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# Transport Properties of Graphene-BiTeI Hybrid Structures

*Z. Tajkov,* D. Visontai, P. Rakyta, L. Oroszlány, and J. Koltai*

**Recent studies have shown that heterostructures comprised of graphene and certain chalcogenides are robust two-dimensional (2D) topological insulators. We developed a simplified model Hamiltonian for such systems and investigated their properties as the function of various parameter values. We mapped the phases of the system that can behave as an insulator, metal or topological insulator. We used this simplistic model to calculate transport characteristics on experimentally relevant sample sizes.**

## 1. Introduction

Graphene has emerged as an excellent substrate for a host of novel electronic applications.[1] One of the more challenging problems of graphene-based electronic devices is controlling the strength of the spin–orbit coupling (SOC). The manipulation of the SOC is theoretically exciting and is capable to revolutionize several industries.[2] Over the last decade, topological insulators, novel topologically protected phases of matter stabilized by SOC,[3,4] have attracted considerable interest due to their potential technological applications in spintronics, topological quantum computation, and thermoelectrics[5,6] elucidated by the topological protection of their surface states. Experimental observations have confirmed the topological protection of this novel phase in HgTe/CdTe[7,8] and in InAs/GaSb[9] quantum wells. However, these experiments are rather difficult to perform and do not lend themselves easily for commercial technologies. In contrast graphene-based heterostructures utilizing the ever growing family of layered two dimensional materials show enticing scalable applications.[1]

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The ORCID identification number(s) for the author(s) of this article can be found under https://doi.org/10.1002/pssc.201700215.

**DOI: 10.1002/pssc.201700215**

In this work, we give an account about a theoretical investigation of a heterostructure consisting of graphene and BiTeI, a layered van der Waals system with a giant SOC.[10] The studied system serves as a template for similar structures, which according to previous calculations[11] can behave as a two-dimensional topological insulator (TI). Based on first principles calculations we distilled an effective model to describe the investigated sandwich structure, and using a new state of the art transport code[12] calculated transport properties of systems with experimentally relevant sample sizes.

## 2. Methods

The crystalline structure of the system considered is illustrated in **Figure 1**. A single layer of BiTeI consists of three atomic layers with triangular lattice of iodide, bismuth, and tellurium in ABC stacking order. Two BiTeI layers sandwich a graphene sheet in a manner that the tellurium layers are beside the graphene sheet on each side. Although a single trilayer of BiTeI lacks inversion symmetry the sandwich system considered here, built of two trilayers and a single sheet of graphene is inversion symmetric with a point-group symmetry $D_{3d}$, which contains threefold rotations, inversion, dihedral mirror planes and their combinations. The experimental in-plane lattice constant of BiTeI bulk is 4.34 Å,[13] whereas the lattice constant of graphene is 2.46 Å. In order to achieve the smallest number of atoms in the unit cell, a rotated $\sqrt{3} \times \sqrt{3}$ supercell of graphene and the unit cell of BiTeI was used. In this configuration, there is a reasonable 1.84% lattice mismatch in the heterostructure. This strain may slightly alter the band structure of the BiTeI layers, albeit our model focuses on the graphene layer, in which this effect is even weaker [11]. After relaxation the effective lattice constant of the system was 4.26 Å, which is indeed the lattice constant of the $\sqrt{3} \times \sqrt{3}$ supercell of graphene. The distance of the graphene sheet and the chalcogenide layers are in a typical vdW distance of 3.45 Å. The interlayer distances of BiTeI monolayer are the following: 1.71 Å of Bi-I distance and 1.83 Å as regards the Bi-Te distance.

All first principles calculations were carried out using the Vienna Ab initio Simulation Package (VASP)[14,15] with the augmented-plane-wave (PAW) method within the generalized gradient approximation (GGA) parametrized by Perdew, Burke, and Ernzerhof.[16] The proposed structure is periodic in the $xy$ plane and separated by vacuum of at least 28 Å along the $z$ direction to avoid the interactions between layers. All the atoms in the unit cell are fully relaxed until the force on each atom is

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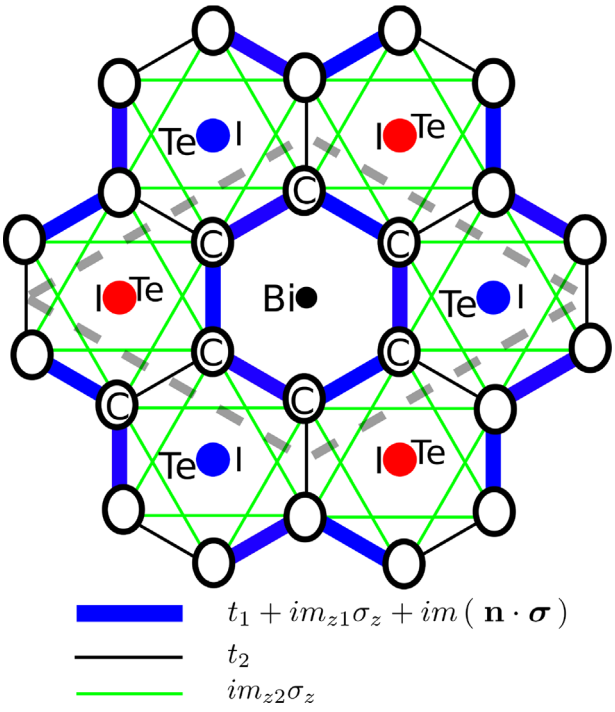


**Figure 1.** Illustration of the BiTeI-graphene sandwich illustrating a top view. The unit cell is designated by the dashed gray lines. The thick blue lines correspond to the first nearest neighbor hopping integral $t_1$, the out-of-plane $m_{z1}$ SOC and the in-plane $m$ SOC. The $\vec{n}$ vector is always perpendicular to the bond. The thin black lines correspond to $t_1$ and the green lines to $m_{z2}$.

less than 0.003 eV Å$^{-1}$. During the relaxation process the SOC was not included. To describe the vdW interaction, a semiempirical correction by Grimme was adopted.[17] The Brillouin zone integration was sampled by a $24 \times 24 \times 1$ $k$-grid mesh. An energy cutoff of 500 eV was chosen for the plane wave basis. After relaxation a self-consistent single-point calculation was done with SOC included,[18] with a reduced $k$-grid mesh of $18 \times 18 \times 1$, due to lack of symmetry. According to the VASP computation, the system is a band insulator with a 36 meV wide energy gap at the $\Gamma$ point.

Our model concentrates on an effective description of the electronic states near the Fermi level of the system. Hence we consider the modification of the graphene $\pi_z$-orbitals induced by spin–orbit interaction due to the presence of the BiTeI monolayers. To construct our Hamiltonian, we consider hopping between the nearest neighbor carbon atoms. Beyond the usual hopping integrals, we assumed spin–orbit interaction on bonds as: $t\mathbf{I} + i\mathbf{m}\boldsymbol{\sigma}$, where $\mathbf{m}$ is a real valued vector, $\boldsymbol{\sigma}$ is the vector of the Pauli matrices, and $\mathbf{I}$ is the $2 \times 2$ identity matrix. The in-plane component of the $\mathbf{m}$ vector on each bond is restricted by symmetry and points perpendicular to the bond. On the second-nearest neighbors we only assumed an out-of plane SOC interaction. After taking into account the symmetries of the system our simple model consists of five different parameters. Two different nearest neighbor hopping integrals $t_1$ and $t_2$, the in-plane $m$ and out-of-plane $m_{z1}$ SOC and the second-nearest neighbor out-of-plane SOC $m_{z2}$. In Figure 1, the thick blue lines correspond to $t_1$, $m$, and $m_{z1}$, the thin black lines to $t_2$, whereas the green lines correspond to $m_{z2}$. The in-plane component of the SOC on the thin black bonds is zero due to symmetry just like the out-of-plane component of the SOC on these bonds. To obtain transport characteristics of the system we used the EQuUs package,[12] designed for transport calculations implementing the equilibrium Green's function formalism developed in Refs. [19–22]. Using our effective model Hamiltonian, we obtained first the Green's function $G = (E - H)^{-1}$ and the associated transmission amplitude matrix $(t)$ finally in the spirit of Landauer's formalism[23,24] the conductance $\mathcal{G}$ is calculated from $t$:

$$\mathcal{G} = \frac{e^2}{h}\mathrm{Tr}\left(t^{\dagger}t\right). \tag{1}$$

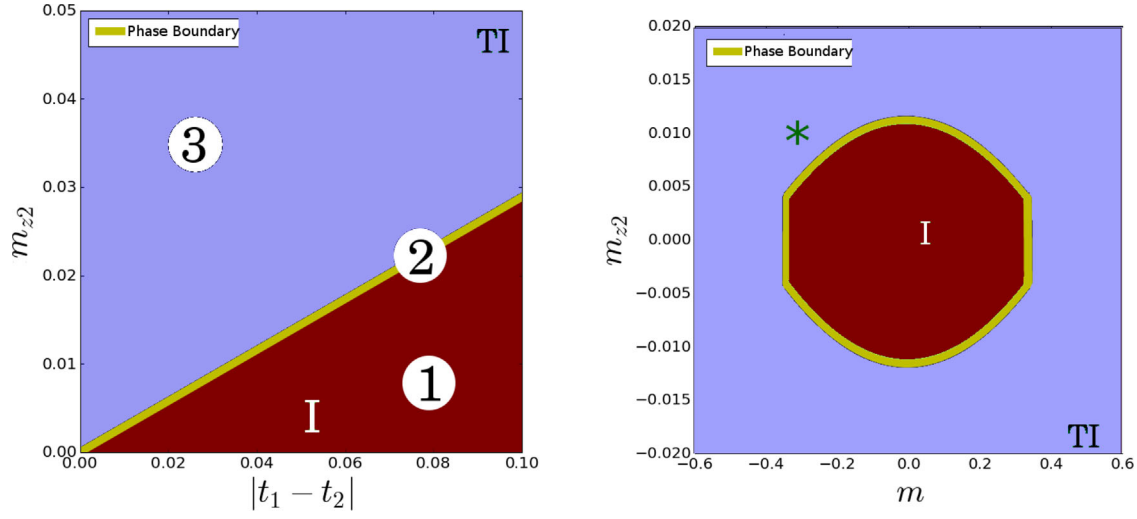


**Figure 2.** Phase diagrams of the system. All units are in eV. If the parameters of the system are in the light blue region then the system is topological insulator, when in the dark red region it is a trivial insulator. On the phase boundary the system is metallic. In the left panel $m_{z1} = 0 = m$, whereas in the right panel $t_1 = 2.20$ eV, $t_2 = 2.19$ eV, and $m_{z1} = 176$ meV. In the right panel the * denotes the parameter values fitted to first principles calculations.


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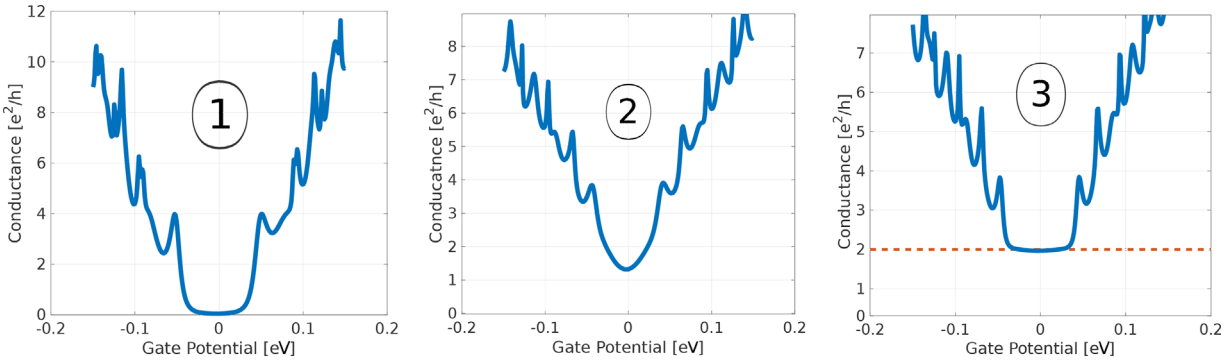


**Figure 3.** Transport properties of the model for different phases. The appropriate parameter values are indicated on the phase diagram in the left panel of Figure 2.

## 3. Results

Depending on the parameters, our model can behave as an insulator, a metal, or a topological insulator.

By calculating the product of the inversion eigenvalues of the occupied states at time reversal invariant momenta, we extract the $\mathbb{Z}_2$ topological invariant of the system.[25] The two different insulating phases of the system can be observed in **Figure 2**. The yellow line is the phase boundary. For parameter values located exactly on the line the model is metallic. The dark red region of the phase diagram indicates that the system behaves as a trivial insulator and the light blue region shows if it is a topological insulator.

We performed transport calculations to obtain the conductance of a clean sample depicted in the abstract figure using the EQuUs package.[12]

We calculated the transmission of the proposed material through a strip of armchair-structured graphene, where the scattering region was the hybrid BiTeI-graphene-BiTeI sandwich. The contacts were modeled by a doped clean armchair-structured graphene sample as it is common practice in the literature.[26] Under the scatterer we assumed a back gate, which can be used to dope the scattering region.

In order to expose the topological character of the investigated system, we have to suppress wavefunction overlap of states located at opposite edges. Choosing a 100 nm long and 100 nm wide geometry, we were able clearly demonstrate signatures of the TI phase, namely a quantized conductance even for model parameter values consistent with the first principles calculations.

The first plot in **Figure 3** shows a trivial insulator, the second plot reveals a metallic state while on the last figure we can observe a plateau in the conductance which is a hallmark of the TI state. The width of the plateau depends on the size of the scattering region and it could be the same as the gap of the band structure at most. These transport characteristics are hence consistent with the phase diagram on the left side figure on 2.

On the right panel of Figure 3, we show the conductance of the system with parameters fitted to VASP calculations. The fitted parameters are indicated on the right panel of Figure 2 by a green star: $t_1 = 2.20$ eV, $t_2 = 2.19$ eV, $m = -309.5$ meV, $m_{z1} = 1.76$ meV, and $m_{z2} = 10.94$ meV.

As shown in **Figure 4** there is a plateau in the conductance, demonstrating that a sandwich structure formed from BiTeI and graphene is a topological insulator, which indicates that our calculations are in agreement with the prediction of Kou et al.

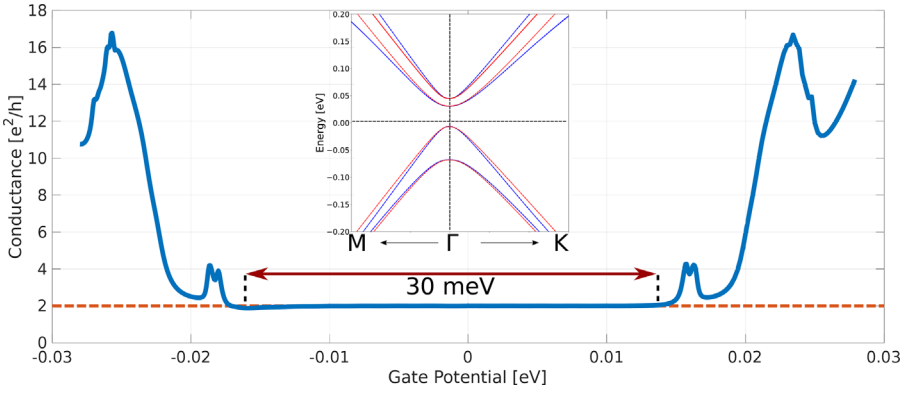


**Figure 4.** Transport properties of the model with parameters fitted to *ab initio* calculations. The band structure of the system near $\Gamma$ point calculated by VASP (blue lines) and by our model (red lines) can be observed in the inset. The width of the plateau corresponds to the gap of the band structure. The energy is measured from the Fermi energy.


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## 4. Conclusions

We present a simple model for a graphene-based topologically nontrivial heterostructure. Our simplified model is suitable for calculating transport properties on the micron scale. Depending on its parameters our model can behave as topological insulator, insulator or metal. Performing first-principles calculations with the VASP package we found material specific parameters for our model and calculated conductance traces for clean systems. Our model transport calculations and *ab initio* results confirm the findings of Kou et al., namely that the investigated system is a topological insulator.

## Acknowledgements

The Hungarian National Research, Development and Innovation Office (NKFIH) grants no. K115608, K108676, and K115575 are acknowledged for support. OL acknowledges the Bolyai program of the Hungarian Academy of Sciences.

## Conflict of Interest

The authors declare no conflict of interest.

## Keywords

BiTeI, graphene, topological insulator, transport

Received: August 1, 2017
Published online:

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