
TOPOLOGICAL INSULATOR: GRAPHENE

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1 Introduction

[Topological insulator](#) is a exotic state on the surfaces of some materials, that's means that the interior of the material or bulk behaves as an insulator. We can connect this state with graphene through Quantum Spin Hall Effect and graphene nanoribbons.

2 Graphene: Description

2.1 Crystal estructure

[Graphene](#) is arranged in a hexagonal lattice of only carbon atoms.

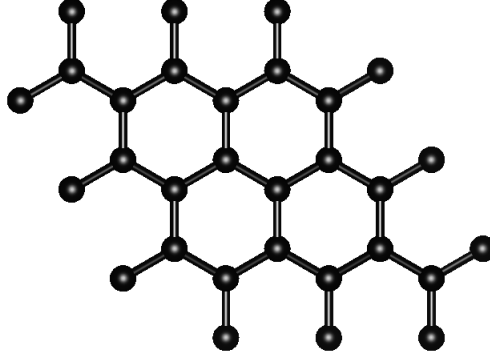


Figure 1: Crystal structure of graphene

Carbon atoms have an electronic configuration $1s^2 2s^2 2p^2$, where their outermost shell has 4 electrons (valence electrons). From this we could expect that these atoms form only 2 covalent bonds, but this is not the case. Since experimentation it is known that the carbon atom actually forms 4 covalent bonds when it interacts with other atoms. This is because a special type of orbital is formed through the hybridization of orbitals, called sp^2 hybridization.

2.2 Primitive vectors of real and reciprocal space

Because we find non-equivalent atoms (A and B) in the hexagonal lattice, we consider the lattice as a superposition of two triangular sublattices.

The primitive vectors are given by:

$$\vec{a}_1 = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \quad , \quad \vec{a}_2 = a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \quad (1)$$

Where $a = \sqrt{3}a_{cc}$ and $a_{cc} = 1.42\text{\AA}$.

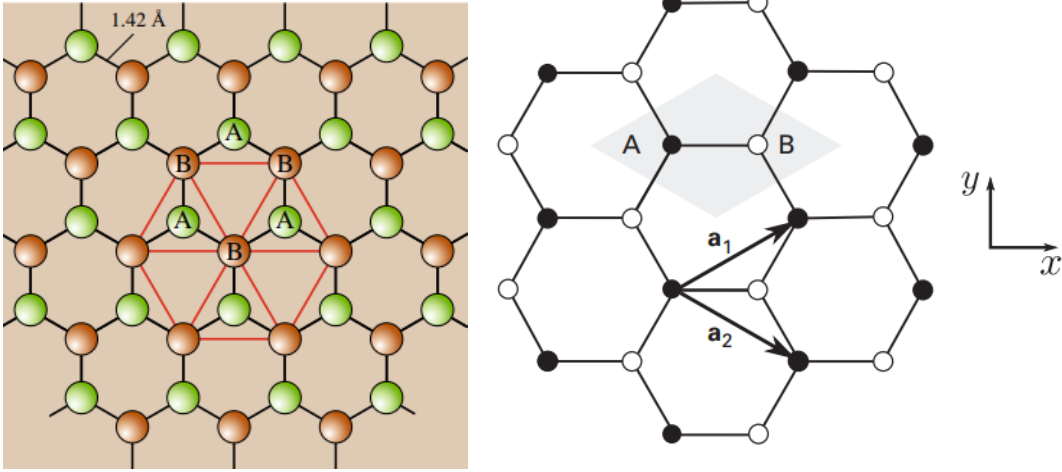


Figure 2: Real space lattice where (a) Superposition of lattice A and B [1] and (b) Base with atoms A and B, and primitive vectors \vec{a}_1 y \vec{a}_2 [2].

In the case of the reciprocal network, we will have that the primitive vectors will be:

$$\vec{b}_1 = \frac{4\pi}{\sqrt{3}a} \left(\frac{1}{2}, \frac{\sqrt{3}}{2} \right) , \quad \vec{b}_2 = \frac{4\pi}{\sqrt{3}a} \left(\frac{1}{2}, -\frac{\sqrt{3}}{2} \right) \quad (2)$$

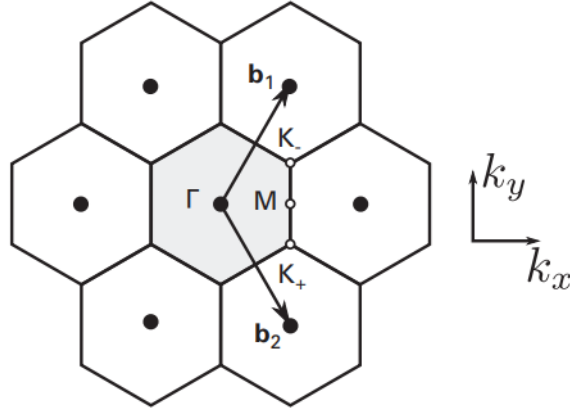


Figure 3: Reciprocal space lattice, where the shaded hexagon refers to the first Brillouin zone [2].

From the first Brillouin zone (Figure 3), we can obtain points of high symmetry (K_- , K_+ , M) which will be very useful to simulate the electronic structure.

$$M = \frac{2\pi}{\sqrt{3}a} (1, 0) , \quad K_+ = \frac{4\pi}{3a} \left(\frac{\sqrt{3}}{2}, -\frac{1}{2} \right), \quad K_- = \frac{4\pi}{3a} \left(\frac{\sqrt{3}}{2}, \frac{1}{2} \right) \quad (3)$$

2.3 Tight binding model

In the π band approximation, it is important to keep in mind that atom A or B are defined by only one orbital per atom since only the p_z orbitals (responsible for forming the π bonds) contribute to the electronic properties.

Eigenfunctions are a linear combination of the Bloch sums of each lattice:

$$\psi(k, r) = c_A(k)\phi^A(k, r) + c_B(k)\phi^B(k, r) \quad (4)$$

So for the π orbitals

$$\phi^A(k, r) = \frac{1}{\sqrt{N}} \sum_{R_j} e^{ik \cdot R_j} \varphi(r - r_A - R_j) \quad (5)$$

$$\phi^B(k, r) = \frac{1}{\sqrt{N}} \sum_{R_j} e^{ik \cdot R_j} \varphi(r - r_B - R_j) \quad (6)$$

If we use Schrodinger's equation to solve the eigenvalue problem:

$$H\psi(k, r) = E\psi(k, r) \quad (7)$$

Expressing it in matrix terms

$$H(k) \begin{pmatrix} c_A(k) \\ c_B(k) \end{pmatrix} = \begin{pmatrix} H_{AA}(k) & H_{AB}(k) \\ H_{BA}(k) & H_{BB}(k) \end{pmatrix} \begin{pmatrix} c_A(k) \\ c_B(k) \end{pmatrix} = E(k) \begin{pmatrix} S_{AA}(k) & S_{AB}(k) \\ S_{BA}(k) & S_{BB}(k) \end{pmatrix} \begin{pmatrix} c_A(k) \\ c_B(k) \end{pmatrix} \quad (8)$$

If we ignore the overlap of neighboring p_z orbitals, we will obtain:

$$S_{\alpha\beta}(k) = \delta_{\alpha\beta} \quad (9)$$

That's means the Bloch sum form an orthonormal set

$$S_{\alpha\beta}(k) = \delta_{\alpha\beta} \quad (10)$$

and the matrix elements of the Hamiltonians are expressed as follows

$$H_{AA}(k) = \frac{1}{N} \sum_{R_i, R_j} e^{ik \cdot (R_j - R_i)} \langle \varphi^{A, R_i} | H | \varphi^{A, R_j} \rangle \quad (11)$$

$$H_{BB}(k) = \frac{1}{N} \sum_{R_i, R_j} e^{ik \cdot (R_j - R_i)} \langle \varphi^{B, R_i} | H | \varphi^{B, R_j} \rangle \quad (12)$$

with $H_{AA} = H_{BB}$ and $H_{AB} = H_{BA}^*$.

Considering equation (8), equation (7) reduces to the following expression

$$\begin{pmatrix} H_{AA}(k) & H_{AB}(k) \\ H_{BA}(k) & H_{BB}(k) \end{pmatrix} \begin{pmatrix} c_A(k) \\ c_B(k) \end{pmatrix} = E(k) \begin{pmatrix} c_A(k) \\ c_B(k) \end{pmatrix} \quad (13)$$

If we restrict the interaction to the first neighbors

$$H_{AB}(k) = \langle \varphi^{A, 0} | H | \varphi^{B, 0} \rangle + e^{-ik \cdot a_1} \langle \varphi^{A, 0} | H | \varphi^{B, -a_1} \rangle + e^{-ik \cdot a_2} \langle \varphi^{A, 0} | H | \varphi^{B, -a_2} \rangle \quad (14)$$

$$H_{AB}(k) = \gamma_0 \alpha(k) \quad (15)$$

Where γ_0 is a transfer integral and $\alpha(k)$ is defined as

$$\alpha(k) = 1 + e^{-ik \cdot a_1} + e^{-ik \cdot a_2} \quad (16)$$

If we choose a reference energy, such that $H_{AA} = H_{BB} = 0$. It allows us to write the Hamiltonian as

$$H = \begin{pmatrix} 0 & -\gamma_0 \alpha(k) \\ -\gamma_0 \alpha(k)^* & 0 \end{pmatrix} \quad (17)$$

Now we have to find the eigenvalue (the energy), this is possible by diagonalizing the Hamiltonian of equation (17)

$$|H(k) - EI| = 0 \quad (18)$$

$$E^\pm(k) = \pm \gamma_0 |\alpha(k)| \quad (19)$$

$$E^\pm(k) = \pm \gamma_0 \sqrt{3 + 2\cos(k \cdot a_1) + 2\cos(k \cdot a_2) + 2\cos(k \cdot (a_2 - a_1))} \quad (20)$$

$$E^\pm(k) = \pm \gamma_0 \sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)\cos^2\left(\frac{k_y a}{2}\right)} \quad (21)$$

To simulate the electronic structure we must take into account that the wave vectors $K = (k_x, k_y)$ must be chosen within the first Brillouin zone [Per10]. And if we take into account the points of high symmetry mentioned above (K_+, K_-)

$$\alpha(k = K_+) = \alpha(k = K_-) = 0 \quad (22)$$

Using equation (21), we can graph

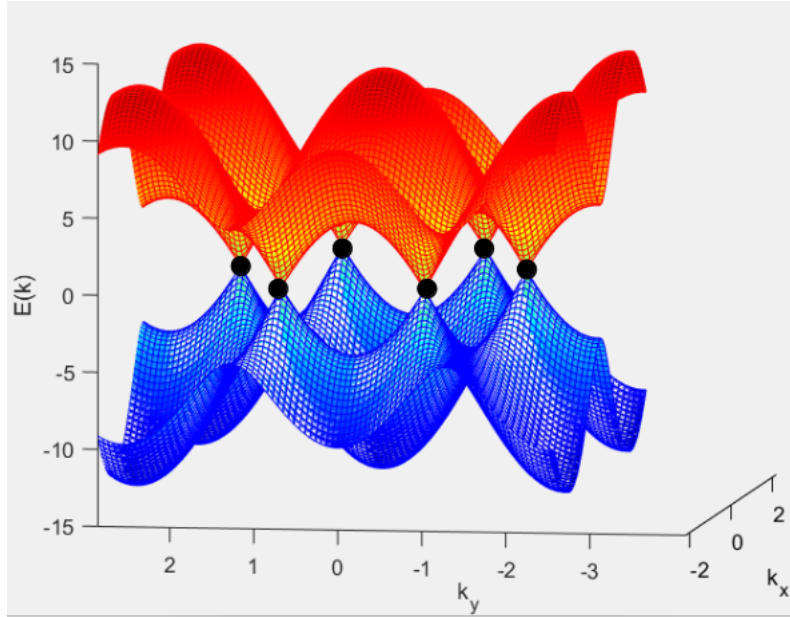


Figure 4: Graphene π and π^* electronic bands .

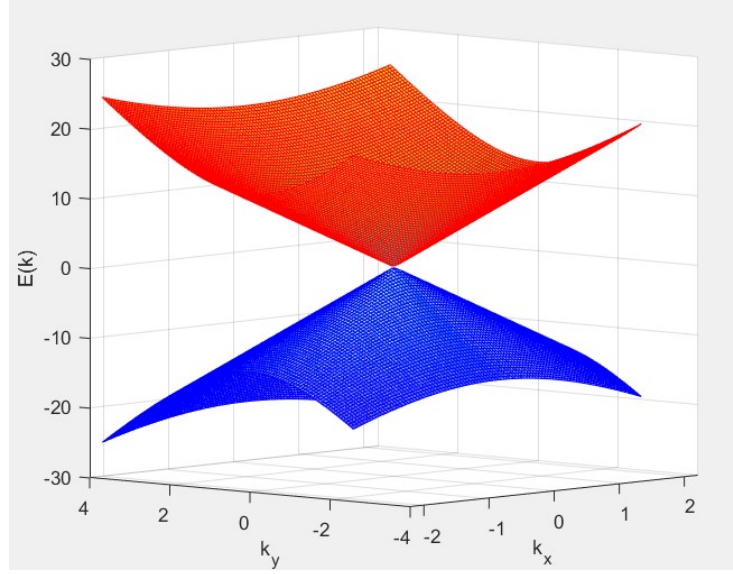


Figure 5: Dirac cones

2.4 Simulation: Band structure

It can be clearly observed that the gap of this material is 0 eV (there is no gap). This is possible to identify since the bands that are represented by the p_z orbitals are responsible for the electronic properties.

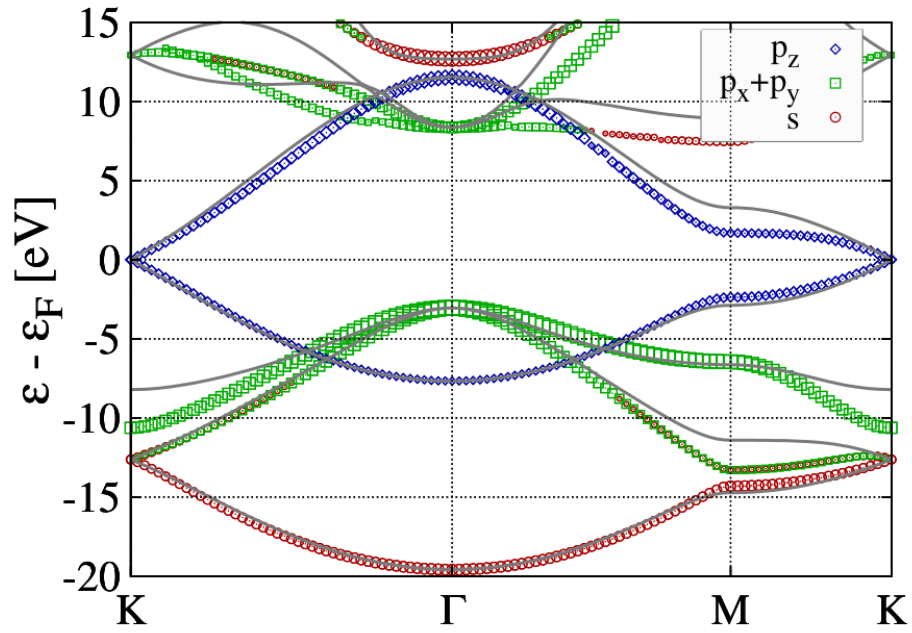


Figure 6: Band structure of graphene [3].

3 Graphene nanoribbons

Graphene nanoribbons are strips of graphene along a certain direction with a finite width.

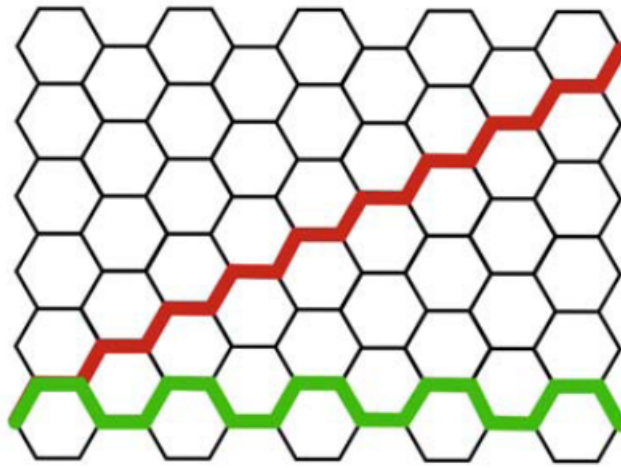


Figure 7: Types of edges: Zigzag (red) and armchair (green) [4].

4 Quantum Spin Hall Effect in graphene

4.1 Classical Hall effect

When a conductor or semiconductor with current flowing in one direction is introduced perpendicularly into a magnetic field, an electric field arises.

- Accumulation of charge occurs on the edge.
- Creates an electric field that counteracts the effect of the magnetic field on the moving charge.

4.2 Quantum Hall Effect

It's a quantized version of the Hall effect which is observed in two-dimensional electron systems to low temperatures and strong magnetic fields.

- Analog of charged object in the presence of a strong, orthogonal magnetic field: Spin-Orbit coupling.
- It's possible to measure Hall conductivity in quantum theory and we find that it is quantized.

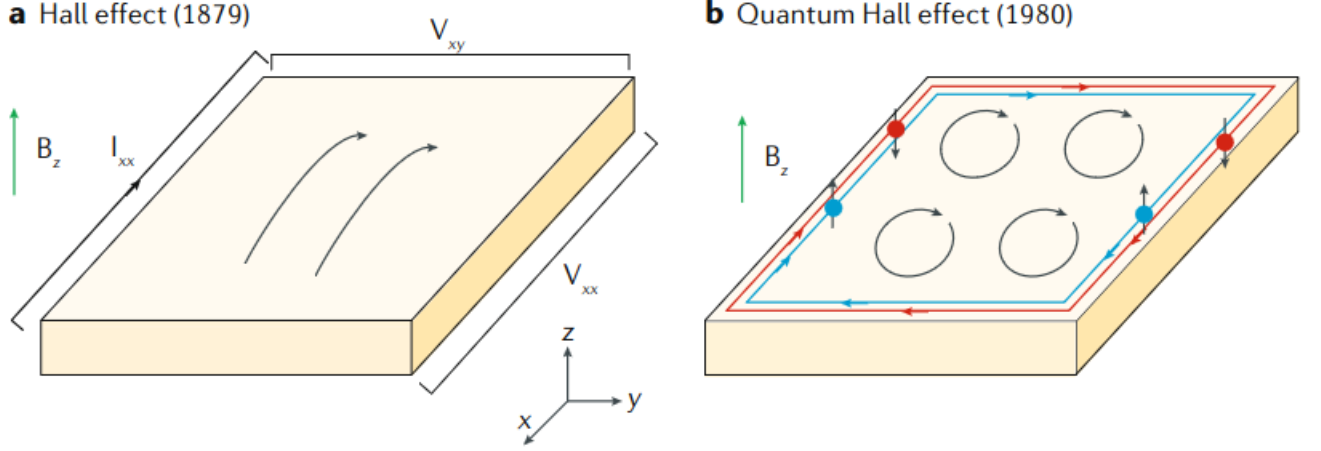


Figure 8: Classical and quantum Hall effect [5].

4.3 Quantum Spin Hall Effect

In a two-dimensional system the quantum spin Hall effect state is characterized by an insulating bulk and two counter propagating helical edge states. These edge channels are protected by time reversal symmetry and spin currents propagate without dissipation [6].

In the case of graphene, the Dirac points are protected by both time reversal (TR) and inversion symmetry. We will add Spin-orbit coupling at low temperatures invariant under TR and inversion symmetry. But to make graphene enter a quantum Hall state, we must open a gap at the Dirac points that's means it's necessary to break the time reversal or inversion symmetry.

Since haldane model we can considerate adding imaginary second-nearest neighbor hoppings, which breaks the TR symmetry. Haldane mentions that through this it is possible to see chiral edges states in graphene nanoribbons and this are topological origin.

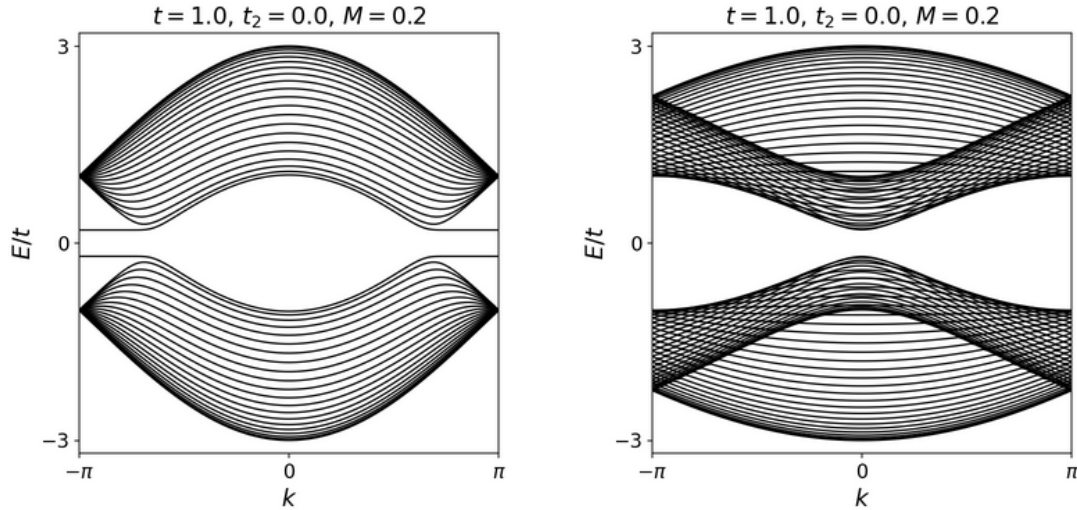


Figure 9: Band structure of graphene nanoribbons (a) Zigzag and (b) Armchair [7].

But Kane and Mele were able to open gaps without breaking any of the symmetries. The main idea is restore TR symmetry taking two copies of the Haldane model.

Through this and calculations performed on zigzag edges, we can see:

- Bands connect gaps.
- Opposite Dirac points and spins.
- Gapless edge states.
- Gapped bulk without magnetic field.
- These bands are localized at the edges of the strip, and each band has degenerate copies for each edge [8].

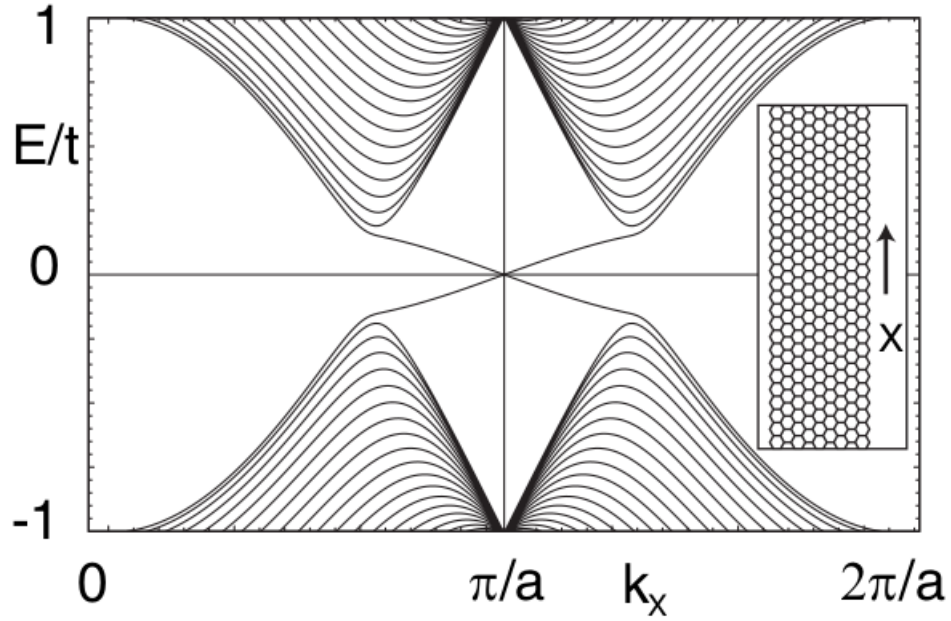


Figure 10: Band structure of zigzag edges [8].

It's a new topological state: Topological insulator.

4.4 Topological insulator: Graphene

This new state have some features, like:

- Edges obey TR symmetry, that's means robust against weak interactions and disorder.
- Dissipationless spin current.
- Non-chiral edges states.

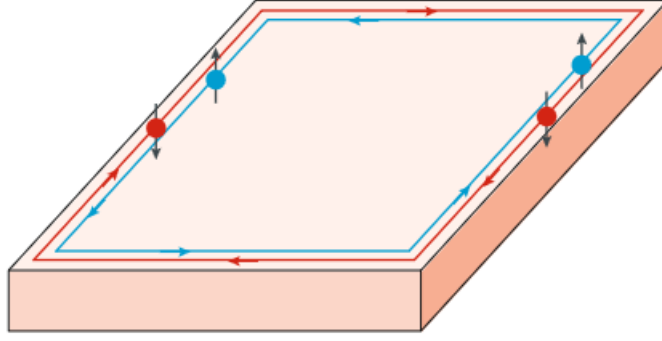


Figure 11: Representation of a topological insulator [5].

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