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Topological phases in Bi/Sb planar and buckled honeycomb monolayers

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ABSTRACT

We investigate topological phases in two-dimensional Bi/Sb honeycomb crystals considering planar and buckled structures, both freestanding and deposited on a substrate. We use the multi-orbital tight-binding model and compare results with density functional theory calculations. We distinguish topological phases by calculating topological invariants, analyzing edge states properties of systems in a ribbon geometry and studying their entanglement spectra. We show that coupling to the substrate induces transition to the Z_2 topological insulator phase. It is observed that topological crystalline insulator (TCI) phase, found in planar crystals, exhibits an additional pair of edge states in both energy spectrum and entanglement spectrum. Transport calculations for TCI phase suggest robust quantized conductance even in the presence of crystal symmetry-breaking disorder.

1. Introduction

Novel topological phases have gained an immense interest of both experimentalists and theorists in the current decade [1–11] due to attractive potential technological applications in spintronic and quantum computing devices [12]. Topological insulators exhibit the energy gap inside the bulk and conduction channels at the edges, inherently protected against certain types of scattering. Quantum spin Hall (QSH) systems are two-dimensional (2D) representatives of the family of Z_2 topological insulators protected by time-reversal symmetry [13]. Topologically nontrivial energy gap is usually inverted by large spin–orbit coupling (SOC), which is a characteristic of heavy elements. QSH systems were experimentally observed in thickness-tunable quantum wells and honeycomb-like systems based on groups of IV [14–16], II–VI [17,18], III–V [19–23] and V [24–27] elements including heavy atoms like bismuth or antimony. Recently, thin films of topological insulators protected by crystalline symmetries were recognized and dubbed topological crystalline insulators [6–11].

Bi and Sb crystals were extensively studied in the context of their topological properties [24,28–38,26,39,32,40,27,41–47,31,43,8]. Murakami [24] has predicted that Bi bilayer is Z_2 topological insulators with helical edge modes propagating in opposite directions. This fact was later confirmed experimentally by scanning tunneling microscopy measurements [28–31]. Several authors investigated robustness of topological properties of Bi(111) and Sb(111) bilayers and few bilayer crystals [32–38]. Sb(111) thin films with less than four bilayers were shown to be topologically trivial [26]. Transitions between topologically trivial and nontrivial phases can be induced by structure modifications involving chemical methods [39], artificial variation of spin–orbit coupling in Bi [32,40], strain [27,41–44] or interaction with a substrate [45–47,31,43]. Recently, TCI phase in flat Bi and Sb honeycomb layers was predicted [8]. In the presence of strain, buckled structures become completely flat, which leads to the formation of bismuthene and antimonene, for Bi and Sb composed crystals, respectively.

In the following work, we investigate various topological phases in planar and buckled Bi and Sb two-dimensional honeycomb layers using multi-orbital tight-binding (TB) model and compare results with density functional theory (DFT) calculations. We analyze whether TB method can be used as a complementary tool to characterize these crystals, as it allows to study larger systems. We distinguish different topological phases for freestanding structures and those deposited on a substrate. These phases are identified by computing topological invariants, examining band structures in a ribbon geometry and analyzing their entanglement spectra (ES).

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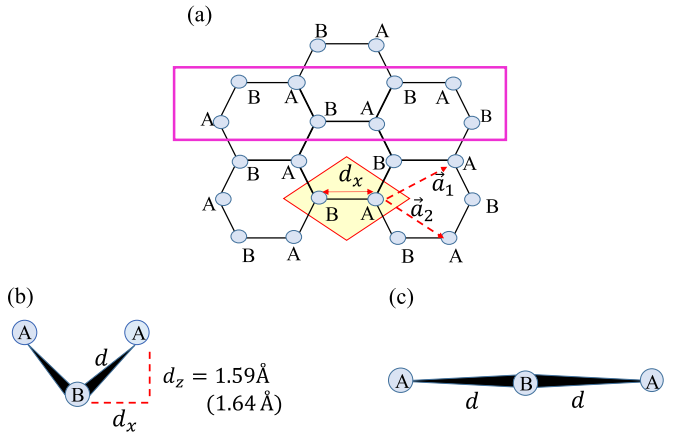

Fig. 1. (a) Top view of a honeycomb crystal structure. $\vec{a}_1$ and $\vec{a}_2$ are the lattice vectors. Rhomboid denotes a unit cell of infinite layer, whereas rectangle corresponds to the zigzag nanoribbon unit cell with periodic boundary conditions in a vertical direction. The atoms from a infinite layer unit cell are labeled as A and B. (b) Side view of bismuth and antimony bilayers. In our TB method, we set the out of plane distortion to $d_z = 1.58$ Å for bismuth and $d_z = 1.64$ Å for antimony. d is the bond length between the nearest neighboring atoms. (c) Corresponding side view of bismuthene and antimonene with interatomic distance d.

We focus mainly on characteristic features of TCI phase and study its topological protection against scattering by calculating conductance in the presence of crystal symmetry-breaking disorder.

The paper is organized as follows. In Section 2 we introduce the methodology. Results from tight-binding method and density functional theory calculations during buckled-flat transitions of freestanding systems are compared in Section 3. In Section 4, we analyze the effect of the interaction with the substrate. In Section 5 we characterize topological phases using entanglement spectrum and in Section 6 transport properties of TCI phase are studied. The results are concluded in Section 7.

2. Methods

2D crystals composed of Bi and Sb are schematically shown in Fig. 1(a). A hexagonal unit cell contains two atoms, denoted by A and B. Freestanding Bi and Sb honeycomb layers have the lowest energy when two atoms are displaced in a direction perpendicular to a lattice plane, thus they are usually called bilayers [24]. While this displacement slightly differs in a literature depending on type of calculations [43,48,49], in our TB method we take $d_z = 1.58$ Å for Bi and $d_z = 1.64$ Å for Sb. We will consider transitions between buckled Bi and Sb bilayers, Fig. 1(b), to flat honeycomb crystals, bismuthene and antimonene (see Fig. 1(c)) caused by an external uniform strain.

2.1. Tight-binding model

We use four-orbital (s, p_x, p_y, p_z) TB method with parametrization introduced by Liu and Allen [50] for bulk bismuth and antimony. The inter-atomic hopping up to the next nearest-neighbors and the atomic spin–orbit coupling (SOC) are parametrized with the Slater–Koster approach [51]. Therefore, we can write Hamiltonian as

$$\begin{aligned} H = & \sum_{\alpha,\sigma,R} |\alpha,\sigma,R\rangle E_\alpha \langle\alpha,\sigma,R| \\ & + \sum_{\alpha,\beta,\sigma,R,R'} \left[|\alpha,\sigma,R\rangle V^{\mathrm{I}}_{\alpha\beta} \langle\beta,\sigma,R'| + H.c \right] \\ & + \sum_{\alpha,\beta,\sigma,R,R''} \left[|\alpha,\sigma,R\rangle V^{\mathrm{II}}_{\alpha\beta} \langle\beta,\sigma,R''| + H.c \right] \\ & + \tfrac{\lambda}{3} \sum_{\alpha,\beta,\sigma,\sigma',R} \left[|\alpha,\sigma,R\rangle \vec{L}\cdot\vec{\sigma} \langle\beta,\sigma',R| + H.c \right], \end{aligned} \tag{1}$$

Table 1
Bismuth and antimony two-center hopping integrals taken from Refs. [42]**, [53]*, [50]. a is a lattice constant, and d_x and d_z denote parallel and perpendicular (buckling) distance between nearest-neighbor atoms in a honeycomb lattice, indicated in Fig. 1(b).

Parameter (eV)	Bi	Sb	Parameter (eV)	Bi	Sb
E_s	−10.906	−10.068	$V^{\mathrm{I}}_{pp\sigma}$	1.854	2.342
E_p	−0.486	−0.926	$V^{\mathrm{I}}_{pp\pi}$	−0.600	−0.582
$V^{\mathrm{I}}_{ss\sigma}$	−0.608	−0.694	$V^{\mathrm{II}}_{pp\sigma}$	0.156	0.352
$V^{\mathrm{I}}_{sp\sigma}$	1.320	1.554	λ	1.5	0.6
a (Å)	4.53	4.30	d_z (Å)	1.58*	1.64**
d_x (Å)	2.62	2.48			

where $\{\alpha, \beta\}$ label orbital $\{s, p_x, p_y, p_z\}$ and $\{\sigma, \sigma'\}$-spin degrees of freedom. $R'(R'')$ denote atomic positions of the nearest, (next-nearest) neighbors to an atom localized at R. E_α corresponds to the on-site energies and $V_{\alpha\beta}$ are Slater–Koster two-center integrals between α and β orbitals (I for nearest and II for next-nearest neighbors). The last term describes the spin–orbit coupling with strength λ. TB parameters are listed in Table 1. 1/3 factor is introduced to renormalize atomic SOC strength λ in order to obtain correct SOC splitting of the valence band [52]. Buckled-flat crystal transitions are modeled by linearly decreasing d_z and at the same time linearly increasing lattice constants of Bi and Sb bilayers up to the values corresponding to completely flat bismuthene and antimonene, with $a = 5.35$ Å and $a = 5.00$ Å, respectively. According to Ref. [31], the effect of SiC substrate is effectively described by shifting p_z orbitals away from the low-energy sector.

2.2. Density functional theory

We study the atomic configurations and electronic properties of relaxed and strained 2D Sb and Bi crystals in the DFT framework. The DFT calculations are done within the generalized gradient approximation (GGA) and the Perdew–Burke–Ernzerhof (PBE) [54] exchange correlation function. The core electrons were model using the norm-conserving pseudo potentials. The cut-off energy for the plane wave expansion and charge density calculations are set to 75/85 Ry and 750/850 Ry respectively for Sb/Bi 2D layers. We note that while usually the ratio between the charge density cutoff to the wave function cutoff is four, here the use of gradient-corrected functional and for pseudopotential without non-linear core correction requires a higher ratio value in order to reach energy convergence with 1 meV/10 meV for Sb/Bi monolayer, respectively. The distance between layers is set to 15 Å to avoid interaction between adjacent image layers. We apply the biaxial tensile strain which saves the hexagonal shape of the relaxed unit cell. The first Brillouin zone integration is performed in the Monkhorst–Pack algorithm [55] using a $15 \times 15 \times 1$ k-grid for relaxation of strained atomic configurations. In the relaxation, the total force on each atom in the final configuration is less than 0.001 (Ry/au). We start DFT relaxation from a completely flat structure and a buckled one to compare the final energy and find the lowest energy configuration. For band structure calculations which include the SOC, we used fully-relativistic pseudo potentials and a fine mesh of $25 \times 25 \times 1$ for k-grid. All DFT calculations presented in this article were performed using the Quantum-Espresso package [56].

The relaxed Bi and Sb honeycomb lattices are buckled and with lattice constants $a = 4.45$ Å and $a = 4.13$ Å, respectively. The equilibrium buckling of relaxed structures are $d_z = 1.64$ Å for Sb and $d_z = 1.69$ Å for Bi 2D planes. Resulting atomic configurations are in a good agreement with previous reports [57,58]. Obtained values differ from chosen tight-binding parameters by less than 10%, and we verify that this discrepancy does not affect results in a qualitative way.

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