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The quasi-two-dimensional electronic gas at the (111) SrTiO₃-based heterostructure interfaces is described by a multiband tight-binding model providing electronic bands in agreement at low energies with photoemission experiments. We analyze both the roles of the spin-orbit coupling and of the trigonal crystal-field effects. We point out the presence of a regime with sizable strain where the band structure exhibits a Dirac cone whose features are consistent with *ab initio* approaches. The combined effect of spin-orbit coupling and trigonal strain gives rise to nontrivial spin and orbital angular momenta patterns in the Brillouin zone and to quantum spin Hall effect by opening a gap at the Dirac cone. The system can switch from a conducting to a topological insulating state via modification of trigonal strain within a parameter range which is estimated to be experimentally achievable.

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I. INTRODUCTION

The discovery [1] of a quasi-two-dimensional electronic gas (q2DEG) formed at the (001) interface between the SrTiO₃ (STO) and LaAlO₃ (LAO) grown on it gave rise to a very rich research field. For example, the q2DEGs formed in these oxide heterostructures are characterized by the simultaneous presence of strong spin-orbit coupling (SOC) [2] and superconductivity [3]. Both these phenomena are tunable by electric field effect [2–4]. Superconductivity can coexist with 2D magnetism [5,6] in q2DEGs with suitable atomic engineering of LAO/STO interfaces [7]. Furthermore, q2DEGs in (001) LAO/STO interfaces have been theoretically proposed to show topological properties in normal [8] and superconducting phases of 2D [9–12] and quasi-1D models [13–17]. It is therefore not surprising that oxides heterostructures, in particular, LAO/STO interfaces, have been proposed for the realization of low-dimensional devices in the field of spintronics and quantum information [18–22].

A general property of heterostructures, among which is LAO/STO, is the possibility of controlling strain at the interfaces by realizing superlattices or using micromembranes

[23–25]. The presence of strain allows the manifestation of phenomena absent in the bulk structure [26–29]. Moreover, these phenomena can be tuned by manipulating the strain itself. In particular, the possibility of a strain-tuned topological phase transition has been theoretically predicted [30] and experimentally realized [31].

After the discovery of the presence of q2DEGs on interfaces with different crystallographic cut directions [32], attention was extended to the (111) LAO/STO interface, in which even more exotic phenomena have been predicted [33]. Recently, anisotropic magnetoresistance both in normal [34] and superconducting states [35,36] has been observed, suggesting the unconventional nature of a superconductivity host by the (111) LAO/STO interface. Further, recent studies [37] have discovered a striking similarity between this interface and graphene due to the presence of a Dirac point in the band structure. This similarity arises by virtue of the similar honeycomb lattice structure formed at the interface when STO is Ti terminated.

The analogy between graphene and q2DEG in the (111) interface suggests the possibility of nontrivial topological effects [38]. In fact, since Haldane's seminal discovery [39], it has been known that q2DEG on honeycomb lattices in an insulating state can manifest quantum Hall effect (QHE) in the absence of magnetic field. The subsequent discovery of the quantum spin Hall effect (QSHE) by Kane and Mele [40,41] showed that topologically protected edge states can appear in graphene even in the presence of time-reversal invariance when SOC is included. This suggested that topological insulators (TIs) can be achieved in materials with strong SOC [42–44]: this was later experimentally confirmed [45–47]. Further studies highlighted the presence of TI in 3D bulk [48] and their nanostructures [49,50].

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Finally, Xiao *et al.* [51] proposed the use of transition metal oxide (TMO)-based heterostructures, in particular, perovskites, in the (111) direction for realizing TIs. This possibility is offered by the presence of strong atomic SOC typical of the TMOs and the peculiar geometry of (111) perovskites. The authors used tight binding (TB) methodologies to show the presence of a QSHE in different materials. This methodology has been widely used to theoretically compute the electronic band structure for LAO/STO (111) [33,52,53].

In this paper, we specifically analyze the properties of the (111) STO interface electronic structure using an effective TB model, focusing on the LAO/STO one. Compared to previous works which adopted TB methodologies, we emphasize the role of the strain at the interface and the atomic SOC in the band-structure properties. Such an approach is useful to have a physical understanding of the mechanisms giving rise to the peculiar features of the system. We perform a comparison with the experimental data available on the (111) interface. In particular, we fix the hopping parameters from angle-resolved photoemission spectroscopy (ARPES) experiments on the bare (111) STO surface. We identify the region of the parameter space in which the Dirac point emerges within the electronic band structure; we find that this happens when a relevant term in the TB treatment is the strain. As already mentioned, the presence of a Dirac point in the electronic band structure of the (111) LAO/STO interface was already predicted in Ref. [37], where density functional theory (DFT) was adopted. The use of TB methodology allows an effective modeling of the band structure near the Dirac point, also including the effects of the SOC with a small computational effort, opening up the way to study the transport properties and the topological invariants of this interface that can be very demanding for first-principles approaches.

We verify the concrete possibility of the regime with sizable strain, studying the relation between the energy parameter in the TB model and the geometry of the physical structure. Furthermore, we include an analysis of the SOC role in the properties of the energy spectra. We also investigate the presence of spin and orbital angular momentum patterns in the Brillouin zone (BZ). In the last part of the paper, we perform a systematic scan of the parameter space to identify the region in which the system exhibits a QSHE. We verify the bulk-boundary correspondence by explicitly showing the presence of edge states on finite-thick zigzag ribbons. Our results suggest the possibility of a strain-induced topological transition for the system.

This paper is organized as follows: In Sec. II, the model Hamiltonian for the STO 2D bilayer is introduced, discussing every contribution we take into account. The methods used to estimate the hopping parameters are also presented. In Sec. III, the properties of the energy spectra are explored, emphasizing the role of the trigonal strain; we also discuss the physical range in which the strain is expected to vary. Furthermore, the presence of spin and angular momentum patterns in the BZ is shown. In Sec. IV, the topological properties of the system are discussed together with the methods used to determine the topological invariant Z_2 . In Sec. V, we report our conclusions.

FIG. 1. (a) Schematic representation of Ti atoms in STO lattice. The red and blue dots represent two different nonequivalent atoms belonging to the two different planes depicted in the figure. (b) Projection on the (111) plane of the Ti atoms with $\tilde{a} = a_0\sqrt{2/3}$; $\vec{R}_1$ and $\vec{R}_2$ identify our choice of the primitive vectors of the lattice.

II. MODEL AND METHODOLOGY

In this section, we discuss the electronic band structure of the q2DEG using a minimal TB approach. This methodology allows us to encode the physical properties of the crystal in a small number of energy parameters to understand their role in the band-structure formation.

The projection of two different Ti atom layers along the (111) direction of the STO results in a honeycomb structure similar to the graphene one, with a lattice constant of $\tilde{a} = 0.3905\sqrt{2/3}$ nm as shown in Fig. 1. The conduction band is obtained by the superposition of the 3d orbitals of Ti atoms of the STO. Due to the approximate cubic geometry, these orbitals split up into a triplet $t_{2g} = \{d_{yz}, d_{zx}, d_{xy}\}$ and a doublet $e_g = \{d_{z^2}, d_{x^2-y^2}\}$ of orbitals as described in Ref. [54]. The t_{2g} orbitals are responsible for the formation of the lower conduction band, so in the following we will only consider them in the description of the energy structure. We consider the two-dimensional structure originating from the projection on a single plane of only two layers of Ti, whose atoms are labeled using the symbols Ti_1 and Ti_2 . We denote by $d_{i\alpha\sigma,\vec{k}}$ the annihilation operator of the electron of 2D dimensionless quasimomenta $\vec{k} = \tilde{a}\vec{K}$, where $\vec{K}$ is the quasimomentum, occupying orbital $i = \{xy, yz, zx\}$ belonging to the layer $\alpha = \{Ti_1, Ti_2\}$ and of spin $\sigma = \pm 1/2$. With this notation, we studied the following Hamiltonian:

$$H = H_{TB} + H_{TRI} + H_{SOC} + H_v. \quad (1)$$

We will discuss the different contributions separately. We start from the TB Hamiltonian which in k -space takes the form

$$H_{TB} = \sum_{\vec{k}} \sum_{i,\alpha\beta,\sigma} t_i^{\alpha\beta}(\vec{k}) d_{i\alpha\sigma,\vec{k}}^\dagger d_{i\beta\sigma,\vec{k}}, \quad (2)$$

where $t_i^{\alpha\beta}(\vec{k})$, also considering the next-nearest-neighbor (NNN) hopping, contain three contributions:

(1) The first and most important contribution will be the head-on overlap of two lobes of the same kind of orbitals for nearest neighbors. This happens between a Ti_1 and a Ti_2 , so this term will describe an interlayer hopping. The amplitude for this hopping will be denoted by t_3 ;

(2) The second contribution will come from the lateral overlap of two lobes of two orbitals of the same type between Ti_1 and Ti_2 . The amplitude of this interlayer term is denoted by t_2 ;

(3) The third and smallest term will be a NNN intralayer hopping caused by the head-on overlap between two orbitals of two Ti's on the same layer. The amplitude of this term will be denoted as t_1 . From best fit calculations, this term will be neglected, as we can show in the following.

The matrix representation of the Hamiltonian Eq. (2) is given in Appendix A [Eq. (A1)]. The values of the hopping parameters have been fixed by comparison with ARPES experiments [55] to the values $t_3 = 0.5$, $t_2 = 0.04$, $t_1 = 0$ eV, obtained as best fit parameters of a maximum likelihood analysis, which is detailed in Appendix A.

H_{TRI} takes into account the possibility of having strain at the interface along the (111) direction. The physical origin of this strain is the possible contraction or dilatation of the crystalline planes along the (111) direction. The strain at the interface can be manipulated via deposition of other crystals, such as LAO. This coupling is taken into account by the following contribution, whose form is fixed by symmetry considerations [56]:

$$H_{TRI} = \frac{\Delta}{2} \sum_{\vec{k}} \sum_{i \neq j, \alpha, \sigma} d_{i\alpha\sigma, \vec{k}}^\dagger d_{j\alpha\sigma, \vec{k}}. \quad (3)$$

In the following, we will refer to this term as the trigonal crystal field. More details about this term will be given in the next section. We initially point out that the sign of Δ determines the kind of the applied strain along the (111) direction: if $\Delta < 0$, a contraction of the Ti atom planes occurs, while for $\Delta > 0$ a dilatation occurs.

Another contribution taken into account is the atomic SOC, which is represented in k -space by

$$H_{SO} = \frac{\lambda}{2} \sum_{\vec{k}} \sum_{ijk, \alpha, \sigma \sigma'} i \varepsilon_{ijk} d_{i\alpha\sigma, \vec{k}}^\dagger \sigma_{\sigma\sigma'}^k d_{j\alpha\sigma', \vec{k}}, \quad (4)$$

where ε is the Levi-Civita tensor and σ^k are the Pauli matrices. Finally, we include a possible interaction with an external electric field orthogonal to the planes of the form

$$H_v = \frac{v}{2} \sum_{\vec{k}} \sum_{i, \alpha, \sigma} \xi_\alpha d_{i\alpha\sigma, \vec{k}}^\dagger d_{i\alpha\sigma, \vec{k}}, \quad (5)$$

where $\xi_{Ti_1} = +1$ and $\xi_{Ti_2} = -1$. This contribution will take into account the possibility of a small perturbation at the interface breaking the inversion symmetry between the two layers.

III. TRIGONAL CRYSTAL FIELD EFFECTS

The purpose of this section is to illustrate the role of the trigonal crystal field in determining the properties of system. We will show two extreme situations: a first one in which Δ is a small perturbation compared to the TB and a second one in which Δ is the dominant parameter. To exemplify the behavior of the system for small values of Δ , we choose a benchmark $\Delta = -0.005$ eV, equal to the trigonal coupling for the unstrained interface [57]. For this choice, the energy

FIG. 2. (a) Energy band structure and (b) density of states for $\Delta = -0.005$ eV, $\lambda = 0$ eV, and $v = 0$ eV. The energy $E = -0.46$ eV corresponding to the states at the K point is highlighted by a dashed line.

band structure and the density of states are shown in Fig. 2. At the K point of the BZ, one can notice an energy dispersion which is linear in lower bands: this could erroneously suggest that a Dirac cone is present within the energy bands. In Appendix B, we discuss a more complete characterization of the energy spectra near the K point, finding that the bands do not have the typical conical structure of the Dirac point in this region.

The band structure drastically changes when the parameter Δ is assumed to be larger, exhibiting a Dirac cone in the low energy region as shown in Fig. 3. In fact, when $|\Delta/t_3| \gtrsim 1$ there is a splitting of the energy levels (neglecting the spin degeneracy) in a pair of bands of lower energy and four bands of higher energy. In the limit of $|\Delta/t_3| \gg 1$, these bands asymptotically become the eigenstates of the trigonal Hamiltonian called, respectively, a_g and e_g^π [56], belonging to the corresponding symmetry group. The hopping contribution causes only a weak mixing between the two groups of states and gives rise to a Dirac cone at the K point in the BZ between the a_g states. Our results are in agreement with the results obtained using DFT methodologies in Ref. [37]. We can locally adopt a perturbative approach near the K point to obtain an effective Dirac Hamiltonian

$$H_{\text{eff}} = \hbar v_F \vec{\delta k} \cdot \vec{\sigma} \otimes \tau_z + \Delta_{SO} \sigma_z \otimes \tau_z + \text{const}, \quad (6)$$

from which we can extract the Fermi velocity of the electron at the Dirac point, which is $v_F = [\frac{1}{2}(t_2 + 2t_3)]/\hbar \approx 2.5 \times 10^5$ m s⁻¹, and Δ_{SO} is the effective coupling induced by the SOC. It depends on the parameters as $\Delta_{SO} \sim (\lambda t_3^2)/\Delta^2$, since it originates from the perturbation to third order in the TB and

FIG. 3. (a) Energy band structure and (b) density of states for $\Delta = -1$ eV, $\lambda = 0$ eV, and $v = 0$ eV. The energy $E = -1.14$ eV corresponding to the Dirac point is highlighted by a dashed line.

SOC contributions. A more detailed discussion is provided in Appendix C. The Dirac point is sensitive to the SOC, which opens a gap between the bands; this is described by the Δ_{SO} term in the Hamiltonian Eq. (6).

The two-dimensional carrier density $n_{2\text{D}}$ needed to fill the bands up to the Dirac point is of the order of 10^{14} cm^{-2} (for $\Delta = -1$ eV, $n_{2\text{D}} = 7.6 \times 10^{14} \text{ cm}^{-2}$, corresponding to 0.34 electrons for each Ti ion). This is comparable with the typical electron densities injected at the LAO/STO interface, making it possible to perform an experimental investigation via field effect technique.

The presence of the trigonal distortion induces some peculiar behavior of the angular and spin polarization between the two layers of Ti atoms. To show this, we evaluated for a fixed

filling μ the following quantity:

$$\langle \mathcal{O}_\alpha \rangle(\vec{k}) = \sum_{E < \mu} \langle E, \vec{k} | P_\alpha \mathcal{O} | E, \vec{k} \rangle \quad (7)$$

where $\mathcal{O}_\alpha$ is the generic component of the angular momentum or spin momentum projected on the α th layer, $|E, \vec{k}\rangle$ is a generic eigenstate of energy E and quasimomentum $\vec{k}$, and P_α is a projection operator on the states localized on the α th layer

$$P_\alpha = \sum_{i, \sigma, \vec{k}} |\psi_{i\alpha\sigma, \vec{k}}\rangle \langle \psi_{i\alpha\sigma, \vec{k}}|, \quad (8)$$

where we defined $\{|\psi_{i\alpha\sigma, \vec{k}}\rangle\}$ as the vector of the original basis of the Hamiltonian. These quantities evaluated throughout the BZ are depicted in Fig. 4 for a benchmark choice of the parameters. This figure shows that a magnetic moment localized in $\vec{k}$ is formed between the two layers, in principle, observable via spin-polarized ARPES experiments. A peculiar feature appears in Fig. 4: When the chemical potential is within the gap formed at the Dirac point, the out-of-plane spin component is totally localized near the K point in the BZ, while the orbital angular momentum is almost zero. The latter can be understood by observing that in the limit $-\Delta/t_3 \gg 1$, the lower orbitals tend to the a_g states which are characterized by $\langle \vec{L} \rangle = 0$. The localization of the spin, instead, can be understood by observing that far from the Dirac point the splitting among the first and second doublets is induced by TB alone, and therefore the mean value of the spin vanishes. On the other hand, near the Dirac point, Eq. (6) shows that the splitting induced by TB vanishes. The gap at the Dirac point is induced by the SOC, represented by the Δ_{SO} term in Eq. (6), leading to a nonvanishing mean value of the spin on each of the two layers oriented along the (111) direction. Of course, in the absence of inversion symmetry, e.g., $v = 0$ in our case, the sum over the two layers of the projected mean values vanishes. This is reasonable and in agreement with literature [58–60]. Furthermore, since the system is time-reversal invariant in the absence of a magnetic field, it does not show magnetic behavior and a many-body interaction is needed to recover ferromagnetic effects: for this reason, the total spin integrated over the whole BZ is always vanishing.

FIG. 4. Mean values of the out-of-plane components of (a) orbital and (b) spin angular momentum, localized on one of the two Ti layers for $\Delta = -1$ eV, $\lambda = 0.1$ eV, and $v = 0$ eV, and with $\mu = -1.14$ eV (within the gap at the Dirac point).

FIG. 5. Cubic structure under a trigonal distortion. The blue sphere is the Ti atom, while the red ones are the O atoms. The pink spheres are the positions of the O atoms in the undistorted structure. The black arrow is the (111) direction. θ represents the distortion angle used for the parametrization of the strain: When $\theta = \arccos(1/\sqrt{3})$ the structure is unstrained; smaller (larger) values of θ lead to dilatation (contraction) along (111) direction.

A. Connection between trigonal coupling and physical strain

We have shown that the possibility for the system to exhibit nontrivial properties is critically connected with the strength of the strain parameter Δ . One can therefore wonder whether it is possible under realistic experimental conditions to achieve the necessary values for the trigonal coupling to have $|\Delta/t_3| \gtrsim 1$. In Refs. [61,62], an analysis of the trigonal strain is performed in the case of a face-sharing octahedral structure. In such a case, a trigonal distortion is a compression or a stretching of the face-shared planes of the oxygen octahedra around a metal ion. When the material is unstrained, the octahedral oxygen cage splits up the d orbitals into t_{2g} and e_g^σ orbitals. When a strain is imposed, the angle M-O-M between two metal ions and an oxygen in between changes, reducing the symmetry of the system from octahedral to trigonal and splitting up the states into three subgroups: e_g^σ , a_g , and e_g^π orbitals. The method of Refs. [61,62] allows a unified treatment of the energy splitting caused by the trigonal distortion and recovers the energy splitting of the octahedral crystal field when the M-O-M angle takes its undistorted value. The same calculation can be used for the case of a corner-sharing structure as in the STO case. The strain at the interface is translated into a rigid shift of the atoms along the (111) direction. This leads to a distortion of the octahedral oxygen cage structure around one Ti atom, analogous to the case of the face-sharing octahedra. This leads to the energy splitting between the a_g , e_g^π , and e_g^σ states, depending on the distortion angle θ between the direction connecting the O ligand with the Ti ion line and the (111) direction as shown in Fig. 5. This energy splitting explicitly depends on the following parameters:

(1) The energy splitting E_0 between the e_g^σ states and the triplet of states a_g and e_g^π , which are degenerate when $\Delta = 0$. This splitting is typically expressed as $E_0 = 10Dq$ [56].

FIG. 6. (a) a_g , e_g^π , and e_g^σ energy level behavior as a function of the distortion angle θ using $E_0 = 2$ eV, $\kappa = 4.93$ and $z^* = 4$. (b) Δ parameter as a function of the distortion angle θ using the same parameters (solid line) and using $\kappa = 12.5$, corresponding to the linearized muffin tin approximation (dashed lines).

(2) $\kappa = a_0^2 \frac{\langle r^2 \rangle}{\langle r^4 \rangle}$, where a_0 is the lattice constant and the mean values of the powers of the radii are evaluated between the orbitals of the conduction band.

(3) The effective nominal charge z^* which affects the electrons in the conduction band. This is evaluated by subtracting from the ion charge Z the charge of the electrons in the complete shells and of those electrons in the noncomplete shells multiplied by a corrective factor (0.35), which takes into account the electron-electron screening.

Using these results for the STO structure, choosing $E_0 = 2$ eV as reported in Ref. [63], $\kappa = 4.93$, as determined for the d orbitals, and $z^* = 22 - 18 = 4$, since Ti^{4+} ions have no electrons in their external shells, we reproduce the energy dependence of the a_g , e_g^π , and e_g^σ orbitals as a function of the distortion angle θ , together with the behavior of the strain parameter $\Delta = (E_{a_g} - E_{e_g^\pi})/2/3$ in Fig. 6. For the latter, we show the results also for $\kappa = 12.5$, corresponding to the muffin tin approximation [62]. The results show that for experimentally accessible distortion angles, Δ reaches absolute values sufficiently large to cause the appearance of the Dirac cone in the band structure. In fact, compared to the equilibrium position $\theta_0 = \arccos(1/\sqrt{3}) \approx 54.7^\circ$ for which there is no splitting between the a_g and e_g^π states, for $\theta \geq 58.7^\circ$ we find $\Delta \leq -0.6$ eV. The muffin tin approximation leads to even smaller values of distortion angle necessary to reach the same value of Δ . For this reason, for the rest of the paper, unless

we specify otherwise, we consider as benchmark the value $\kappa = 4.93$ which leads to conservative estimates for Δ .

We observe that our results do not take into account the correction due to the crystal field originating from the metal ions in the structure; the introduction of such a correction only increases the strength of the trigonal coupling in absolute value. Our results are therefore meant as a lower bound on the realizable coupling Δ , and they show that, already at this level, the trigonal dominated regime proposed in the previous sections seems to be experimentally achievable. These conclusions are further strengthened in Appendix D, in which we show that they are robust by accounting for the modification of the hopping parameters induced by the distortion angle. Let us finally discuss the change in the in-plane lattice constant induced by the biaxial strain along the (111) direction. As reported in Ref. [64], a biaxial (111) strain in the bulk STO could lead to transition to a ferroelectric phase if the strain is tensile. We first point out that, in the realistic case corresponding to $\Delta = -0.65$ eV and a distortion angle of 2° evaluated using the muffin tin approximation, the compression of the lattice constant is about 5%. To maintain the volume of the lattice cell constant, the in-plane hexagonal lattice has to expand by about $\sim 2.5\%$ of the lattice constant along the $[110]$ and $[112]$ directions. This would result in a dilation of the side of the hexagon by the same relative amount, preserving the C_{3v} symmetry of the 2D lattice. For this reason, we neglected this effect in our paper. Furthermore, given that the considered strain for negative Δ is compressive, we expect a paraelectric phase for the STO, according to Ref. [64], which does not modify the predicted results, up to a redefinition of the electric field coupling v .

IV. TOPOLOGICAL PROPERTIES

Due to the simultaneous presence of the SOC, the Dirac cone in the electronic band structure, and the time-reversal invariance, we expect that, at least for $|\Delta/t_3| \gtrsim 1$, the system could exhibit QSHE. In this section, we scan the parameter space of the system to determine which are the conditions for this to happen.

Since in the strained interface all the conditions for QSHE are met, we simulated a finite-thick (20–100 sites) zigzag ribbon, whose representation is shown in Fig. 7, obtaining numerical evidence of edge states. The latter are represented by the band inversion in the energy dispersion along the k_x coordinate, the momentum in the orthogonal direction to the finite length of the ribbon. The results for a 20-site ribbon are represented in Fig. 8, where we highlight in color the edge states. Notice that the SOC is chosen to be 0.1 eV for ease of visualization (the typical values are smaller [52]). We also show the value of the Z_2 invariant computed for each of the Kramers doublets according to the method of the Wannier charge centers (WCCs). In this method, we identify the fundamental direction of the reciprocal lattice, named λ_1 and λ_2 , and we compute the WCCs, namely, the mean value of the position $i \frac{\partial}{\partial \lambda_i}$, for both of the states of a Kramers doublet as a function of the periodic variable λ_2 . For each doublet, we subsequently count the number of discontinuities of the mean WCC along half a period of λ_2 . The sum modulo 2 of the number of discontinuities is equal to the Z_2 invariant. The specific

FIG. 7. Schematic representation of a finite-thick zigzag ribbon. The system is confined along the vertical Y axis while is unlimited along the X axis.

details of how to choose a continuous gauge along the BZ are discussed in more detail in Refs. [65,66]. The edge states are always formed in between the nontrivial bands. The localized nature of these states is confirmed by the rapid decreasing of the occupancy probability away from the edge for the red band. The choice of showing the results for a 20-site ribbon is to highlight this rapid decreasing. For a 100-site ribbon we find, as expected, the same qualitative behavior. A particularly interesting conclusion is the fact that edge states can form at the K point, in between the Dirac cone; this constitutes a further similarity between our heterostructure and graphene.

The general topological characterization of the system has been obtained by computing the Z_2 topological invariant for each of the six Kramers doublets and subsequently determining the phase diagrams in the $\lambda - \Delta$ plane. In Fig. 9(a), we show the phase diagram for the lowest energy doublet. The diagrams for the other doublets can be found in Appendix E. We can deduce from the figure that the first energy doublet is always nontrivial when λ and Δ are nonzero.

To achieve a QSHE, the necessary requirements are a chemical potential within the energy gap in the band structure and a value equal to 1 for the Z_2 invariant; the latter is the sum modulo 2 of the Z_2 of the filled doublet. A topologically nontrivial behavior is therefore expected when the chemical potential lies between the first and second Kramers doublets. We emphasize the behavior of the first doublet, since it is easier to access experimentally, but, referring to Fig. 8, a nontrivial behavior is also expected if the bands are filled up to the second doublet.

Finally, we studied the stability of the topological properties against an external electric field. To do this, we evaluated the Z_2 invariant for a fixed value of $\lambda = 0.1$ eV, varying v and the trigonal parameter Δ in a region in which the system exhibits an insulating behavior. The results are depicted in Fig. 9(b), showing how the topological structure for the lowest bands is preserved for electric potentials of $v \sim 0.004$ eV for $\lambda = 0.1$ eV. This corresponds to an electric field between the two layers of Ti of the order of 10^7 V/m over a thickness of $\tilde{a} \sim 0.3$ nm. Generally, with the decreasing of the strain $|\Delta|$, a larger field is needed to bring the system into the normal state. We studied the stability against weak perturbations also

FIG. 8. (a) Energy dispersion for a finite-thick zigzag ribbon of 20 sites, for $\Delta = -1$ eV, $\lambda = 0.1$ eV, and $v = 0$ eV. The colored lines represent the edge states of the system, where there is an energy band inversion within the gap. (b) Energy band structure for the same parameters and the corresponding Z_2 invariant for each band. (c) The probability of a carrier occupation of a site for $k_x = \pi/\sqrt{3}$ for the red curve in the (a) panel.

varying the SOC, since it could, in principle, be different from the value used in the previous analysis: we fixed the trigonal parameter to $\Delta = -1$ eV obtaining the phase diagram shown in Fig. 9(c). To prove the possibility to induce a topological transition via modification of the strain, we show in Fig. 10 the energy gap between the bands as a function of the strain parameter, together with the chemical potential for a fixed value of the surface carrier density n_{2D} . We have chosen this density value so the chemical potential μ lies within the energy gap

for $\Delta = -0.65$ eV and for benchmark values of $\lambda = 0.1$ eV and $v = 0$ eV. From Fig. 10, it is evident that decreasing Δ , and therefore increasing the strain, the chemical potential moves through the bands passing in the orange region. Here the two conditions of a nontrivial topological structure for the lower band and an insulating regime for the material are simultaneously met, so the system can exhibit a QSHE.

V. CONCLUSIONS AND DISCUSSION

In this paper, we investigated the properties of the (111) STO-based heterostructure interface via TB methodologies. We took into account the contribution of the electron hopping in the bilayer of STO at the surface, the interfacial trigonal strain, the SOC, and the electric field orthogonal to the bilayer. The values of the main hopping parameters were obtained by comparison with the ARPES experiments. The remaining parameters were systematically studied in order to identify the features of the electronic structure. We identified two different regimes: one in which the strain is a small perturbation compared to the hopping parameters and the other in which it is a relevant contribution. In the former situation, our model is able to capture the main features of the band structure previously obtained in literature [53,55,67]. In the latter, the system exhibits a Dirac point in the structure of the low-energy bands for experimentally accessible values of the carrier density. Compared with Ref. [37], which obtained the same behavior with DFT methodologies, we accurately discussed the role of SOC and assessed the regime of the trigonal strain where a Dirac cone is expected. We found that the presence of the Dirac point requires values of the trigonal distortion such that $|\Delta/t_3| \geq 1$. Our assumption was supported by a systematical study of the dependence of the energetic parameter Δ on the physical strain applied at the interface. We also showed the presence of nontrivial spin and orbital angular momentum patterns in the BZ, finding that in the presence of the trigonal distortion there can be a nonvanishing magnetic dipole moment between the two layers of Ti at a fixed $\vec{k}$ in the BZ. In agreement with the expectation of time-reversal invariance, this magnetic moment vanishes when integrated over the whole BZ; nevertheless, these results are potentially accessible using spin-polarized ARPES experiments. Interestingly, in the regime with sizable strain, when the chemical potential is within the gap at the Dirac point, the out-of plane components of the spin are completely localized near the K point in the BZ. These features suggest a nontrivial spin behavior and open the way to a systematic analysis of the spin properties of (111) STO heterostructures. We determined these properties in a minimal model using only two layers of Ti atoms. The presence of thin films over the STO, in particular, LAO layers, are included as a *reservoir* of electrons, and its possible role in generating distortion is completely contained within the strain parameter Δ and v . Moreover, we did not include in our study the Coulomb interaction. This allowed us to obtain flexible results from the model with small computational effort: Indeed, we plan to use this model as a starting point for studying different phenomena. Furthermore, we expect the Coulomb interaction to be weak in the low filling region. Its effect should mainly be a renormalization of the energy spectra for the occupied bands

FIG. 9. Phase diagram for the first Kramers doublet (a) in the $\lambda - \Delta$ plane with $\nu = 0$ eV, (b) in the $\nu - \Delta$ plane fixing $\lambda = 0.1$ eV, and (c) in the $\lambda - \nu$ plane fixing $\Delta = -1$ eV. The red region corresponds to $Z_2 = 1$, while the white one corresponds to $Z_2 = 0$. Diagram (a) has been computed using an energy step of 0.05 eV, diagram (b) has been computed using an energy step for Δ (ν) of 0.05 (0.001) eV, and diagram (c) using an energy step for λ (ν) of 0.005 (0.001) eV.

[53], locally increasing the Fermi velocity. This conclusion should still be valid in the regime of interest $|\Delta|/t_3 > 1$ near the Dirac point, as shown in Ref. [68]. Here it is shown that the Coulomb interaction cannot open a gap in the band structure by itself, even though it widens the energy gap opened by SOC. Therefore, the main effects of Coulomb interactions that are not included in our paper should be a renormalization of the Fermi velocity and the energy gap induced by SOC at the Dirac point. We point out that we did not investigate a possible antiferrodistortive transition which can occur at low temperature in the bulk STO, and using (111) biaxial strain as predicted in Ref. [64]. Moreover, we did not investigate the possible presence of charge-ordered modes as predicted in Ref. [37] under suitable conditions. These questions can be investigated in future studies.

The low-energy region in the regime with sizable strain is particularly interesting also due to its nontrivial topological properties. We computed the topological invariant of the system using the WCC method proposed by Soluyanov and Vanderbilt [65,66]. We found that the first Kramers doublet is characterized by a $Z_2 = 1$ in the presence of the inversion

FIG. 10. Energy gap between the first and the second Kramers doublet as a function of the strain parameter Δ . The green (red) curve represents the minimum (maximum) energy $E_{\min}^I$ ($E_{\max}^I$) of the upper (lower) Kramers doublet after subtraction of the quantity $\bar{E} = (E_{\max}^I + E_{\min}^I)/2$; the dashed line is the chemical potential $\mu - \bar{E}$ with a fixed surface density. The orange section is the region in which the system exhibits QSHE.

symmetry. This property is preserved in the presence of weak perturbations due to an external electric field. Finally, we showed that the system can exhibit a QSHE; this property has been investigated via finite-thick zigzag ribbon simulations, which show that edge states can be present under suitable conditions at the Dirac point. We found that a topological transition can occur since the system can be tuned from a conducting to an insulating state via strain manipulation.

In conclusion, as a result of a sizable strain, our TB scheme predicts a nontrivial topological phase for LAO/STO (111), including a gap at the Dirac point. The possibility to engineer the applied trigonal strain at the interface suggests that the transition to the nontrivial topological phase can be controlled in a parameter range which is experimentally achievable.

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APPENDIX A: MAXIMUM LIKELIHOOD ANALYSIS FOR t_1, t_2, t_3 PARAMETERS

In this Appendix, we discuss the methodology used to extract the values of the hopping parameters of the matrix $t_i^{\alpha\beta}$ in Eq. (2). In literature, STO bare-surface ARPES data are available [55], which allow us to fix the hopping parameters t_1 , t_2 , and t_3 , since the qualitative behavior of the interface depends on the ratio between them and Δ . As a first approximation, we can fix $\Delta = 0$, since its value is of the order of the meV for the bare STO [57], $\lambda = 0$ and $\nu = 0$. In this framework, we can extrapolate analytically the eigenvalues of the system Hamiltonian, reported here in a matrix form for

simplicity¹:

$$H = \sum_{\vec{k}} \begin{pmatrix} d_{yzTi_1, \vec{k}}^\dagger \\ d_{zxTi_1, \vec{k}}^\dagger \\ d_{xyTi_1, \vec{k}}^\dagger \\ d_{yzTi_2, \vec{k}}^\dagger \\ d_{zxTi_2, \vec{k}}^\dagger \\ d_{xyTi_2, \vec{k}}^\dagger \end{pmatrix}^T \begin{pmatrix} \gamma_{yz} & 0 & 0 & \epsilon_{yz} & 0 & 0 \\ 0 & \gamma_{zx} & 0 & 0 & \epsilon_{zx} & 0 \\ 0 & 0 & \gamma_{xy} & 0 & 0 & \epsilon_{xy} \\ \epsilon_{yz}^* & 0 & 0 & \gamma_{yz} & 0 & 0 \\ 0 & \epsilon_{zx}^* & 0 & 0 & \gamma_{zx} & 0 \\ 0 & 0 & \epsilon_{xy}^* & 0 & 0 & \gamma_{xy} \end{pmatrix} \begin{pmatrix} d_{yzTi_1, \vec{k}} \\ d_{zxTi_1, \vec{k}} \\ d_{xyTi_1, \vec{k}} \\ d_{yzTi_2, \vec{k}} \\ d_{zxTi_2, \vec{k}} \\ d_{xyTi_2, \vec{k}} \end{pmatrix}, \quad (A1)$$

where the intralayer, diagonal, contributions are

$$\begin{aligned} \gamma_{yz} &= -2t_1 \cos\left(\frac{-\sqrt{3}}{2}k_X + \frac{3}{2}k_Y\right), \\ \gamma_{zx} &= -2t_1 \cos\left(\frac{\sqrt{3}}{2}k_X + \frac{3}{2}k_Y\right), \\ \gamma_{xy} &= -2t_1 \cos(\sqrt{3}k_X), \end{aligned} \quad (A2)$$

and the interlayer contributions are

$$\begin{aligned} \epsilon_{yz} &= -t_3 \left(1 + e^{i(\frac{\sqrt{3}}{2}k_X - \frac{3}{2}k_Y)}\right) - t_2 e^{-i(\frac{\sqrt{3}}{2}k_X + \frac{3}{2}k_Y)}, \\ \epsilon_{zx} &= -t_3 \left(1 + e^{-i(\frac{\sqrt{3}}{2}k_X + \frac{3}{2}k_Y)}\right) \\ &\quad - t_2 e^{i(\frac{\sqrt{3}}{2}k_X - \frac{3}{2}k_Y)}, \\ \epsilon_{xy} &= -2t_3 \cos\left(\frac{\sqrt{3}}{2}k_X\right) e^{-i\frac{3}{2}k_Y} - t_2, \end{aligned} \quad (A3)$$

where $\vec{k} = k_X \hat{u}_{110} + k_Y \hat{u}_{\bar{1}\bar{1}2}$ is the dimensionless in-plane k vector of the BZ. We emphasize that the coupling among different t_{2g} orbitals are all equal by virtue of the C_3 symmetry of the interface. The possibility of exact diagonalization is evident due to the fact that the TB interaction does not mix the different d_i orbitals with one another but only the two layers. The matrix is therefore in a 2×2 block diagonal form. The eigenvalues, which are doubly degenerate in the spin, are the following:

$$\rho_i(\vec{k}) = \gamma_i(\vec{k}) \pm |\epsilon_i(\vec{k})|, \quad (A4)$$

where i runs over yz, zx, xy , $\gamma_i(\vec{k})$ in which we have explicitly expressed the $\vec{k}$ dependence. In $\vec{k} = 0$ (Γ point in the BZ), the eigenvalues referring to the lower band ($-$ sign) have a three-fold degenerate minimum (neglecting the spin degeneracy):

$$E_{\min} = 2t_1 - (2t_3 + t_2). \quad (A5)$$

Near the bottom of the bands an approximate expression for the energies is

$$\rho_i(k_X, k_Y) = E_{\min} + \frac{\hbar^2 k_X^2}{2(m_{\Gamma K}^*)_i} + \frac{\hbar^2 k_Y^2}{2(m_{\Gamma M}^*)_i} + \alpha_i k_X k_Y, \quad (A6)$$

¹The double spin degeneracy is understood.

FIG. 11. Detail of the bottom of the bands near the Γ point, along the line connecting M with Γ (k_Y direction) on the left side and the line connecting Γ with K (k_X direction) on the right side. The dashed line represents the bands using only the TB model while the solid line includes a small trigonal strain parameter. The splitting induced by the latter is of the order of $3/2\Delta$. The minima of the bands in the two cases have been shifted to coincide for ease of visualization.

where we defined

$$\begin{aligned} (m_{\Gamma K}^*)_{yz} &= (m_{\Gamma K}^*)_{zx} = \frac{4\hbar^2}{3(2t_1 + \frac{t_3(3t_2+t_3)}{t_2+2t_3})}, \\ (m_{\Gamma M}^*)_{yz} &= (m_{\Gamma M}^*)_{zx} = \frac{4\hbar^2}{9(2t_1 + \frac{t_3(t_2+t_3)}{t_2+2t_3})}, \\ (m_{\Gamma K}^*)_{xy} &= \frac{2\hbar^2}{3(4t_1+t_3)}, \quad (m_{\Gamma M}^*)_{xy} = \frac{2\hbar^2(t_2+2t_3)}{9t_2t_3}. \end{aligned} \quad (A7)$$

These quantities represent the effective masses in the free particle approximation along the directions connecting, respectively, the Γ and K points and the Γ and M points in the BZ. The numerical values of the parameters have been fixed using ARPES data [55] shown in Fig. 11: From the dashed curves, we have extrapolated the values of the effective masses, together with a confidence range. In this way, a χ^2 analysis has been performed to search for the best fit combination of the three parameters. The best fit values are

$$t_3 = 0.5 \text{ eV}, \quad t_2 = 0.04 \text{ eV}, \quad t_1 = 0 \text{ eV}. \quad (A8)$$

We do not provide the confidence interval since this is meant only to be a qualitative analysis. Nonetheless, we show in Fig. 12 the χ^2 contours in the $t_3 - t_2$ plane. From the contours, we see that the number of digits for the parameters is chosen coherently with their uncertainty on them. Analogous studies in literature [67] have found similar values for the parameters. In Fig. 11 (solid line), we show the effect of a weak trigonal strain on the pure TB curves. The strain changes the effective masses near the Γ point and induces a splitting between the first and the other two doublets of the order of $3/2\Delta$. However, the splitting is not sufficient to induce an effective gap between the first two doublets and the third one.

APPENDIX B: EFFECTIVE MODEL NEAR THE K POINT FOR THE UNSTRAINED INTERFACE

In the case of unstrained interface, the value of Δ is fixed to be -0.005 eV. As we discussed above, at the K point there is an intersection of bands that, along the high symmetry lines, has a structure similar to the Dirac point in the graphene.

FIG. 12. Contours of exclusion at 68%, 95%, and 99.7% confidence level in the $t_2 - t_3$ plane: The best fit point is marked in black.

We will now detail the differences between our case and the graphene one.

In the same way, as we did for the Γ point in Appendix A, we will provide an analytical approximation for the energy eigenvalues in the case of pure TB. The 3D structure near K , corresponding to $\vec{k} = (\frac{4\pi}{3\sqrt{3}}, 0)$, is represented in Fig. 13 for the lower bands, where we set $\Delta = 0$. The structure represents the intersection of three planes in the K point, which is different from the Dirac cone. Thus near the K point, the eigenvalues in Eq. (A4) can be expanded both for the upper and the lower bands to first order as

$$\rho_i \simeq \rho_0 + \hbar \vec{v}_{Fi} \cdot (\vec{k} - \vec{k}_0), \quad (\text{B1})$$

where $\vec{k}_0 = (\frac{4\pi}{3\sqrt{3}}, 0)$, and $\rho_0 = t_1 \pm |t_2 - t_3|$ with the minus (plus) sign referring to the lower (upper) bands. We will focus on the lower bands; the values of $\vec{v}_{Fi}$ depend on the orbital

FIG. 13. Structure of the lower bands near their intersection at the K point: The bands behave linearly as planes near the K point.

FIG. 14. (a) Detail of the band structure near the K point for the pure tight-binding model. (b) Same as above in the presence of a trigonal crystal field $\Delta = -0.005$ eV: the degeneracy is partially split.

FIG. 15. (a) Detail of the band structure near the K point in the presence of a spin-orbit coupling $\lambda = 0.01$ eV: the degeneracy is partially split. (b) Same as before, with the simultaneous presence of $\Delta = -0.005$ eV and $\lambda = 0.01$ eV.

FIG. 16. (a) Geometrical representation of the strain δ and the corresponding change in the bond length between two Ti: the angle $\theta_0 = \arccos(1/\sqrt{3}) \sim 54.7^\circ$. (b) Dependence of the TB parameters on the distortion angle δ . We show the behavior both of the strain parameter $|\Delta|$, for two benchmark values of κ (black, solid and dashed), and of the hopping parameter t_3 (red) as a function of δ .

under examination:

$$\begin{aligned}\vec{v}_{Fyz} &= \frac{1}{\hbar} \left(\frac{3}{4} \left(2t_1 + \frac{t_3(t_3 - t_2)}{\sqrt{(t_3 - t_2)^2}} \right), \frac{3\sqrt{3}}{4} \left(2t_1 + \frac{t_3\sqrt{(t_3 - t_2)^2}}{t_2 - t_3} \right) \right); \\ \vec{v}_{Fzx} &= \frac{1}{\hbar} \left(\frac{3}{4} \left(2t_1 + \frac{t_3(t_3 - t_2)}{\sqrt{(t_3 - t_2)^2}} \right), \frac{3\sqrt{3}}{4} \left(2t_1 + \frac{t_3(-t_2 + t_3)}{\sqrt{(t_3 - t_2)^2}} \right) \right); \\ \vec{v}_{Fxy} &= \frac{1}{\hbar} \left(-3t_1 + \frac{3}{2} \frac{t_3(t_2 - t_3)}{\sqrt{(t_3 - t_2)^2}}, 0 \right).\end{aligned}\quad (\text{B2})$$

It is possible to write an effective Hamiltonian in the proximity of the K point. The eigenvectors of the 2×2 matrices of Eq. (A1) are

$$|\psi_{i,k}^\pm\rangle = \frac{1}{\sqrt{2}} (|\psi_{i\text{Ti}_1,k}\rangle \pm e^{i\varphi_i(\vec{k})} |\psi_{i\text{Ti}_2,k}\rangle), \quad (\text{B3})$$

with the sign referring to the lower or the upper bands, $e^{i\varphi_i(\vec{k})} = \frac{|\epsilon_i(\vec{k})|}{\epsilon_i(\vec{k})}$. We have neglected the spin index for simplicity. Thus we can write the effective Hamiltonian as

$$H_K = \sum_{\vec{k} \simeq \vec{k}_0} \sum_{i,\lambda,\sigma} \lambda \hbar \vec{v}_{Fi}^\lambda \cdot (\vec{k} - \vec{k}_0) d_{i\sigma,k}^{\lambda\dagger} d_{i\sigma,k}^\lambda, \quad (\text{B4})$$

with $\lambda = \pm$ discriminating between the upper or the lower bands and $d_{i,k}^{\lambda\sigma}$ is the annihilation operator referring to the states in Eqs. (B3).

We conclude that the K point in this case is quite different from the Dirac point in graphene: in the latter, in fact, there are no states near the Dirac point, while in our case there is a large quantity of states corresponding to the intersection of the three plane bands. This is also seen from the density of states in Fig. 2 at the dashed line. To experimentally realize an electron filling up to the K point, an electron surface density of $n_{2D} = 1.59 \times 10^{15} \text{ cm}^{-2}$ is needed, which is large compared with the typical charge carriers densities measured or predicted at the interface under examination.

We will now discuss the stability of the degeneracy of the K point upon including the perturbations. First, using the trigonal crystal field coupling of $\Delta = -0.005 \text{ eV}$ the band structure changes as in Fig. 14. The degeneracy is partially split, without the formation of a gap.

The presence of v does not influence the existence of the degeneracy: its effect is limited to pushing the upper and lower band further and further apart.

The SOC, on its own, is not able to remove the degeneracy as shown in Fig. 15. On the other hand, the simultaneous presence of the trigonal field and the spin-orbit interaction completely removes the degeneracy which leads to the intersection of the bands. Of course, for sufficiently small values of λ and Δ , the effect is limited only to an extremely narrow region near K , and the behavior returns to be quasilinear as we go far from the K point.

APPENDIX C: EFFECTIVE DIRAC HAMILTONIAN NEAR THE K POINT FOR STRAINED INTERFACE

The case of the strained surface is particularly interesting due to the presence of the structure resembling the Dirac point. Since $\Delta = -1 \text{ eV}$, it is possible to analyze the proximity of the point thanks to a perturbative approach in which the TB terms are treated as small. In fact, we can consider the two lower bands as originating only from the $|a_g\text{Ti}_1, \vec{k}\rangle$ and $|a_g\text{Ti}_2, \vec{k}\rangle$ Bloch orbitals belonging to layer Ti_1 and Ti_2 : this would be an exact statement in the case of infinite Δ . Even though $\Delta = -1 \text{ eV}$ is not exactly in the range of applicability of perturbation theory (because $t_3 = 0.5 \text{ eV}$), this would be enough to give us a semiquantitative understanding of what happens at the K point.

In the subspace of degeneracy constituted by the two states $|a_g\text{Ti}_1, \vec{k}\rangle$ and $|a_g\text{Ti}_2, \vec{k}\rangle$, the perturbation induced by the TB is

$$H_{\text{eff}} = \frac{1}{3} \begin{pmatrix} \gamma_{yz} + \gamma_{zx} + \gamma_{xy} & \epsilon_{yz} + \epsilon_{zx} + \epsilon_{xy} \\ \epsilon_{yz} + \epsilon_{zx} + \epsilon_{xy} & \gamma_{yz} + \gamma_{zx} + \gamma_{xy} \end{pmatrix}. \quad (\text{C1})$$

Near the K point, the latter can be expanded to first order due to the fact that the sum of the ϵ vanishes in that point,

$$H_{\text{eff}} = \begin{pmatrix} t_1 & \frac{1}{2}(t_2 + 2t_3)(\delta k_X - i k_Y) \\ \frac{1}{2}(t_2 + 2t_3)(\delta k_X + i k_Y) & t_1 \end{pmatrix}, \quad (\text{C2})$$

where we used the notation of $\delta k_X = (k_X - \frac{4\pi}{\sqrt{27}})$. We can write this Hamiltonian introducing the very compact notation of the Pauli spin matrices σ_i :

$$H_{\text{eff}} = \hbar v_F \vec{\delta k} \cdot \vec{\sigma} + \text{const}, \quad (\text{C3})$$

where $\vec{\delta k}$ is the k vector centered around the K point, $\hbar v_F = \frac{1}{2}(t_2 + 2t_3)$, and we neglected the constants because we are interested in the qualitative behavior. Using $t_2 = 0.04 \text{ eV}$ and $t_3 = 0.5 \text{ eV}$, we obtain $v_F \approx 2.5 \times 10^5 \text{ m s}^{-1}$ which is smaller than the graphene one ($v_F \sim 10^6 \text{ m s}^{-1}$). The eigenstates of this Hamiltonian are

$$|A_{g\pm}, \vec{k}\rangle = \frac{1}{\sqrt{2}} (|a_g\text{Ti}_1, \vec{k}\rangle \pm e^{i\theta_k} |a_g\text{Ti}_2, \vec{k}\rangle), \quad (\text{C4})$$

FIG. 17. Evolution of the band structure for increasing strain applied to the surface. We show the band structure for a distortion angle increasing from $\delta = 1^\circ$ (a), $\delta = 3.2^\circ$ (b), $\delta = 6^\circ$ (c). The dashed line corresponds to the filling needed to reach the intersection of the first two doublets at the K point, namely, $\mu = -0.56$ eV (a), $\mu = -0.815$ eV (b), and $\mu = -1.04$ eV (c). The electric field at the interface is fixed to $v = 0$; the spin-orbit coupling is taken as $\lambda = 0.01$ eV.

where the phase $e^{i\theta_k} = \frac{\delta k_x \mp i k_y}{|\delta \vec{k}|}$, so θ_k coincides with the geometrical angle between $\delta \vec{k}$ and k_x . The degeneracy near the K point is repeated six times throughout the hexagonal BZ, however, these six points are not all equivalent. In particular, near the K' point, the Hamiltonian is the same with a change in sign in σ_x . If, for this second class of Dirac points, we reverse the ordering of the states in the matrix form of the Hamiltonian, we find that the form of the Hamiltonian is equal and opposite to the one near K . Thus, with the new ordering of states, we can write the effective Hamiltonian near K' as

$$H'_{\text{eff}} = -\hbar v_F \delta \vec{k} \cdot \vec{\sigma} + \text{const.} \quad (\text{C5})$$

The eigenstates of this Hamiltonian now become

$$|A'_g \pm, \vec{k}\rangle = \frac{1}{\sqrt{2}} (|a_g \text{Ti}_2, \vec{k}\rangle \mp e^{i\theta_k} |a_g \text{Ti}_1, \vec{k}\rangle). \quad (\text{C6})$$

The degenerate points therefore group into three points equivalent to K and three points equivalent to K' , forming two independent sublattices. This is again exactly what happens in graphene, where in the usual treatment a two-valued degree of freedom is introduced, generally named valley degree of freedom, corresponding to which class of Dirac point is under analysis. In the space of this new degree of freedom, one can introduce new Pauli matrices, which we will denote by τ_i , so

FIG. 18. Phase diagram for each of the six Kramers doublets in the $\lambda - \Delta$ plane with $v = 0$ eV. The panels are ordered from lowest to the highest energy doublet. The red region corresponds to $Z_2 = 1$, while the white one corresponds to $Z_2 = 0$. Every diagram has been computed using an energy step of 0.05 eV.

FIG. 19. Phase diagram for each of the six Kramers doublets in the $v - \Delta$ plane fixing $\lambda = 0.1$ eV for small values of v in the topologically interesting region. The panels are ordered from lowest to the highest energy doublet. The red region corresponds to $Z_2 = 1$, while the white one corresponds to $Z_2 = 0$. Every diagram has been computed using an energy step for $\Delta(v)$ of 0.05 (0.001) eV.

the full Hamiltonian can be written as

$$H_{\text{eff}} = \hbar v_F \vec{\delta} \mathbf{k} \cdot \vec{\sigma} \otimes \tau_z + \text{const}, \quad (\text{C7})$$

where the state is now a four-spinor. We conclude that there is a resemblance between graphene's Dirac cone and (111) LAO/STO interface. An experimentally relevant difference is the fact that the Dirac point in the graphene stands exactly at the neutrality point of the system, between the conduction and valence band, while the Dirac point in the LAO/STO interface resides fully in the conduction band. Therefore, to investigate that point we need to fill sufficiently the $|A_g\rangle$ lower bands: the numerical predicted value (for our choice of parameters) is $n_{2D} = 7.6 \times 10^{14} \text{ cm}^{-2}$. This value is comparable in order of magnitude with the typical charge carrier density predicted at these interfaces by the polar catastrophe model.

We now discuss the presence of the effective emergent coupling due to the SOC at the Dirac point. The energy splitting induced by SOC has to be treated carefully since, as we mention in the text, the mean value of $\vec{L}$ is equal zero on the a_g states, leading to no induced splitting to first order in the SOC. Moreover, both the SOC and the TB terms are to be treated as small perturbations to the larger trigonal strain term. We explicitly verified that a gap among the a_g states at the Dirac point only opens to third order in perturbation theory: In particular, the gap opening is well-described by the perturbative term in the Hamiltonian

$$H_Z = \Delta_{\text{SO}} \sigma_Z \otimes \tau_z, \quad (\text{C8})$$

with

$$\Delta_{\text{SO}} = 0.337 \frac{\lambda t_3^2}{\Delta^2}. \quad (\text{C9})$$

In these formulas, for simplicity we set $t_2 = 0$. Therefore, the complete Hamiltonian on the Dirac points is well described by

$$H_{\text{eff}} = \hbar v_F \vec{\delta} \mathbf{k} \cdot \vec{\sigma} \otimes \tau_z + \Delta_{\text{SO}} \sigma_Z \otimes \tau_z + \text{const}. \quad (\text{C10})$$

APPENDIX D: STRAIN INFLUENCE ON HOPPING PARAMETERS

In this section, we will discuss the effect of the strain on the hopping parameters. We will demonstrate that, even if the trigonal strain does change the hopping parameters, mainly due to the change in the bond lengths, the regime of $|\Delta|/t_3 > 1$ described in the text can always be reached. As we discussed in the main text, a trigonal distortion is a rigid shift of one layer with respect to the other along the (111) direction. First, this shift preserves the relative magnitude of the hopping parameters in different directions: Since the trigonal strain preserves the C_3 symmetry, it does not give rise to new types of TB couplings violating C_3 , and therefore it only affects the numerical values of the parameters t_1 , t_2 , and t_3 . The numerical change is induced by two factors: the different angle in the projection of the orbitals and the different bond lengths in the

FIG. 20. Phase diagram for each of the six Kramers doublets in the $\lambda - \nu$ plane fixing $\Delta = -1$ eV. The panels are ordered from lowest to the highest energy doublet. The red region corresponds to $Z_2 = 1$, while the white one corresponds to $Z_2 = 0$. Every diagram has been computed using an energy step for $\lambda(\nu)$ of 0.005 (0.001) eV.

two centers Slater-Koster (SK) overlap integrals

$$E_{lm,l'm'} = \int d\vec{r} \bar{\psi}_{lm}(\vec{r} - \vec{d}) V(\vec{r} - \vec{d}) \psi_{l'm'}(\vec{r}), \quad (\text{D1})$$

where $\psi_{lm}(\vec{r})$ is the wave function of the electrons localized on $\vec{r}$ and V is the ionic potential which mediates the hopping between the two sites. We discuss the two dependencies in turn.

On the one hand, the cosine of the angle δ between the Ti-Ti joining line and the z direction, which would be 1 in the equilibrium configuration (see Fig. 16), changes in the distorted configuration. Since the (SK) integrals depend regularly on the $\cos(\delta)$, this will affect the hopping parameters by powers of $\cos \delta \simeq 1 - \delta^2/2$, so even for large angle of distortion, e.g., $10^\circ \sim 0.17$ rad, the correction of the hopping parameters is of the order of 1.5%. We will neglect the correction due to the distortion angle in comparison with the one due to the bond lengths.

On the other hand, the distances between two Ti atoms are changed by the distortion of the crystalline planes. The unperturbed angle between one side of the cubic lattice and the (111) direction is $\theta_0 \simeq 54.7^\circ$. Under contraction of the crystalline planes, this angle increases to $\theta_0 + \delta$. The distance between two Ti atoms is decreased from a_0 to $a_0 \sin \theta_0 / \sin(\theta_0 + \delta)$. The SK integrals, and therefore the t_3 parameter, depend on the distance as $d^{-(l+l'+1)}$ [26], and since we are in the subspace of the $\{t_{2g}\}$ which have a quenched angular momentum, $l = 1$, $l' = 1$, and thus $t_3 \propto d^{-3}$. For

a representative value $\delta = 10^\circ$ (which is large compared to the angles needed to reach the regime $|\Delta| > t_3$), the hopping parameter t_3 changes from 0.5 eV to $0.5 \text{ eV} / (0.9)^3 \simeq 0.7 \text{ eV}$. Therefore, due to the small values of the distortion angles needed to reach the regime of $|\Delta|/t_3 > 1$, the change in the hopping parameters is not expected to significantly influence our results. We emphasize in any case that our results are based on choices for the numerical parameters which are conservative: for example, for the constant κ we have taken a value $\kappa = 4.93$. The linearized muffin-tin orbitals approximation predicts larger values for κ , leading to $|\Delta|$ which are even larger, therefore requiring even smaller distortion angles to enter the regime of $|\Delta|/t_3 > 1$. In Fig. 16, we show the dependence of t_3 and Δ as a function of the distortion angle. We can see that, since t_3 grows slower than $|\Delta|$, it is possible to reach the $|\Delta|/t_3 > 1$ regime already for $\delta \sim 3^\circ$. In Fig. 17, we show the evolution of the band structure for decreasing Δ , taking into account the correction to the hopping parameters due to the distortion angle δ . The result shows that already for $\delta = 6^\circ$ the Dirac cone is present, corresponding to $\Delta = -0.81$ eV.

APPENDIX E: TOPOLOGICAL PHASE DIAGRAMS

In this Appendix, we show the topological phase diagrams for all the six Kramers doublets. In Figs. 18, 19, and 20 we show, respectively, the Z_2 behavior in the $\Delta - \lambda$ plane, in the $\nu - \lambda$ plane, and in the $\nu - \Delta$ plane.

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