Structure and binding of stanene on the Al\(_2\)O\(_3\)(0001) surface

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Stanene, the two-dimensional monolayer form of tin, has been predicted to be a 2D topological insulator due to its large spin–orbit interaction. However, a clear experimental demonstration of stanene’s topological properties has eluded observation, in part because of the difficulty of choosing a substrate on which stanene will remain topologically nontrivial. In this paper, we present first-principles density functional theory (DFT) calculations of epitaxial monolayer stanene grown on the (0001) surface of alumina, Al\(_2\)O\(_3\). We perform a detailed analysis of the binding energy and electronic structure of stanene on Al\(_2\)O\(_3\), and demonstrate that it is a quantum spin Hall insulator. In addition, we discuss the relevance of decorated stanene and dumbbell stanene on the alumina surface.

I. INTRODUCTION

Two-dimensional topological insulators (2DTIs) have received attention in recent years due to their potential for hosting robust symmetry-protected current-carrying edge states \([1]\). The buckled hexagonal monolayer form of tin, known as stanene, is of particular interest \([2,3]\) since its band gap (\(\sim 0.1\) eV) is large enough for room-temperature applications \([4,5]\). Stanene’s band gap can be further enhanced by functionalization, in particular with halogen atoms. Proposed uses of stanene include spintronic nanoribbon devices \([6,7]\); tunable field-effect transistors \([8]\); a surface for adsorption of molecules including CH\(_2\)O, CH\(_4\), CO, NO, N\(_2\)O, and NH\(_3\) \([9,10]\); and room-temperature demonstration of the quantum spin Hall effect \([5,11]\) and quantum anomalous Hall effect \([12,13]\).

However, the electronic structure of epitaxial stanene is sensitive to both strain and surface interactions, so choosing an appropriate substrate is vital \([14]\). Stanene is metallic on many substrates, including Ag(111) \([15,16]\), Au(111) \([17,18]\), Sb(111) \([19]\), and Bi\(_2\)Te\(_3\)(111) \([20,21]\). Ultraflat stanene grown on Cu(111) shows evidence of nontrivial edge states but is metallic overall \([22]\), while buckled stanene on PbTe(111) is gapped but is topologically trivial due to in-plane compressive strain \([23]\). InSb(111) is a promising substrate for globally gapped topological stanene, though reported results remain somewhat inconclusive \([24,25]\). A fuller suite of potential stanene substrates is important to enable robust continued work.

Alumina (Al\(_2\)O\(_3\)) is a wide-gap insulator whose growth is well-characterized and commonly performed. Cleaved along its (0001) surface, alumina has a surface lattice parameter within a few percent of the free-standing stanene lattice parameter. Previous work has examined one possible structure for stanene on Al\(_2\)O\(_3\) and elucidated basic aspects of the resulting electronic bands \([27,28]\). In this paper, we describe several critical results regarding the structure, stability, and topological character of stanene on alumina: hexagonal stanene (the assumed structure in the prior works) is indeed stabilized on stanene compared to other structures that are favored as isolated 2D sheets, the strength of the binding of stanene to the alumina surface turns out to be surprisingly large, the binding is strong enough to create an epitaxial 2D layer of stanene on alumina, and the resulting electronic bands of the heterostructure show a large gap as well as the desired topological character of a quantum spin Hall insulator. We end with an outlook for the potential of stanene synthesis on alumina.

![Image](317x208 to 562x374)

**FIG. 1.** a,d: Top (a) and side (d) views of the bare Al\(_2\)O\(_3\)(0001) slab used as a substrate. The three inequivalent exposed Al atoms are labeled A, B, and C. The blue arrow in (a) indicates the viewing direction of panels d–f. b,e: Top (b) and side (e) views of second-most-stable registry choice A/B for stanene on Al\(_2\)O\(_3\), placing the upper and lower Sn atoms in positions A and B, respectively. Black arrows in e label the bond length \(d\), the buckling \(b\), and the vertical binding distances \(h_1\) and \(h_2\), whose values are found in Table I. c,f: Top (c) and side (f) views of the most stable registry choice A/C for stanene on Al\(_2\)O\(_3\), placing the upper and lower Sn atoms in positions A and C, respectively.

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TABLE I. Structural data for free-standing stanene in its bare, hydrogenated, and fluorinated forms.

|                        | Bare stanene | Hydrogenated stanene | Fluorinated stanene |
|------------------------|--------------|-----------------------|---------------------|
| Lattice parameter a (Å)| 4.68         | 4.72                  | 5.02                |
| Sn–Sn buckling b (Å)   | 0.85         | 0.82                  | 0.53                |
| Sn–Sn bond length d (Å)| 2.83         | 2.85                  | 2.95                |
| Band gap (eV)          | 0.069        | 0.214                 | 0.306               |
| Topological insulator? | YES          | NO                    | YES                 |

TABLE II. Structural and energetic information for the two most favorable registries of stanene on Al₂O₃.

|                  | A/B structure | A/C structure |
|------------------|---------------|---------------|
| Buckling b (Å)   | 1.03          | 1.18          |
| Bond length d (Å)| 2.95          | 3.01          |
| Binding distance h₁ (Å)| 3.06 | 2.90 |
| Binding distance h₂ (Å)| 3.43 | 3.47 |
| Binding energy E₅ per unit cell, no Grimme (eV) | 0.31 | 0.50 |
| Binding energy E₅ per unit cell, with Grimme (eV) | 1.02 | 1.26 |
| Band gap (eV)   | 0.247         | 0.263         |

II. METHODS

Density functional theory (DFT) calculations were performed using the Quantum ESPRESSO software package [29]. Fully relativistic projector augmented-wave (PAW) pseudopotentials with spin–orbit interaction were used, along with the Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation to the exchange-correlation functional [30]. A plane-wave basis set with a wave-function energy cutoff of 680 eV and a charge density plane wave cutoff of 6,800 eV was used, and atomic relaxations were performed until all axial forces were below $2.5 \times 10^{-3}$ eV/Å. Calculations were performed at the theoretical relaxed lattice parameters of bulk alumina; however, since Quantum ESPRESSO cannot perform automated variable-cell relaxations with fully relativistic pseudopotentials, those lattice parameters were found by atomically relaxing bulk structures on a grid of lattice parameter values and fitting to find the minimum in energy. We estimate that this is equivalent to performing an automated variable-cell relaxation until all uniaxial stresses are below 5 kbar. Calculations used a $12 \times 12 \times 1$ $k$-point mesh and 14 meV of Gaussian thermal broadening.

Substrate-based calculations were carried out on an Al-terminated slab of Al₂O₃ cleaved along the (0001) surface. In-plane lattice parameters were taken from a theoretical relaxation of bulk Al₂O₃, which yielded a lattice parameter of 4.792 Å. Four stoichiometric layers of the Al₂O₃ slab were included to ensure convergence in atomic positions and formation energies. Monolayers of stanene were placed on both surfaces of a symmetric slab to retain inversion symmetry and avoid the need for a dipole correction in the vacuum. The Grimme DFT-D2 van der Waals correction was used to account for noncovalent interaction between the substrate and the stanene overlayer [31].

For isolated 2D tin-based monolayers, topological characters were computed from occupied band parities at time-reversal invariant momenta using the method of Fu and Kane [32].

III. RESULTS

A. Free-standing stanene monolayers

We performed variable-cell structural relaxations for free-standing monolayers of bare stanene, as well as fully functionalized fluorinated stanene (SnF) and hydrogenated stanene (SnH). In each calculation, both the lattice parameter and the atomic positions were relaxed to minimize stresses and forces. Each structure is “low-buckled,” with a unit cell containing two vertically-displaced Sn atoms. The optimal structural parameters and DFT band gap, shown in Table I, are in good agreement with previous results [5]. According to the Fu–Kane method of determining topological character using band parities at time-reversal invariant momenta [32], bare and fluorinated stanene are topological insulators, while hydrogenated stanene is a normal insulator. The topological properties of each of these freestanding materials are examined in greater detail in Section III.D below.

B. Stanene structures on Al₂O₃(0001)

For our substrate-bound calculations, we focused on undecorated stanene. When bound epitaxially to alumina, low-buckled stanene retains its basic structure but is under ~2.4% tensile strain. We found that the most stable structures are obtained when Sn atoms are placed atop Al atoms.
FIG. 2. a,c: Side view of free-standing stanene layer and stanene bound to the Al$_2$O$_3$(0001) slab, respectively. b: Side view of bare alumina slab. The yellow features are an isosurface of the local density of states (LDOS) integrated from the Fermi level ($E_F$) to 1.0 eV above $E_F$. d,e,f: Density of states (DOS) plots for free-standing stanene, bare alumina, and bound stanene on alumina, respectively. In the plot for the full system, the DOS is also projected onto the Löwdin orbitals of the tin atoms and the aluminum/oxygen atoms.

The Al-terminated alumina slab has three exposed aluminum atoms per unit cell, which are labeled A, B, and C in Figure 1(a). Atom A terminates the slab, while atoms B and C are roughly coplanar (∼0.2 Å vertical separation) and located under a layer of oxygen atoms. We examined a 3 × 3 grid of possibly registry alignments for stanene within the alumina unit cell, each of which permits two structures that are obtained by swapping the up-buckled and down-buckled Sn atoms. For each of these 18 inequivalent stanene-on-alumina registries, we relaxed each atom in the $z$-direction. The two most favorable registries, shown in Figures 1(b) and 1(c), place the upper tin atom directly over atom A and the lower tin atom directly over either atom B or C. The structural parameters, binding energies, and band gaps of each structure are found in Table II. The A/C structure is the most energetically favored by a margin of 0.24 eV per two-atom stanene unit cell. This structure, which was predicted by similar previous work [27, 28], will be taken as the ground state structure.

Since stanene must be placed under 2.4% tensile strain to bind epitaxially to the Al$_2$O$_3$(0001) surface, we checked for the possibility of incommensurate rather than epitaxial binding. In a case of incommensurate binding at the free-standing lattice parameter, the Sn monolayer will be unstrained, but most of the monolayer’s area will not attain its preferred registry with respect to the alumina substrate. Therefore, the competition between epitaxial and incommensurate binding depends on a comparison of the strain energy of the stanene monolayer to the energy penalty for placing the monolayer on a non-optimal registry.

The energy to strain a free-standing stanene monolayer from its equilibrium lattice parameter of $a = 4.68$ Å to the relaxed Al$_2$O$_3$ lattice parameter of $a = 4.792$ Å is 25 meV per unit cell. For low strain, an incommensurate overlayer on a substrate can be treated as a long-wavelength superlattice, with each unit cell of the superlattice sampling a different registry. If we label the in-plane position of the lower Sn atom (Sn atoms B or C in Figure 1) by $x = u_1a_1 + u_2a_2$, then the average energy of a single unit cell in such an incommensurate overlayer is approximately

$$E_{\text{incomm}} = \int_{-1}^{1} \int_{-1}^{1} E(u_1a_1 + u_2a_2) \, du_1 \, du_2,$$

where $E(x)$ is the energy of a single commensurate unit cell with a lower Sn atom placed at $x$. We estimate this integral using the registry calculations performed earlier, considering only the 3 × 3 grid of structures that are lateral shifts of the optimal A/C structure. The incommensurate structure is estimated to be 463 meV per unit cell higher in energy than the optimal registry; this value represents the energy penalty of incommensurate binding. Since this is an order of magnitude greater than the strain energy, the incommensurate structure is irrelevant and that stanene will bind epitaxially on the alumina substrate.

C. Alternative stanene structures

We considered the “dumbbell” stanene structure proposed by Tang et al., which contains 10 Sn atoms in a multilayered analogue of a 2 × 2 stanene supercell [33]. In an isolated monolayer, out-of-plane $sp^3$ hybridization renders dumbbell stanene lower in energy than low-buckled stanene by 0.18 eV per Sn atom [33]. However, we find that dumbbell stanene binds only weakly to Al$_2$O$_3$, collapsing into a disorderly structure that is 0.46 eV per Sn atom higher in energy than the bound low-buckled configuration. This occurs because the highly
buckled dumbbell structure prevents a close wetting interaction between Sn atoms and the substrate. Therefore, dumbbell stanene is not predicted to be a relevant phase when considering epitaxial stanene on alumina.

D. Binding energy analysis

The binding energy $E_b$ equals the total energy of the bound stanene-substrate complex $E_{\text{bound}}$, minus the sum of the energies of the free-standing stanene layer $E_{\text{stanene}}$ and the bare alumina slab $E_{\text{Al}_2\text{O}_3}$:

$$E_b = E_{\text{bound}} - (E_{\text{stanene}} + E_{\text{Al}_2\text{O}_3}). \quad (2)$$

We calculated this value both with and without the van der Waals Grimme DFT-D2 functional [31] to assess the importance of noncovalent interactions in the binding. We found that including the Grimme functional modifies the interatomic distances listed in Table 1 by less than 0.5%, indicating that the physical structure is determined largely by chemical rather than van der Waals interactions. However, the binding energy increased dramatically from 0.50 eV per stanene unit cell without Grimme to 1.26 eV per unit cell with Grimme, suggesting that both noncovalent and covalent interactions are needed to fully describe the absolute magnitude of the binding energy of stanene to alumina.

The fact that the chemical binding is quite substantial at 0.50 eV/unit cell requires some explanation: naively, one might expect a wide-gap material such as alumina to be relatively inert. To identify the chemical interaction that drives the binding, we plotted the density of states (DOS) of the free-standing stanene layer, the bare alumina slab, and the stanene-substrate complex (Figures 2(d-f)). The bare alumina slab displays a peak in the DOS just above the Fermi level, which represents a surface state localized to “dangling” orbitals on the top layer of exposed Al atoms (left panel of Figure 2(b)). This state vanishes upon the binding of stanene—as can be seen from Figure 2(f), the states of the full complex near the Fermi level are dominated by Sn orbitals. The unoccupied alumina orbital hybridizes with various Sn orbitals, spreading out in energy over the former alumina gap. In particular, a portion of this orbital forms a new bonding orbital between $-2$ and 0 eV in Figure 2(f).

We confirmed that the originally empty “dangling” states of the alumina slab remain localized to the vicinity of the exposed Al atom by examining the redistribution of electron density shown in Figure 3. During binding, electron density redistributes from the cyan regions to the yellow regions, including a large $\sigma$-like region between the surface Al atom and the Sn atom above it. This indicates that the formerly-vacant Al orbital becomes filled as it moves lower in energy and hybridizes with nearby Sn orbitals: a heteropolar covalent bond has formed, explaining the substantial binding energy of 0.50 eV even without van der Waals interactions.

E. Free-standing and bound band structure

Next, we performed a thorough investigation of the band structure and topological index of free-standing stanene. Figure 3(a) shows the evolution of the band gaps of free-standing bare stanene, fluorinated stanene, and hydrogenated stanene as a function of lattice parameter, highlighting regimes in which the material is a topological insulator, a topological material with negative gap, and a normal metal. For metallic materials, examination of the band structures shows they have a “negative gap” (the conduction band minimum drops below the valence band maximum compared to nearby insulating structures), and for them we compute the topological index that we would obtain if the valence and conduction bands were pulled apart far enough to create a global gap without further modification of the electronic structure. This hypothesis allows for a prediction of topological behavior on substrates without performing expensive calculations in large unit cells: if the primary effect of the substrate is to introduce a gap without modifying the character of the electronic bands, then a metallic material can become topological if its occupied bands have the proper parities.

The four band structure plots in Figure 3(b-e) illustrate how the bands of isolated stanene evolve under strain. For large compressive strain (Figure 3(b)), the valence band at $\Gamma$ sits well above the Dirac cone at K, resulting in a (negative gap) metal. As the lattice parameter increases (Figure 3(c)), the gaps at $\Gamma$ and K line up, forming a globally gapped topological insulator. For small tensile strain (Figure 3(d)), the gap at $\Gamma$ is pushed below the Dirac cone at K: this is the regime of strain in which stanene on Al$_2$O$_3$ lies, so the substrate is necessary to open the global band gap (we will see that is also sufficient below). Finally, for tensile strain somewhat larger than that applied by Al$_2$O$_3$ (Figure 3(e)), the gap closes between the negative-parity $s$-type conduction band at
FIG. 4. a: Evolution of the band gap of bare stanene (blue), fluorinated stanene SnF (orange), and hydrogenated stanene SnH (yellow) as a function of lattice parameter. The computed lattice parameter of Al$_2$O$_3$ is indicated with a vertical black line. Positive values on the y-axis indicate the size of a global band gap, while negative values are the signed difference between the valence band maximum and the conduction band minimum for semimetallic materials. For each structure, a dashed line indicates a trivial topological index of $Z_2 = 0$, while a solid line indicates a topological material with $Z_2 = 1$. In the negative gap regime, the material will become a topological insulator if its conduction and valence bands are pulled apart rigidly in energy to create a global gap. b, c, d, e: Band structures of bare stanene at selected lattice parameters. Bands are colored by their s-orbital (red) and p-orbital (blue) characters. The zero of band energy is the Fermi level $E_F$.

FIG. 5. Band structure plots showing the change of topological character via band inversions in fluorinated stanene SnF (top row) and hydrogenated stanene SnH (bottom row). The zero of band energy is the Fermi level $E_F$. In each case, the negative-parity s-band crosses down from the conduction band into the valence band as the lattice parameter increases. Due to their different equilibrium lattice parameters, free-standing SnF ($a = 5.02\,\text{Å}$) is a topological insulator, while SnH ($a = 4.72\,\text{Å}$) is a trivial insulator, but either material can be tuned to the other regime under strain. Figure 4(a) also illustrates the onset of topological behavior for decorated, free-standing SnF and SnH. At their equilibrium lattice parameters, SnF is a topological insulator while SnH is a trivial insulator. However, the two materials are actually quite similar electronically: both materials are trivial insulators under sufficient compressive strain and topological insulators under sufficient tensile strain. The difference between them at equilibrium is simply due to the relative ordering of the lattice parameter of the topological transition and the equilibrium lattice parameter. This fact is illustrated in Figure 5 in which band structures of SnF and SnH near their respective phase transitions are juxtaposed. In each case, a negative parity antibonding band constructed from Sn s orbitals moves down through the conduction band, and crosses over to the valence band at $\Gamma$, inducing a band

\[ \Gamma \]
FIG. 6. Band structure plot for epitaxial stanene on alumina. Bands are colored by their Sn $s$-orbital (red) and Sn $p$-orbital (blue) characters. The DFT band gap is calculated to be 0.263 eV.

inversion and leading to a nontrivial topological index.

Figure 6 shows the band structure of the full stanene-on-alumina system. It differs from the bare-stanene band structure (Figure 4(d)) in several important ways. First, the presence of the substrate breaks inversion symmetry, which, when combined with the spin–orbit interaction, leads to a Rashba splitting of the conduction band away from the Γ point. By comparing the band structures for alumina slabs of different thickness, we confirmed that the $k$-dependent splitting of other bands away from the Γ point is also due to inversion symmetry breaking (rather than evanescent coupling between the two surfaces of the alumina slab).

Finally, the Dirac cone at K has vanished due to the partial saturation of the stanene $p_z$ orbitals by the alumina surface, and the ordering of $s$-type and $p$-type orbitals at Γ has become inverted. These latter features also appear in the band structure of topological SnF, and are necessary for the existence of topological behavior in stanene on a substrate [5]. Hence, low-buckled hexagonal stanene on alumina has every indication of being topological.

IV. DISCUSSION AND OUTLOOK

The combination of strong epitaxial binding with band inversion at Γ and $p_z$-orbital saturation at K indicates that alumina is a promising substrate for the synthesis of bare monolayer stanene. Such a material offers an opportunity for experimental observation of the quantum spin Hall effect [3] [11] as well as a substrate for a variety of technological applications [6] [10]. In addition, the spin separation in the conduction band due to the Rashba splitting can be harnessed for applications in spintronics and topological superconductivity [34].

Controlled functionalization, e.g., by hydrogen or fluorine, is also an important avenue of stanene research, since functionalization both enhances the band gap and protects against unwanted environmental interactions with Sn $p_z$ orbitals [5]. Generally speaking, two-dimensional materials can be synthesized either by epitaxial deposition or by the exfoliation of multilayered van der Waals materials [1]. The latter method is attractive since it is flexible and modular, but is impractical for materials like bare stanene whose 3D bulk phase (α-tin) is not intrinsically layered. However, the epitaxial growth of stanene on alumina should kinetically trap the tin atoms in the 2D hexagonal stanene structure, perhaps making it possible to functionalize the monolayer in situ. The functionalized sheet, now weakly bound to the alumina, could be exfoliated for use in heterostructure and device applications.

In summary, we have shown that monolayer stanene binds strongly and epitaxially to the Al$_2$O$_3$(0001) surface, with a buckled structure and a sizable global band gap. We have examined the chemical character of the binding and presented evidence for the topological nature of stanene on alumina. With its wide surface band gap and relative inertness, alumina is a promising substrate for future experimental fabrication and characterization.

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