surfaces, Bi/InSb(110)-(1×2) is expected to exhibit a structure corresponding to the missing-row model [24,25]. However, the structure of Bi/InSb(110)-(1×3) is unique to InSb and still unclear. Thus, the Bi/InSb(110) system is ideal for investigating variable Bi content and the electronic effect of tunable Bi surface reconstruction.

In this work, we investigated Bi-induced 1D chains on InSb(110) surfaces, with varying Bi amounts and surface reconstructions, using complementary surface characterization techniques including scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), and angle-resolved photoelectron spectroscopy (ARPES). The Bi-induced structures include (1×2) and (1×3) reconstructions as well as an intermediate arrangement. The atomic arrangement of Bi/InSb(110)-surface reconstructions is observed experimentally and confirmed using *ab initio* density functional theory (DFT) simulations. The low Bi concentration surface, i.e., (1×3) reconstruction, exhibits a larger Rashba splitting value than the (1×2) surface, but both surface arrangements display a value resulting in giant splitting parameter, $\alpha_R > 3 \text{ eV \AA}$. Furthermore, using surface-sensitive x-ray photoemission spectroscopy (XPS), both Sb-Bi and stable In-Bi bonds are observed at the Bi-InSb interface. The III-Bi compounds, such as InBi, are predicted to be topological insulators, but are considered unstable and cannot be realized yet experimentally using conventional synthesis approaches [26]. Thus, Bi/InSb(110) provides a platform for efficient spintronics applications with a variable magnitude of spin splitting and a template for epitaxial growth of advanced quantum materials.

II. METHODS

Surface preparation: An oxide-free InSb(110) surface is achieved by cleaving a piece of an InSb(100) wafer in ultra-high vacuum along the natural cleave directions $\langle 110 \rangle$. Bi was deposited using an effusion cell (from MBE Components), heated at 450 °C. The Bi/InSb(110) surface was then annealed to get different surface reconstructions.

Experimental characterization: XPS and ARPES measurements were performed at the FinEstBeAMS and BLOCH beamlines of the MAX IV Laboratory, Sweden. The In *4d*, Sb *4d*, and Bi *5d* core levels were recorded at 130 eV photon energy and 5 eV pass energy. The recorded spectra were background fitted with the Shirley background function and deconvoluted assuming pseudo-Voigt functions, using the Igor Pro software. The parameters used in spectral fitting are included in Table S1 of the electronic Supplemental Material [33]. For ARPES, the band dispersion was measured using linearly polarized light and a Scienta DA30-L spectrometer. The energy resolution is expected to be $< 10 \text{ meV}$. The STM studies were performed in an Omicron VT-STM, using electrochemically etched tungsten tips. All structural characterization was performed at room temperature, unless otherwise mentioned.

Density functional theory: All first-principles calculations were performed using the Vienna *Ab Initio* Simulation Package (VASP) within density functional theory [27–29]. The projector augmented-wave (PAW) method and the Perdew-Burke-Ernzerhof (PBE) functional were adopted with a

plane-wave cutoff energy of 300 eV [30–32]. A Γ -centered $6 \times 6 \times 1$ k-point mesh and a 15 Å vacuum layer were used for the Bi/InSb heterostructure. Atomic structures were relaxed until forces were below $10^{-2} \text{ eV/\AA}$, with the bottom three layers fixed as the substrate, and the energy convergence threshold set to 10^{-7} eV . The spin-orbit coupling is included in all the DFT electronic-structure calculations.

III. RESULTS AND DISCUSSION

The freshly cleaved InSb(110) forms an unreconstructed surface with a rectangular unit cell, as confirmed by LEED and STM results presented in Fig. S1 of the Supplemental Material [33]. The ARPES band dispersion shows gapped parabolic dispersion, and the typical features of the valence band (VB), including heavy hole, light hole, and split-off bands, are also highlighted in Fig. S1. The In *4d* and Sb *4d* core-level XPS of the cleaved InSb sample are plotted in Fig. 4 (in comparison to other sample treatment conditions). The spectra can be fitted with one main component and another surface component (fitting parameters are available in Table S1 of the Supplemental Material [33]), consistent with the previously reported work [34].

Depending on the annealing conditions, Bi deposition on InSb(110) is known to result in multiple surface reconstructions [22,23,35]. Here, Bi was first deposited onto the sample at room temperature, followed by stepwise annealing to obtain different surface reconstructions.

Upon annealing at approximately 200 °C, the surface shows self-assembled and periodic atomic chains of Bi, following ($1 \times n$) type surface reconstruction, as indicated by the LEED image shown in Fig. 1(a). Two LEED diffraction spots are visible between (10) and (11) diffraction spots from the substrate, along the $[001]$ direction. The surface diffraction spots correspond to an intermediate phase of Bi-induced surface reconstruction between (1×2) and (1×3). The STM image of the same surface (Fig. S2(a) of the Supplemental Material [33]) also shows atomic chains with varying distances between them, corresponding to an intermediate phase between (1×2) and (1×3) surface reconstructions. The (1×2) surface reconstruction is reported to be unstable and to occur in a narrow temperature range; thus, it is challenging to have large-scale (1×2) periodicity [22,23]. From the STM and LEED images, we conclude that the atomic chains extend along the $\langle 110 \rangle$ or Γ -X direction.

The band dispersion along the Bi chains (i.e., along the Γ -X symmetry direction), mapped by ARPES, can be seen in Fig. 1(b). It shows splitting of bands along the momentum vector, symmetrically centered around the Γ point, which is consistent with the typical Rashba effect [4,11]. From the ARPES results and their second derivative, we obtain a momentum offset between the spin-split bands of $\Delta k_0 = 0.14 \text{ \AA}^{-1}$ and an energy difference between the VB maximum and the crossing point of the spin-split bands at the Gamma point of $\Delta E_R \approx 300 \text{ meV}$, as indicated in Fig. 1(b). This results in a Rashba parameter $\alpha_R = 2 \times \Delta E_R / \Delta k_0$ of about $4.3 \text{ eV \AA}$, which is considered a giant Rashba splitting [8,9] and is one of the largest reported Rashba splitting magnitudes. We attribute the observation of such a large Rashba splitting here to the large spin-orbit coupling in Bi/InSb, supported by

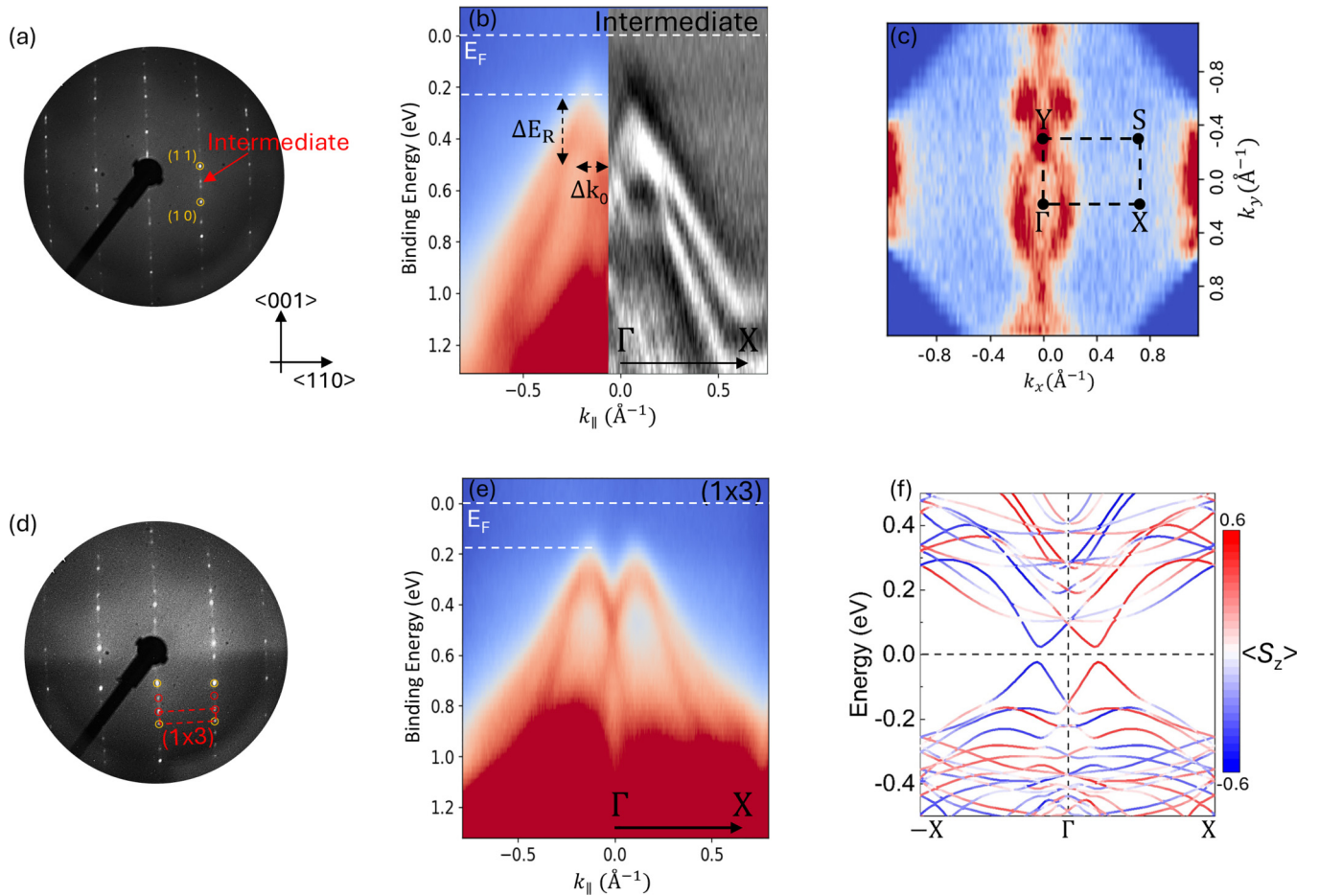


FIG. 1. Bi deposition on InSb(110) surface: (a) LEED image of the intermediate surface reconstruction from Bi/InSb(110)-(1 $\times$ 2) and Bi/InSb(110)-(1 $\times$ 3), the yellow circles highlight the substrate unit cell; (b) corresponding ARPES image along the direction of the atomic chains showing band splitting, second derivative of the band dispersion is stitched to the right, (c) Fermi surface map obtained at 300 meV BE, overlaid with the rectangular InSb(110) unit cell in reciprocal space, displaying quasi-1D dispersion perpendicular to the chains, i.e., along Γ -Y direction; (d) LEED image corresponding to the Bi/InSb(110)-(1 $\times$ 3) surface reconstruction, the red dashed rectangle highlights the (1 $\times$ 3) surface unit cell; (e) corresponding band dispersion along the atomic chains, i.e. along Γ -X direction imaged by ARPES, and (f) calculated spin-polarized states in the Bi/InSb(110)-(1 $\times$ 3) surface band dispersion. All ARPES results were taken at a photon energy of 60 eV, and the dashed lines indicate (b), (e), (f) the Fermi level at 0 eV BE and (b), (e) the VB maximum.

the induced surface corrugation, as will be explained later. A Fermi surface map, obtained at a binding energy (BE) of 300 ± 50 meV, is shown in Fig. 1(c). It confirms the Rashba splitting along the Γ -X symmetry direction, and it shows anisotropic dispersion and 1D states along the Γ -Y symmetric direction, i.e., perpendicular to the Bi chains. The waving feature and dispersion perpendicular to the chain direction indicate electronic interaction across Bi chains and are considered as quasi-1D surface states [4,36]. The absence of Rashba splitting perpendicular to the Bi chains, i.e., along the Γ -Y symmetric direction, can also be seen directly in a corresponding ARPES map shown in Fig. S2(b) of the Supplemental Material [33].

The VB maximum of the Bi/InSb(110) surface is found in Fig. 1(b) at about 200 meV below the Fermi level, while it is located very close to the Fermi level for clean InSb(110) (as shown in Fig. S1(e) [33]). Considering the small InSb bandgap of 0.17 eV, this indicates that the Bi/InSb(110) structure has a larger bandgap than clean InSb, and Bi deposition induces semiconducting character. This is in

contrast to the semimetallic character reported previously for Bi/III-V(110) surfaces [37]. Additional ARPES measurements were obtained at a low sample temperature of 19 K from a Bi/InSb(110) surface prepared under nominally identical conditions, shown in Fig. S2(c) of the Supplemental Material [33]. They confirm the semiconducting character, with a VB maximum observed again at about 200 meV below the Fermi level, as well as a similar magnitude of Rashba splitting along the Bi chains.

The sample was then annealed to a higher temperature, 250 $^{\circ}$ C, which facilitates the desorption of Bi from the InSb surface. A large-scale (1 $\times$ 3) surface reconstruction along the (001) direction is observed, according to the LEED image in Fig. 1(d). The transformation from (1 $\times$ 2) to (1 $\times$ 3) has been reported due to the desorption of excess Bi upon sample annealing [22,23,35]. The corresponding band dispersion is shown in Fig. 1(e), and Rashba splitting along Γ -X can still be observed, with almost the same Rashba parameter as obtained before. In comparison to the band dispersion in Fig. 1(b), the VB maximum is slightly shifted by about 50 meV towards

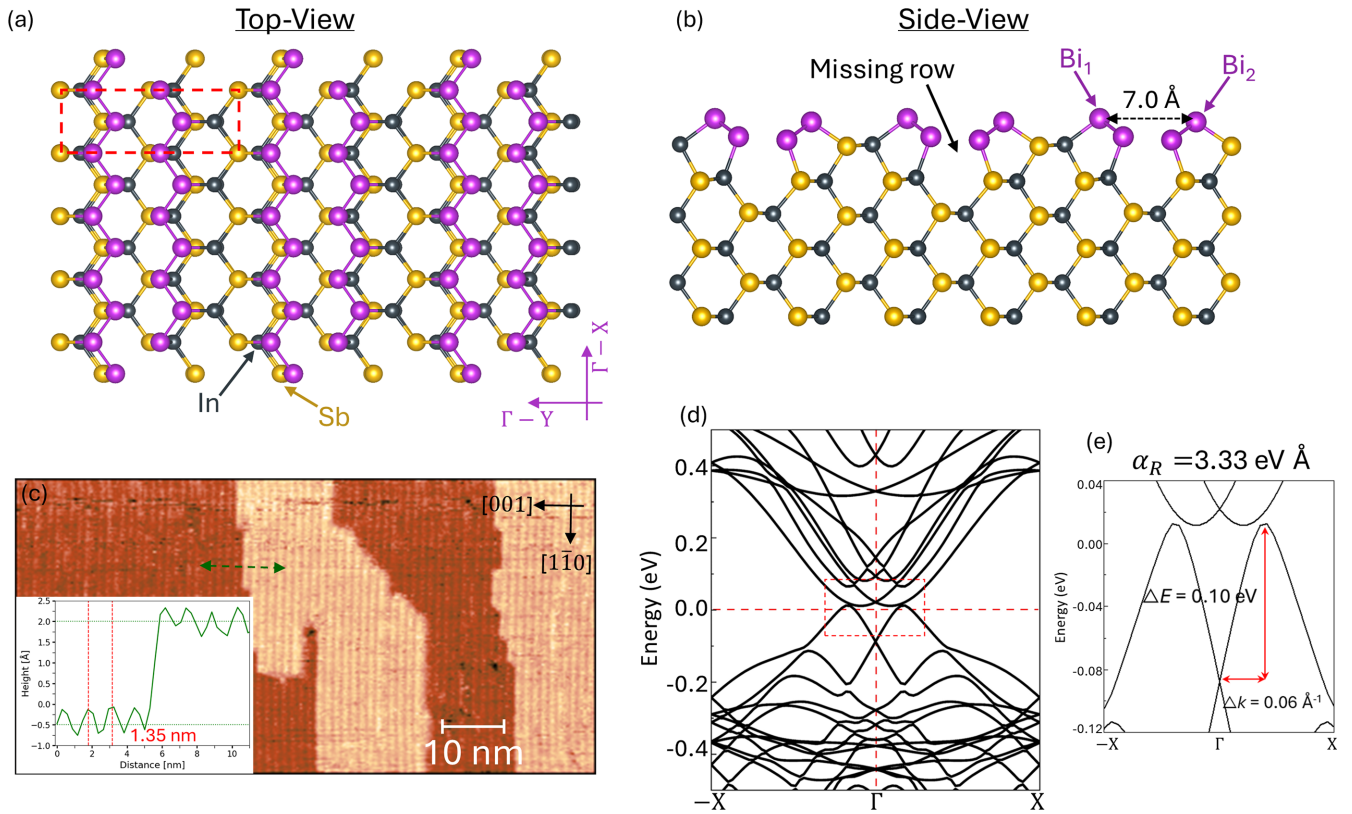


FIG. 2. Bi/InSb(110)-(1 × 2): (a) Top-view and (b) side-view model of the Bi/InSb(110)-(1 × 2) surface, resulting from DFT after energy relaxation. The black, yellow, and purple color spheres correspond to In, Sb, and Bi atoms, respectively. The (1 × 2) surface unit cell is indicated in (a) by a red rectangle (dimensions 1.33 × 0.47 nm²). Bi atoms are bonded to either In or Sb atoms, marked in (b) as Bi₁ and Bi₂. (c) STM filled-state image of the Bi/InSb(110)-(1 × 2) surface ($V = -1.8$ V, $I = 130$ pA), with an STM line profile across a surface step in the inset. (d) Band dispersion along Γ -X calculated for the structure shown in (a,b), including spin-orbit coupling. The area around the Γ -point, as indicated by the red rectangle, is magnified in (e), where the Rashba splitting parameters are highlighted.

the Fermi level, and the parabolic bands are more defined, with fewer electronic states around the dominating bands. The similar Rashba parameter and the comparison of band dispersion in Figs. 1(b) and 1(e) confirm that the surface resulting in Fig. 1(b) has to be understood as an intermediate surface reconstruction between (1 × 2) and (1 × 3), where the corresponding electronic states either overlap or contribute to the broader background around the dominating parabolic bands. Figure 1(f) shows the simulated spin polarization in the band splitting using DFT (explained below) corresponding to the Bi/InSb(110)-(1 × 3) surface, showing that the Bi-induced band splitting is spin polarized. It should be noted that the absolute energy positions in the experimental and DFT electronic band structures differ due to the well-known tendency of standard DFT calculations to underestimate the semiconductor bandgap [38,39].

DFT has been employed to simulate the atomic structure of the Bi/InSb(110) surfaces, in accordance with the experimental STM and ARPES results. Figures 2(a) and 2(b) shows the top-view and side-view model of the Bi/InSb(110)-(1 × 2) surface, compared with the STM image shown in Fig. 2(c). Pairs of Bi zigzag atomic chains are formed on top of the InSb(110) surface with a missing InSb atomic row, called the missing-row model, which has also been reported for other Bi/III-V semiconductor surfaces [4,11]. The structure results in a significant surface corrugation and in the (1 × 2) surface

reconstruction. Note that only the topmost Bi atoms contribute to the filled-state STM image and that the image resolution is not sufficient to resolve individual atoms within each pair of Bi chains. Interestingly, in each pair of chains, the Bi atoms are bonded equally to both In and Sb surface atoms, while for each chain, the Bi atoms bond either fully to In or fully to Sb atoms.

The corresponding calculated band dispersion along the Γ -X symmetry direction with spin-orbit coupling considered is shown in Fig. 2(d), and the bands at the Γ -point are highlighted in Fig. 2(e). The dispersion shows Rashba splitting, and the calculated Rashba parameter amounts to $\alpha_R = 3.33$ eV Å. It is smaller than the experimental value obtained from the ARPES results shown in Fig. 1(b), but it is still in the range of giant Rashba splitting. We further simulated the contribution from different elements to the surface band dispersion. Interestingly, the main contribution to the bands at the Γ -point, where giant Rashba splitting is observed, comes from In and Sb atoms rather than Bi, as shown in Fig. S3(a)–S3(c) of the Supplemental Material [33]. Accordingly, the deposited Bi itself is not the only reason for electronic band splitting, which has been expected before [4,11]. For comparison, the electronic band corresponding to the surface structures without Bi but with the same surface corrugation is also calculated, shown in Fig. S3(e). Removing Bi not only removes the Bi atomic spin-orbit contribution, but

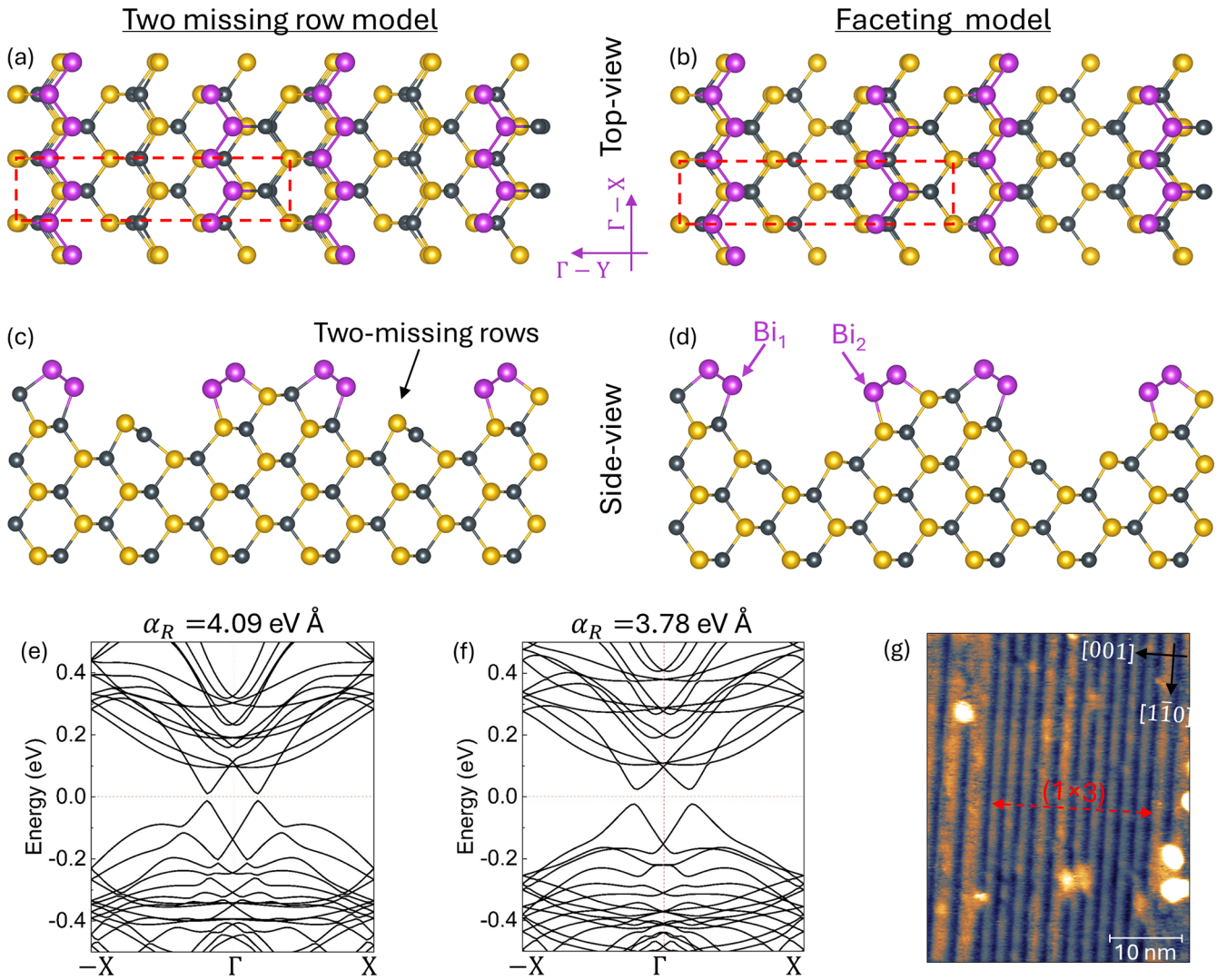


FIG. 3. Bi/InSb(110)-(1 × 3): DFT results for the Bi/InSb(110)-(1 × 3) surface. (a), (c), (e) refer to the two-missing-row model and (b), (d), (f) refer to the faceting model. (a), (b) Top-view and (c), (d) side-view models of the surface, resulting from DFT after energy relaxation. The black, yellow, and purple color spheres correspond to In, Sb, and Bi, respectively. The (1 × 3) surface unit cell is indicated in (a), (b) by a red rectangle. (e), (f) Band dispersion along Γ -X calculated for the structures shown in (a)–(d), including spin-orbit coupling. The corresponding Rashba parameters are indicated; (g) STM image of the Bi/InSb(110)-(1 × 3) surface taken at $V = -1.5$ V, $I = 160$ pA, the distance across atomic chains indicates Bi-induced (1 × 3) surface reconstruction.

also the Bi-In and Bi-Sb bonding and the associated surface electron-passivation effect. Consequently, the corrugated InSb surface without Bi shows multiple surface bands across the Fermi level, and a clean and isolated Rashba-split band cannot be unambiguously observed. Although the contribution of Bi to the Rashba-split bands is less significant, the presence of Bi is important. Bi adsorption stabilizes the reconstructed 1D chain geometry, and this reconstruction enhances the asymmetric surface potential gradient, especially the out-of-plane and transverse components, which are also responsible for the spin-dependent energy splitting [18]. Thus, the giant Rashba splitting in Bi/InSb is the interplay of spin-orbit coupling from Bi and an induced large in-plane potential gradient from the surface geometry along the $\langle 110 \rangle$ symmetry direction.

As mentioned above, the Bi-induced (1 × 3) reconstruction is unique to the InSb(110) surface, and the stable Bi surface arrangement has not been known yet. Thus,

several structural models are plausible for Bi/InSb(110)-(1 × 3) reconstruction. In the present work, we investigated two representative structures by DFT, namely the two-missing-row model and the faceting model. These models can be regarded as analogous to the missing-row model associated with (1 × 2) surface, and similar reconstruction motifs have previously been reported for (1 × 3)-type reconstruction on other heavy-metal surfaces, such as Pt(110) and Ir(110) [40]. The two simulated models are shown in Fig. 3, in both configurations, again a pair of Bi atomic zigzag chains is formed on top of the InSb(110) surface, but here resulting in a (1 × 3) surface reconstruction. It means that the density of Bi atoms on these surfaces is only 2/3 of that of the (1 × 2) surface, estimated simply by considering the number of Bi atoms per square unit area from the STM image in Figs. 2(c) and 3(g) [22]. Still, in each pair of chains, the Bi atoms are bonded equally to In and Sb atoms, as shown in Fig. 3. From the

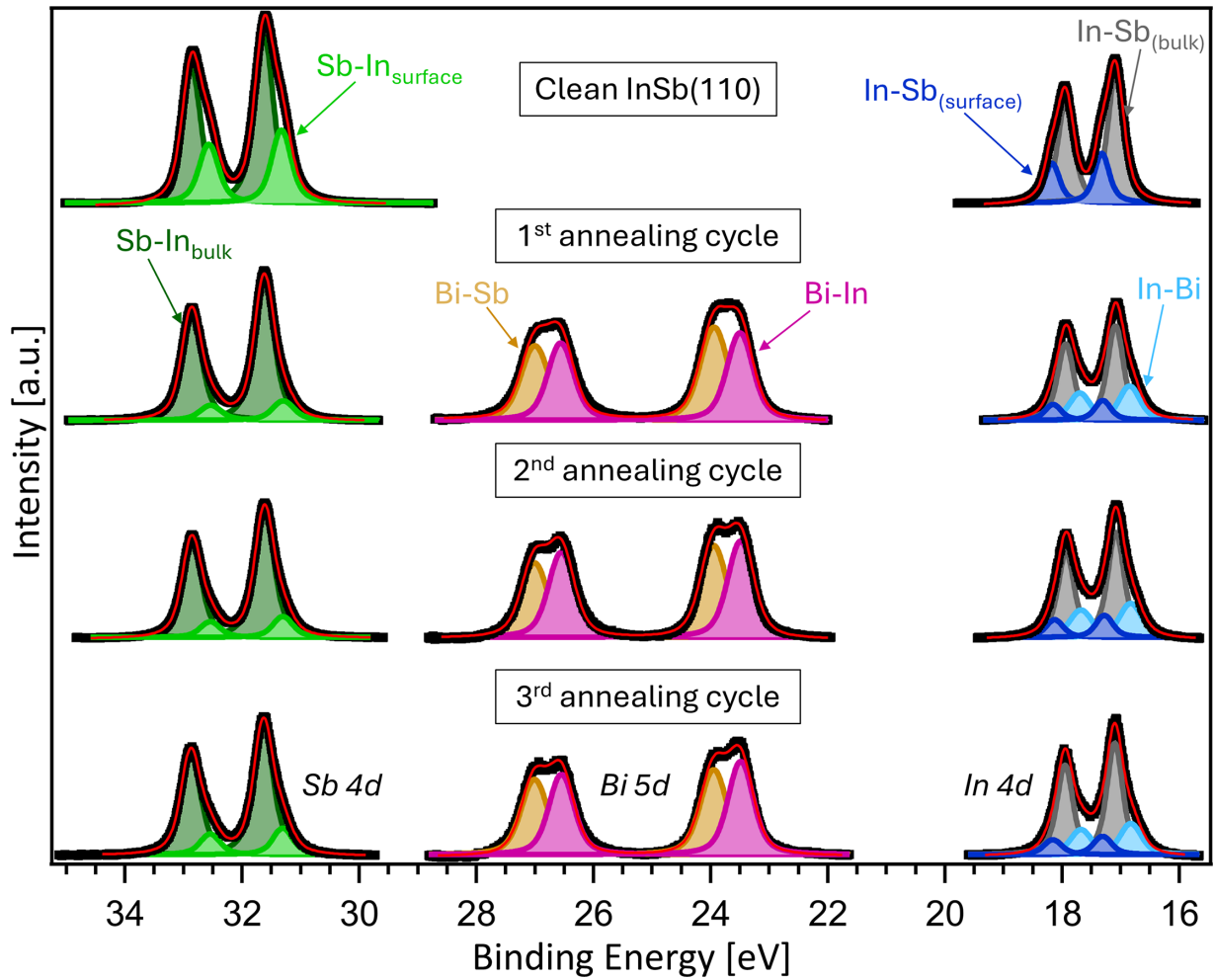


FIG. 4. Chemical characteristic of Bi/InSb(110): Comparison of Sb 4d, Bi 5d, and In 4d core level spectra after different sample treatment steps. The spectrum labeled “clean InSb(110)” corresponds to the freshly cleaved sample in UHV, followed by Bi deposition and subsequent sample annealing cycles. The In 4d and Sb 4d intensities are normalized to those of the spectra from the clean InSb(110). Photon energy was 130 eV for all spectra.

DFT results, we also calculated the chemical adsorption energies for the two configurations, and found that the faceting configuration is more stable, with chemical adsorption energy of -1.3 eV/Bi atom, compared with -1.24 eV/Bi atom for the two-missing-row configurations. The chemical adsorption energy was calculated by subtracting the energy of the pristine InSb(110) slab and the energy of pristine Bi chains from the total energy of the Bi/InSb heterostructure [41]. Giant Rashba splitting is obtained for both the possible surface configurations, with Rashba parameters of 3.78 eV Å and 4.09 eV Å. These values are closer to the experimentally obtained parameter of 4.2 eV Å for Bi/InSb(110)- (1×3) . Importantly, the calculated Rashba parameters for the two (1×3) surface structures are larger than those for the (1×2) surface, despite the lower Bi density. This further confirms that the interaction between Bi atoms and the InSb surface corrugation is more important for giant Rashba splitting than just the amount of Bi atoms.

We investigated the Bi-substrate interaction using synchrotron-based core-level XPS to study the chemical state and bonding of Bi, In, and Sb under various sample annealing conditions. Figure 4 shows the comparison and

deconvolution of In 4d, Sb 4d, and Bi 5d core-level spectra after different sample treatment steps. The fitting parameters are shown in Table S1, and the obtained binding energies in Table S2 of the Supplemental Material [33]. From the clean InSb surface, we obtain two doublets for both the In 4d and Sb 4d core-levels, which can be attributed to dominating bulk peaks (i.e., In-Sb and Sb-In, respectively) and surface components. The latter ones are found at higher BE than the bulk peak in In 4d and at lower BE in Sb 4d, in agreement with the literature [42]. These surface components decrease when Bi is deposited, but the bulk peaks remain almost the same. In the case of In 4d, one more component at low BE is required to fit the spectrum for Bi/InSb(110) samples. We assign this component to In-Bi bonding [43], which is further explained later.

For the Bi 5d spectrum, two prominent doublets can be observed. Based on reported work, the high BE component is assigned to Bi-Sb bonding [42], while analyzing the low BE component is not so straightforward because the Bi-Bi and Bi-III components (for different group-III elements) have been reported to overlap in BE [43]. To investigate the origin of the low-BE Bi component, systematic steps of sample annealing

were employed to desorb excessive Bi. Thus, a decrease in the Bi-Bi component compared to Bi-Sb is expected. On the contrary, a slight increase in the low BE component of the Bi 5*d* core level is observed from the second annealing cycle. Simultaneously, an increase in low BE shoulder to the In 4*d* core level peak is observed, reported as In-Bi bonding [43]. The last annealing cycle temperature was $>300^\circ\text{C}$, high enough to initiate desorption of metallic Bi (Bi-Bi component); thus, the increase in the lower BE component of Bi 5*d* core level is associated with stable Bi-In bonding. The almost equal amount of Bi-Sb and Bi-In peak area indicates equal bonding of the atomic chain to the Sb and In from underneath the substrate. The DFT calculations further confirmed the equal Bi-Sb and Bi-In bonding with the underneath surface, as shown in Figs. 2(a)–2(b) and 3(a)–3(d). On the other hand, the Sb 4*d* peak does not show a significant change in the peak shape, which has been reported before because of overlapping Sb-In/Sb-Bi peaks [3,42].

Here, we highlight the high-temperature stability of In-Bi bonds and the role of a non-polar substrate for Bi bonding to group III elements. III-Bi has been predicted as a Dirac-Weyl semimetal with electronic band inversion [44,45]. However, bulk growth of III-Bi has not been realized yet, and even the growth of III-Bi on a periodic surface using conventional techniques has been challenging [26]. Bi deposition on nonpolar substrates such as InSb(110) can thus provide a template for periodic InBi growth.

IV. CONCLUSIONS

In conclusion, we have combined experimental techniques and *ab initio* simulations to establish Bi-induced (1×2) and (1×3) surface structures, which host a tunable giant Rashba spin splitting along one-dimensional atomic chains. The giant Rashba parameter along the chains, exceeding $3\text{ eV \AA}$, varies with surface reconstructions. It was found that the Rashba splitting is the interplay between Bi adsorption and the corrugation of surface atoms. Density functional theory further showed that, while spin-orbit coupling from Bi is essential, the significant contribution of spin splitting arises from the InSb

substrate. The formation of stable Bi-In and Bi-Sb bonds also highlights the potential of this system for controlled growth of InBi compounds. These findings identify Bi/InSb(110) as a versatile platform for spintronics and next-generation quantum materials.

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The authors declare no conflict of interest.

DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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