Doctoral School of Physics - Eötvös Loránd University (ELTE)

Semester Report 2

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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].

In my research work, l placed 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 l 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.

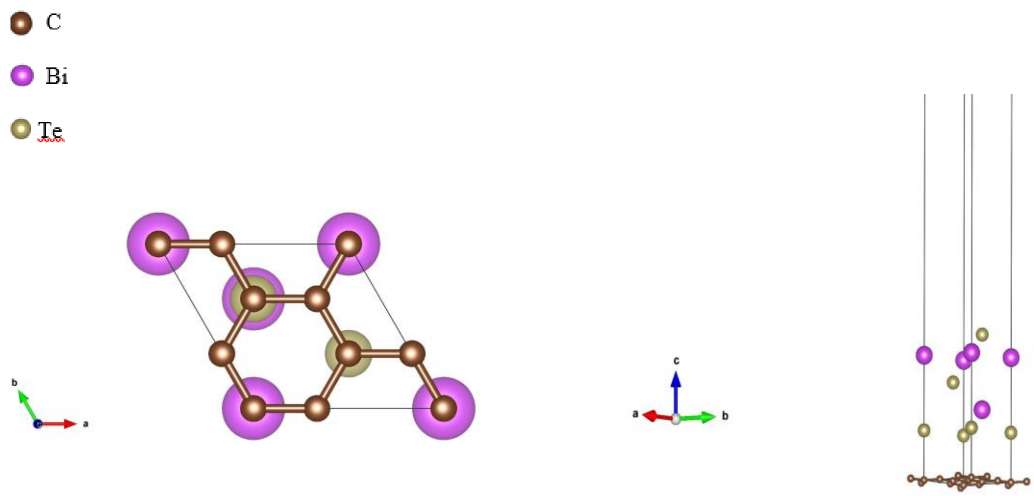

Figure 1. Lattice structures of graphene and Bi_2Te_3 topological insulator heterostructures (top and side view).

The electronic structure calculations are performed by density functional theory (DFT) which is implemented in SIESTA package. Self-consistent calculations 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.

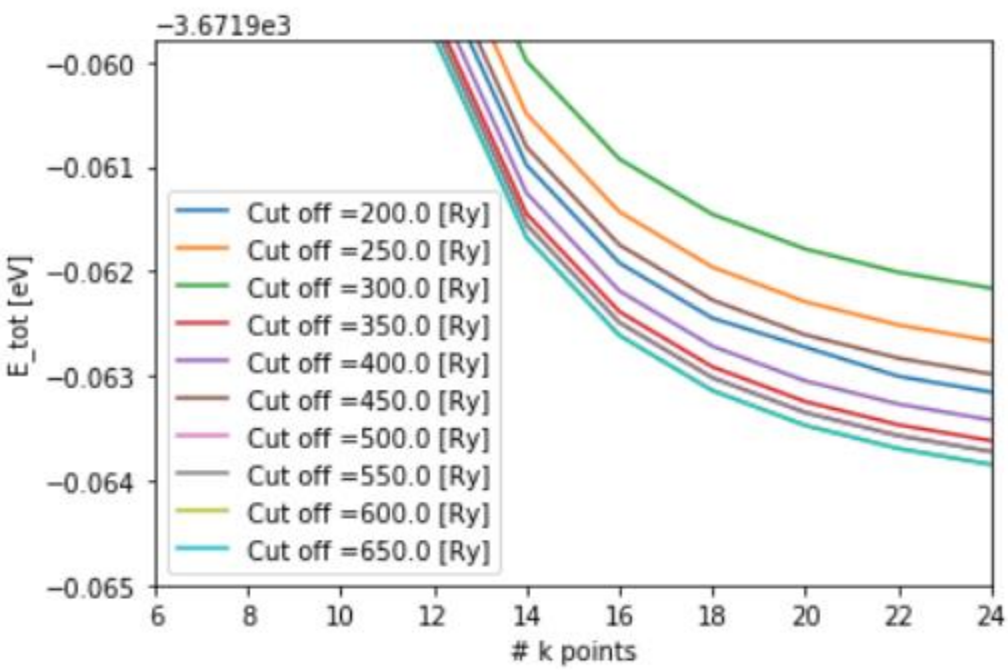

Figure 2. Convergence of K point and Mesh-Cutoff

As a next step, in order to investigate topological properties of the above mentioned material, the spin-orbit interaction is included and we are in calculation of the electronic band structure in the presence of the spin-orbit interaction. Finally, in order to provide smoking gun proof of the topological properties of the considered material the Z2 topological invariant via SISL package. Note that, until now, we have done the calculations only for the **T** phase and all the calculations should be repeated for the **H** and **B** phase, accordingly.

Description of educational activities carried out in current semester

l have registered three subjects during this semester: Carbon Nanostructures, Fractal Growth, Deep learning and machine learning in natural science.

Carbon Nanostructures - In this course, Prof. Kürti Jenő taught us combined theoretical and experimental description carbon allotropes: diamond, graphite, C60 (buckminsterfullerene or buckyball), single-walled carbon nanotube or buckytube. Specifically, l have learned the history of C60 [5] and its symmetry, energy levels, band structures, optical properties. Moreover, l learned how to calculate the number of pentagons and hexagons in fullerenes based on Euler's rule, vibrational analysis of C60 by using the character table of icosahedral symmetry to find the vibrational modes, one-electron energy levels of C60, reduction of the 60 dimensional reducible representation, spanned by the 60 p_z atomic orbitals, reduction of the 180 dimensional reducible representation spanned by the displacement vectors of the 60 atoms (nuclei) [6].

Fractal Growth – In this course, l have carried out a project which was aiming at creating an interactive Diffusion Limited Aggregation (DLA) simulation in a form of a python notebook. By simulating DLA l introduced interactive growth process of DLA cluster [7]. l calculated the objects fractal dimension by using correlation dimension. Simply using the definition and multiple pivot points, l calculated the objects multifractal spectrum [8] and plot some interactive plots about the growing cluster and the attachment of particles to the cluster.

Deep learning and machine learning in natural science – l have completed two challenges during this course. The first challenge was about Photometric redshift estimation. The data consists of the magnitudes of galaxies measured with various filters, celestial positions, shape properties and spectroscopic, which was measured using spectrography. l predict the redshift of galaxies based on only the photometric data. The dataset was generated with the Sloan Digital Sky Survey. l calculated the empirical photo-z method and estimated the redshift via local regression method on a spectroscopic training set based on Beck, Róbert, et al paper [9], then fitting a spectrum template to obtain K-corrections and absolute magnitudes [10], [11].

The second challenge was image classification challenge about tiger mosquito. By using deep learning model which called the convolution neural network (CNN) l build a classifier that can correctly decide if the presented image contains a tiger mosquito or not. Convolution neural network (CNN) is very interested in machine learning and has excellent performance in hyperspectral image classification, recognition problem and objects detection and. Deep learning CNN models to train and test, each input image will pass it through a series of convolution layers with filters. Convolution of an image with different filters can perform operations such as edge detection, blur and sharpen by applying filters [12], [13].

Additionly, l review new recent articles about Condensed matter physics on https://arxiv.org/ weekly [14], [15], [16]. By this task l improved my skills in efficient ways of reporting and presenting. During my first year of doctoral studies, I strengthened and expand my knowledge in physics and related computational stuff.

Awards

Stipendium Hungaricum Scholarship

Hungarian Quantum Technologies Excellence Project

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