Doctoral School of Physics - Eötvös Loránd University (ELTE)

Semester Report 3

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PhD Program: Statistical Physics, Biological Physics and Physics of Quantum Systems

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Ph.D. Thesis title: Investigation of Layered Topological Insulators

Description of research work carried out in current semester

Graphene can be thought as the prototype of 2D topological insulators with negligible spin-orbit coupling [1] albeit the non-trivial gap is too small. Bi2Te3 prototypical three-dimensional topological insulators supply surface states which against back scattering inside the bulk band gap and protected by time reversal symmetry caused by spin-orbit coupling-induced topology [2].

In order to overcome the shortage of negligible band gap of the graphene, several conceptually different mechanisms have been exploited to open a band gap in graphene. The spin−orbit coupling (SOC) can be enhanced by using diluted heavy adatoms which in turn can open a gap in graphene. Another options for opening band gap in graphene are breaking of the sublattice symmetry on a substrate of proper symmetry or inducing inequivalent hopping rates between the sublattice site leading to scattering of the Dirac electrons [3].

Here, we represent a systematic study of the electronic properties of monolayer graphene on the surface of Bi2Te3 topological insulators, giant spin-orbit coupling is induced by the proximity effect [4]. In order to analyze spin projection of the Dirac electrons, I prepared the geometry with VESTA. We consider a quintiple layer of Bi_2Te_3 with lattice constant a = b = 4.38 Å and a 15 Å thick vacuum layer was introduced to avoid possible effects between image supercells.

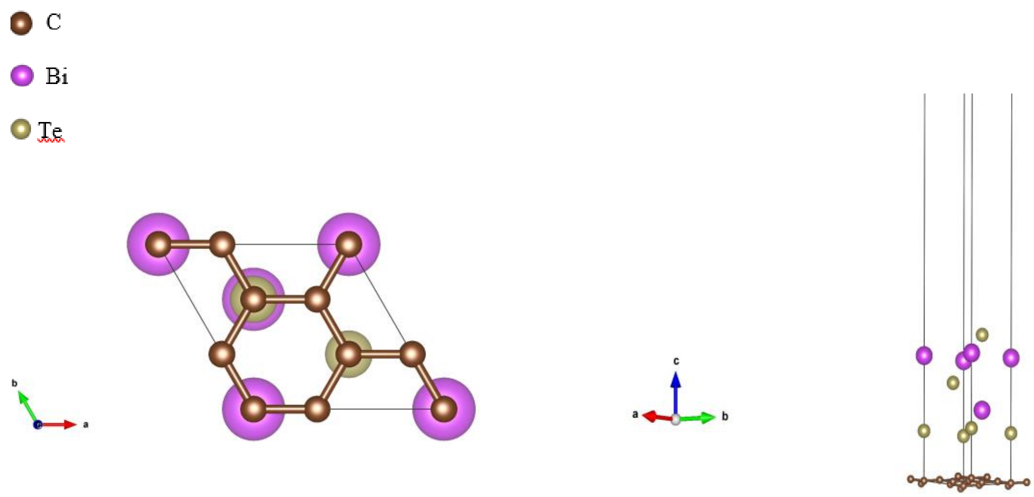

Figure 1. Lattice structures of graphene and Bi_2Te_3 topological insulator heterostructures

T Phase (top and side view).

The electronic structure calculations are performed by density functional theory (DFT) which is implemented in SIESTA package. Self-consistent calculations for T phase are performed for the k-point sampling from 6x6x1 till 24x24x1 by 2 increments and cutoff energy from 200 Ry to 650 Ry by 50 increments. Energy cutoff and K-points optimizations yield Ecut = 300 Ry and K-points as 18x18x1.

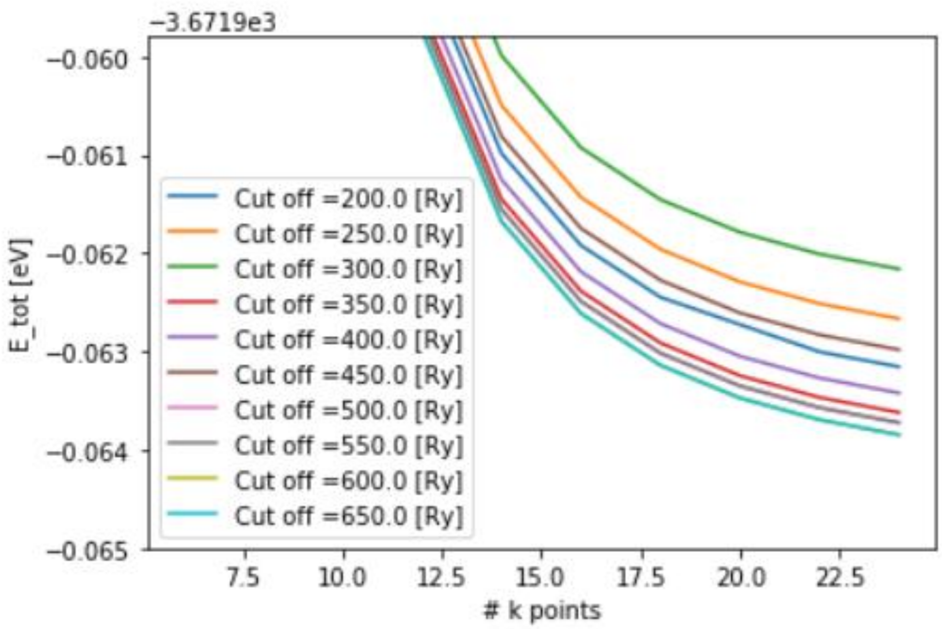

Figure 2. Convergence of K point and Mesh-Cutoff for T Phase

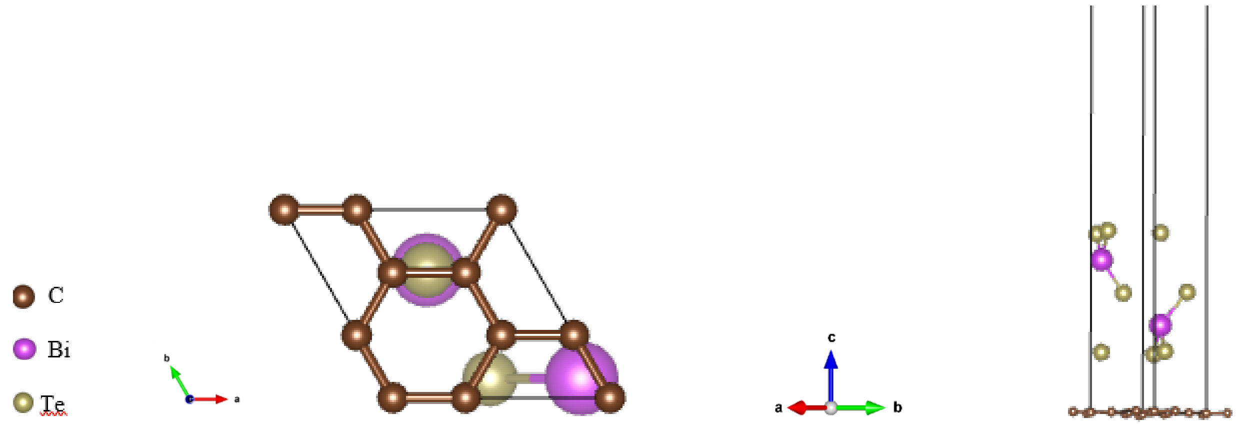

Figure 3. Lattice structures of graphene and Bi2Te3 topological insulator heterostructures

B Phase (top and side view).

Self-consistent calculations for B phase are performed for the k-point sampling from 6x6x1 till 24x24x1 by 2 increments and cutoff energy from 200 Ry to 650 Ry by 50 increments. Energy cutoff and K-points optimizations yield Ecut = 350 Ry and K-points as 20x20x1.

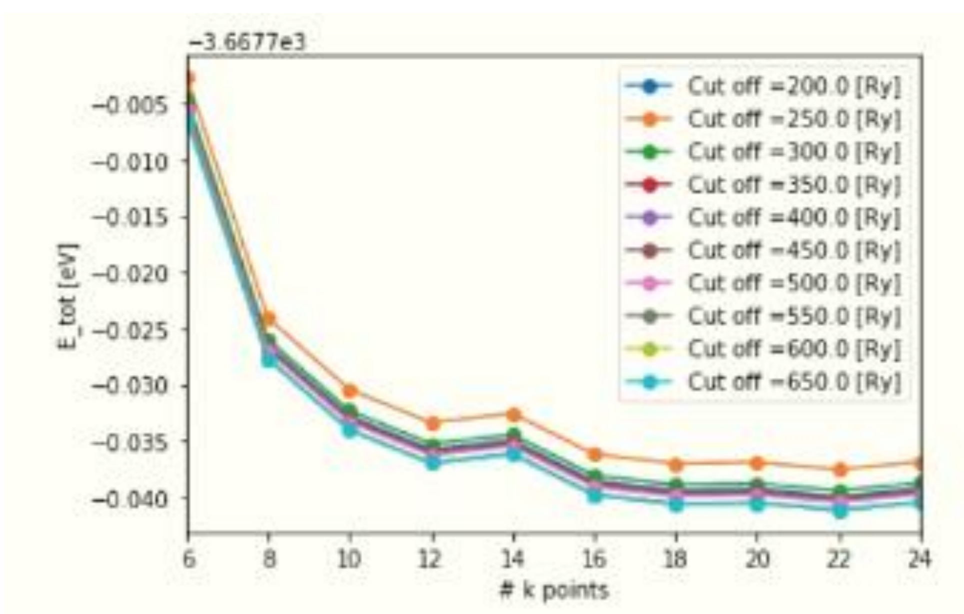

Figure 4. Convergence of K point and Mesh-Cutoff for B Phase

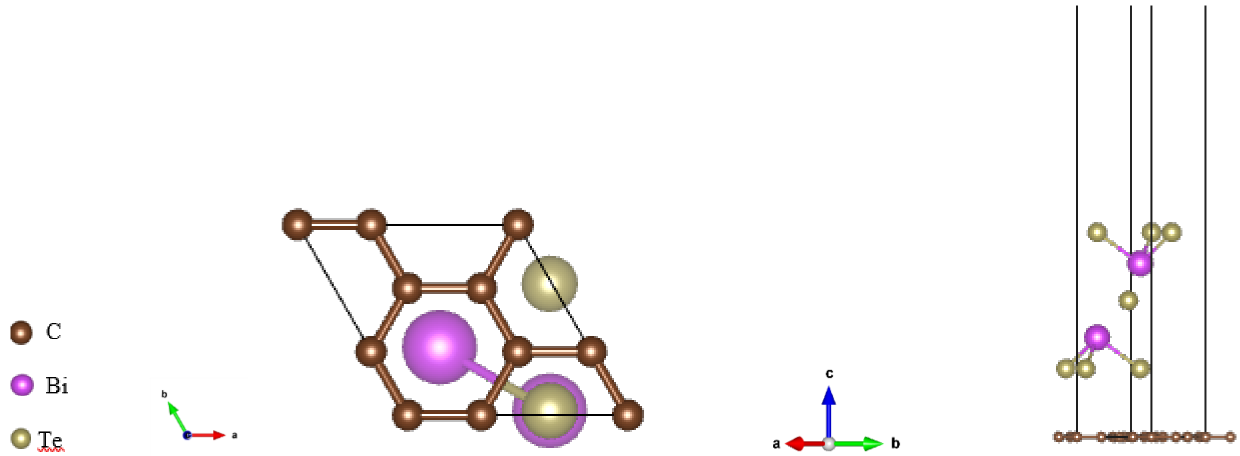

Figure 5. Lattice structures of graphene and Bi2Te3 topological insulator heterostructures H Phase (top and side view).

Self-consistent calculations for H phase are performed for the k-point sampling from 6x6x1 till 24x24x1 by 2 increments and cutoff energy from 200 Ry to 650 Ry by 50 increments. Energy cutoff and K-points optimizations yield Ecut = 350 Ry and K-points as 20x20x1

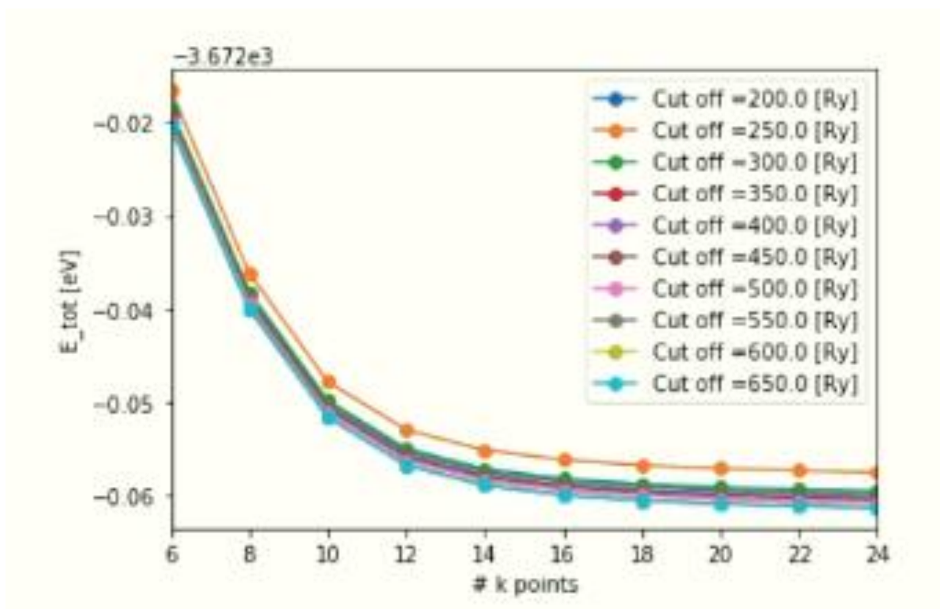

Figure 6. Convergence of Mesh-Cutoff and K point with SOC for H Phase

For the gap opening in these heterostructure, it is tempting to treat spin orbit coupling (SOC) effects. Therefore, after relaxation geometry on each phases l performed calculations with k-point sampling from 18x18x1 till 54x54x1 by 6 increments and cutoff energy from 300 Ry to 900 Ry by 50 increments for T, B and H phases.

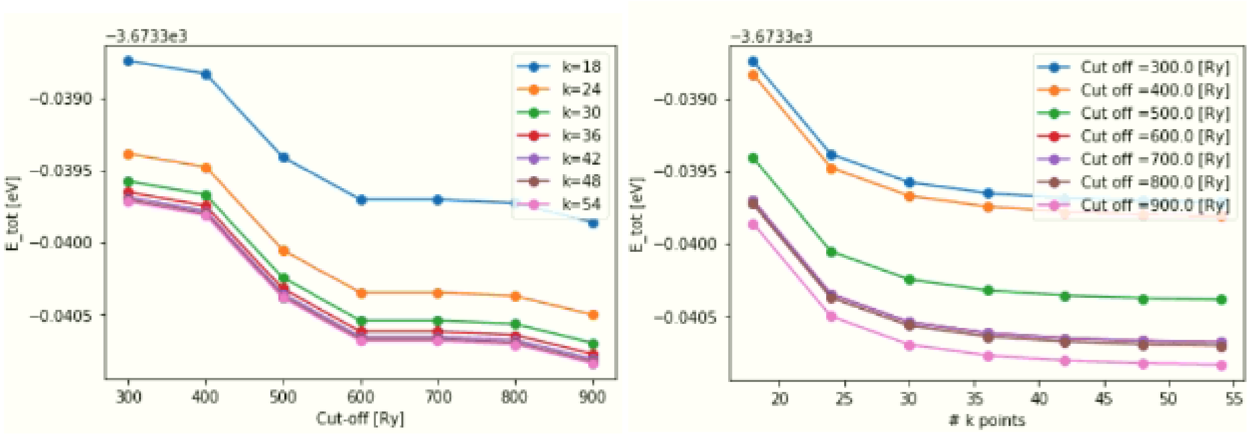

Figure 7. Convergence of Mesh-Cutoff and K point with SOC for T Phase

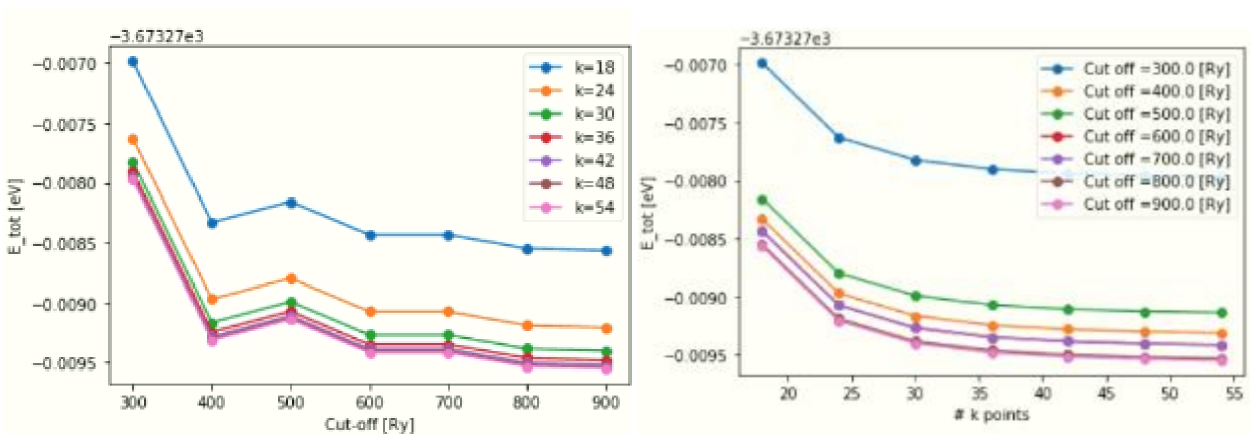

Figure 8. Convergence of Mesh-Cutoff and K point with SOC for B Phase

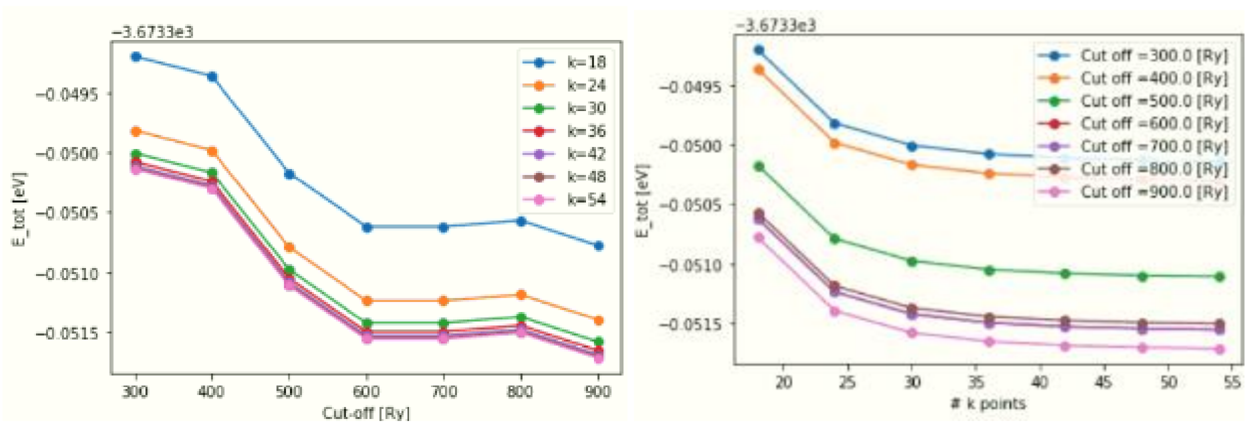

Figure 9. Convergence of Mesh-Cutoff and K point with SOC for H Phase

As a next step, in order to investigate topological properties of the above-mentioned material, we are in calculation time-reversal symmetry in the presence of the spin-orbit interaction. Ultimately, the light of these evidences of the topological properties of the considered material will be given by the Z2 topological invariant calculation via SISL package.

Description of educational activities carried out in the current semester

I have taken two new subjects during this semester which are: Grid Errors I, Transmission electron microscopy and electron diffraction.

Grid Errors I - Prof. Dr Jenő Gubicza guided us to obtain valuable information about various important properties of crystals which are controlled by imperfections, the interpretation of the plastic mechanical properties of crystalline solids, general description of twinning in hexagonal crystal, etc. out of his accumulated experience [5], [6]. I have reviewed the body-centered cubic, face-centered cubic (cubic close-packed), and hexagonal close packed crystal structures and also the closest packed planes, and closest packed directions and the relationships between them for each of the structures. Moreover, I have advanced my calculation skills in the means of c:a ratio for the hexagonal close packed (HCP) crystal structure, miller indices of planes and directions in a crystal structure and so on.

Transmission electron microscopy and electron diffraction – During the course, I have studied on the construction of a TEM: optical elements, electromagnetic lenses, image formation in the TEM, imaging of the lattice defects, the dislocations and three-dimensional defects, electron diffraction by amorphous materials and by crystals [7], [8].

Furthermore, I follow up reading newly published scientific articles about Condensed Matter Physics regularly on https://arxiv.org/. Reporting essential articles under the scope of our team I managed to refine my scientific analysis skills [9], [10]. On the other hand, I broaden my knowledge in physics as well as in related computational part within the current period of my PhD studies.

The Coding School's Qubit by Qubit's Introduction to Quantum Computing with IBM Quantum The Quantum Computing is an additional course out of the university curriculum which is organized by The Coding School and IBM Quantum Computing Research. It is a first-of-its-kind course aimed at making quantum computing accessible to university students.

The full course period divided into two semesters:

Semester 1 focused on the foundational math, programming, and physics concepts necessary for quantum computing. I expanded my understandings of the Classical Computing, Quantum Computing in the Abstract, Math: Introduction to Vectors and Complex Numbers, Probability Math for Quantum Mechanics, Introduction to Python Programming and learned making measurements on circuit composer by using quantum gates. I have attended laboratories and seminars, submitted every assignment on weekly basis. I started to the second term of the course after successfully completing the Semester 1.

When it comes to the Semester 2, it focuses on the Quantum Mechanics, Quantum Information and Computation, and Quantum Algorithms. The second part of the above-mentioned course will guide and explain me the ways using Qiskit and IBM Quantum Experience to run quantum simulations on real quantum hardware.

Conference - CMD2020GEFES

It was a large international conference covering all aspects of Condensed Matter Physics. The conference combines the biennial meeting of the Condensed Matter Divisions of the Spanish Royal Physics Society (RSEF-GEFES) and of the European Physical Society (EPS-CMD).

Awards

Stipendium Hungaricum Scholarship

Hungarian Quantum Technologies Excellence Project

References

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