

MULTIFUNCTIONAL NANOMATERIALS AND NANODEVICES BASED ON TOPOLOGICAL INSULATORS

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Abstract: The discovery of topological insulators has become one of the most exciting recent developments in condensed matter physics. Some aspects of emergent multifunctional materials and nanodevices based on oxide compounds and topological insulator materials are highlighted. After physics and they become the materials platform for a new emergent multifunctional nanoelectronics and nanospintronics. The surfaces of topological insulators enable the transport of spin-polarized electrons while preventing the "scattering" typically associated with power consumption. Because of such characteristics, these materials hold great potential for use in future transistors, memory devices and magnetic sensors that are highly energy efficient and require less power. The first step to field effect transistor is illustrated for Bi₂Te₃ nanoribbons. The device potential for topological insulator nanotubes are analyzed. New memory device concept based on the intrinsic topological insulator attribute- Berry curvature is revealed.

I. Introduction

More than three decades ago there was established that spin-orbit interaction (SOI) has an important pattern on band structure of solid state matter. Among different qualitative features induced by SOI the band inversion of electronic spectrum near the Fermi level has been discovered. Such type of electronic spectrum was identified in different type of semimetallic and narrow-gap semiconductors Bi_{1-x}Sb_x, Pb_{1-x}Sn_xTe, Bi₂Te₃, HgTe, TlBiTe₂ etc. Last years investigations [1] have reopened the interest to materials with inverted band spectra. Due to new type of the symmetry break like that characteristic for the integer and fractional quantum Hall effects the electronic states was shown to have topological nature and materials have been named topological insulators (TI). In these materials new state of condensed matter is realized and on their basis a new platform for nanoelectronics and spintronics is developed in the last years. In TI a new state of matter appear, distinguished from a regular band insulator by a nontrivial time-reversal topological invariant, which characterizes its band structure, and non-trivial interplay of charge and spin degree of freedom of band electrons. In results new physics and phenomena related to this states have greatly emerged.

Part of interest in TIs stems from the fact that they represent a new topological phase of noninteracting electrons: the TI character of a material is its bulk property, nontrivially encoded in the wavefunctions of the occupied (valence band) states. However, it is the presence of the helical edge/surface states which leads to observable consequences. Their surface states are protected by time-reversal symmetry and show the Dirac cones connecting the inverted conduction and valence bands [1]. Like the Hall state the "bulk" of the electron gas of TI is an insulator, but along its surface, the states can be gapless. Within a certain parameter range the surface states of TI are well described by a Dirac cone, allowing for parallels with graphene and relativistic physics, and prohibiting backscattering. These Dirac cones constitute the topological transport regime, which has the gapless conducting and spin-momentum locked surface states leading to the suppression of backscattering. Such extraordinary surface states of the three-dimensional topological insulators may occur, as the term "surface" already suggests, only at the surfaces

or, more generally, interfaces where the topological invariant changes [2].

Unlike graphene, the states on the Dirac cone on the surface of the TI are spin filtered; they have fixed spin directions for each wave number k . In such way among many new topics developed in such materials and nanostructures, the most exciting one may be spintronics. Spintronics (or spin-electronics) is the term to express a field of electronics utilizing both charge and spin degrees of freedom possessed by an electron, which have been treated independently until recently. Because the state at k and that at $-k$ have the opposite spins, the perfect backscattering from k to $-k$ is forbidden. The gapless helical surface states with linear dispersion is similar to photons. Therefore, when two different TIs are attached together, the refraction phenomenon similar to optics is expected at the junction.

Exploring the properties of nanoscale topological insulators is a growing area of research and the present paper reveals some aspects of new interface and device physics of such materials. The spectrum and characteristics of topological interface states (TIS) depending on geometrical configuration can be manipulated by different factors: electrical and magnetic fields, strain and deformation etc. For this reason TI are being explored with a view towards applications, as a potential platform for tailoring nanostructures and nanomaterials properties. This topic covers the main part of the paper. Thermoelectric aspect of TSS are discussed in the context of TI materials Bi₂Se₃ and Bi₂Te₃ knowing as the best thermoelectric.

II. Topological Insulator Materials

An ordinary insulator such as glass cannot conduct electricity because electrons are not free to move through the material, but physicists have recently discovered a special type of insulator that behaves somewhat differently. The electrons inside or in the bulk of these 'topological insulators' behave like the electrons in conventional insulators. However, topological insulators have surface states in which electrons can flow as easily as in a metal.

The discovery of topological insulators has become one of the most exciting recent developments in condensed matter physics [6-7]. Topological insulators

are electron systems with a bulk gap and gapless edge states which are robust at presence of time-reversal symmetry. In two-dimension, a topological insulator has counter-propagating edge states with opposite spin polarization. Since the edge states carry unidirectional spin current, this state is also known as the ‘‘quantum spin Hall (QSH) insulator’’ [6]. The key reason that the QSH insulator is a new state of matter is that the back-scattering between left and right moving edge states is forbidden due to Kramers degeneracy [6]. The suppression of back-scattering can be understood intuitively as a consequence of perfectly destructive interference between two back-scattering processes in which the spins are rotated clockwise and counter-clockwise [7]. The surface state of a simplest three-dimensional topological insulator is a 2D ‘‘Dirac fermion’’ with linear dispersion and spin locked with the direction of velocity, which is a direct generalization of the QSH edge states. The same argument of back-scattering suppression holds for the surface states of three-dimensional topological insulators.

Because topological order is a global, non-local property, it is rather difficult to measure in the general situation. In a few important cases, such as the integer and fractional quantum Hall effects, and the topological insulators, the topological properties give rise to certain quantized responses [6-7]. These examples have topologically protected gapless boundary modes that dominate the responses. However, often there is no obvious ‘‘nice’’ response that can be computed or observed in experiment. The entanglement entropy and the entanglement spectrum have emerged as two important measures of the quantum entanglement and the topological properties.

One important result to emerge from the study of the ES of topological insulators is that a gapless ES can persist under some conditions where the physical edge spectrum becomes gapped. For example, applying a magnetic field to an topological insulator will gap the surface states but leave the entanglement spectrum gapless. These exotic properties result from the combined effect of spin-orbit interactions and time-reversal symmetry, and thus topological insulators are usually composed of heavy elements (Bi, Se, Te, Hg and so forth) because the larger nuclear charges of such elements lead to stronger spin-orbital coupling.

III. Topological Insulator Nanostructures and Nanomaterials

TI open new ways in nanoscale properties tailoring based on its heterostructure engineering. The electronic states of such materials are described by the low-energy effective 3D Hamiltonian [3], which has the 4×4 matrix form and can be expressed in general form as

$$H = \begin{pmatrix} \Delta(z) + V(z) & \bar{\sigma} \bar{p} - i(\bar{\sigma} \bar{u} + L) \\ \bar{\sigma} \bar{p} + i(\bar{\sigma} \bar{u} + L) & -\Delta(z) + V(z) \end{pmatrix} \quad (1),$$

where σ are the Pauli matrices, $\Delta = Eg/2 + M_1 k_2 z + M_2 k_2^2$, $\bar{p} = -i\hbar(v_{\perp} \nabla_x, v_{\perp} \nabla_y, v_{\parallel} \nabla_z)$, v_{\parallel} , v_{\perp} are the electron Fermi velocities, and $V(z)$ is the potential,

which incorporates the change in the work function in the structure and applied gate voltage. Following the results of our early works [4] we introduced the vector parameters u which describes the electrical polarization and the scalar L to describe the antiferromagnetic ordering with the antiferromagnetic vector along z -axis.

The junction breaks translation symmetry in the z -direction, and we let $kz \rightarrow -i\partial/\partial z$ to obtain a system of second order homogeneous differential equations $H(k \rightarrow -i\partial/\partial z)\chi = E\chi$. They are solved with the ansatz of the effective mass approximation. We first analyze topological states bound to the interface of TI and BI like PbTe/SnTe without antiferromagnetic ordering $L=0$ and electrical polarization $u=0$. In this case the energies of

$$E = E_0 \pm \frac{v_{\perp} k_{\perp} D}{\Delta_1 - \Delta_2}, \quad \text{where}$$

$$D^2 = (\Delta_1 - \Delta_2)^2 - (V_1 - V_2)^2 \quad \text{and}$$

$$E_0 = (\Delta_1 V_2 - \Delta_2 V_1)(\Delta_1 - \Delta_2)^{-1}$$

This helical nature of surface topological states of TI leads to new interface physics of heterojunction of two TI. In the case of two TIs, at the junction we expect a coupling between two surface states belonging to different TIs. In the framework of a simple model [5] which includes phenomenological coupling between massless relativistic states of the two TIs, it was shown earlier that the properties of the junction surface states strongly depend on the relative sign of the Fermi velocities of the two TIs.

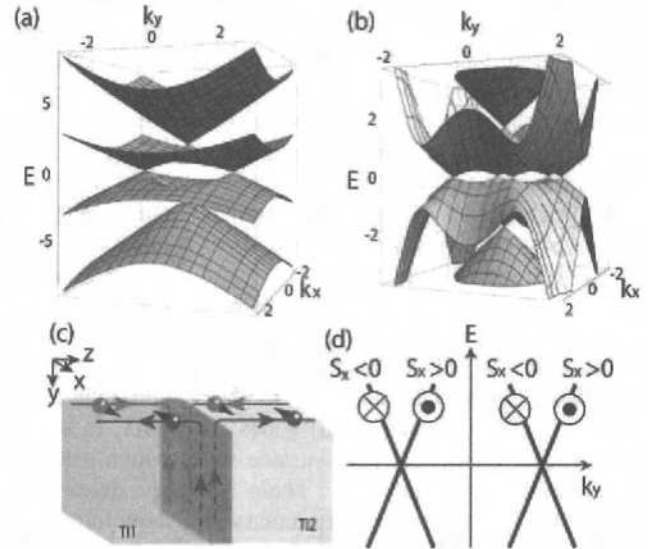


Fig.1. Dispersion on the TIS between the two TIs in Eq. (5) with different velocities

The analysis was performed on the basis of the refraction phenomena on the junction between the two TI surfaces with different velocities. The resulting reflectance and transmittance reflect the backscattering-free nature of the surface states of TIs. When the velocities of the TI surface states for the two TIs have different signs, we show that the gapless states appear on the interface (Fig.1). The existence of the gapless states

is shown by using the mirror Chern number, and thus is topologically protected by the mirror symmetry.

A systematic study of the possible combinations of TIs was performed in [7] using a quantitative model for a strong TI and the existence of different types of topological interface states was demonstrated (Fig.2). These interface states are not protected in the same manner as the surface states of a single TI, instead they are protected by mirror symmetry. The physics of this system resembles certain aspects of bilayer graphene, because both result from the hybridization of Dirac cones.

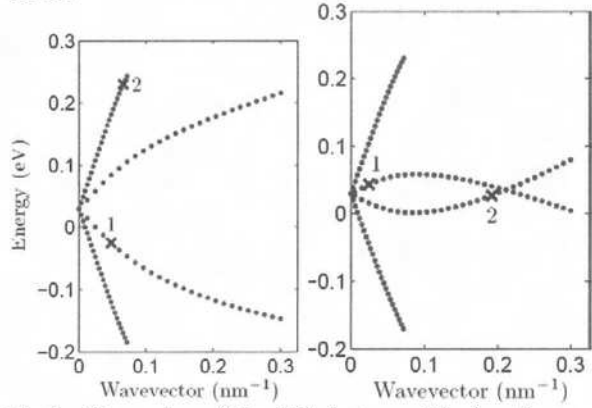


Fig.2. Dispersion of the TIS between TIs for the cases: i) when the velocities in the junction are opposite sign, but in the perpendicular direction – the same; ii) when both velocities change the sign across the junction.

Further we analyse on the basis of the Hamiltonian (1) the TIS for topological insulator heterostructures with incorporated electrical polarization u . Using the method of supersymmetric quantum mechanics we obtain the energy spectrum of the TIS which is not degenerate in terms of spin and it is determined by

$$E = \left\{ \begin{array}{l} -\Delta_+ (V_0 \Sigma_- + Du_-) + \\ (\pm p_\perp + u_+) (D\Delta_- + V_0 u_-) \end{array} \right\} (\Delta_-^2 + u_-^2)^{-1}, (2)$$

for $(V_0 D - \Delta_- u_-) (u_-^2 - V_0^2)^{-1} \geq 0$, where

$$D = (\Delta_-^2 + u_-^2 - V_0^2)^{1/2} \text{ and } V_0 \leq (\Delta_-^2 + u_-^2)^{1/2}.$$

This solution determines two-dimensional boundary electronic states of the TIS type, which are localized near the interface. TIS exist in limited intervals of the energy and the transverse momentum $p_\perp = \hbar v_\perp k_\perp$. The proposed TI heterostructures driven by electrical polarization has many unique advantages, including: 1) it can be realized based on commonly used semiconductors and be integrated into various devices; 2) it is driven by large intrinsic polarization fields; 3) the TI state can be manipulated by applying external fields or injecting charge carriers and can be adjusted by standard semiconductor techniques, including doping, alloying and varying the QW thickness; 4) The proposed TI has many unique advantages, including: 1) it can be realized based on commonly used semiconductors and be integrated into various devices; 2) it is driven by large intrinsic polarization fields; 3) the TI state can be

manipulated by applying external fields or injecting charge carriers and can be adjusted by standard semiconductor techniques, including doping, alloying and varying the QW thickness; 4) the polarization field can induce a large Rashba SOI in this system containing only light elements, which provides a new approach to manipulating spin freedom in such systems. can induce a large Rashba SOI in this system containing only light elements, which provides a new approach to manipulating spin freedom in such systems.

To illustrate the generation of TI states driven by the polarization field recently [8] the edge states of a Hall bar of GaN/InN/GaN quantum well have been analysed (Fig.3). The kp simulations show that the band structure of the GaN/InN/GaN QW is inverted when the QW width is larger than 1,55 nm. The edge states are topologically invariant under scattering, and therefore the corresponding mean free paths of the carriers can be exceedingly large.

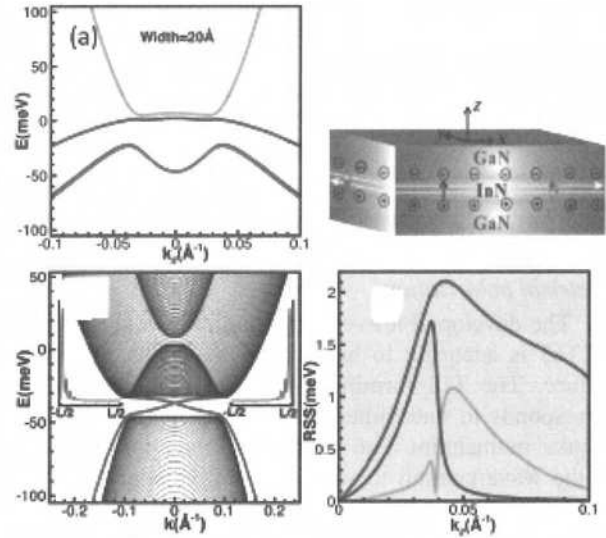


Fig.3 Band structure of a GaN/InN/GaN QW obtained on the basis of band kp model.

Another opportunity to tailor the TIS is offered by the antiferromagnetic ordering of the materials, which constituted heterostructure. In the simplest form this situation is described by Hamiltonian (1). After the transformation

$$U = \begin{pmatrix} i\sigma_z & 0 \\ 0 & 1 \end{pmatrix}, \text{ the Hamiltonian (1) become}$$

$$H = \begin{pmatrix} \Delta(z) & ip_z + W + u \\ -ip_z + W + u & -\Delta(z) \end{pmatrix}, (3)$$

where $W = \vec{\sigma} [p\vec{u}] + \sigma_z L$.

The energy spectrum of bulk materials consists of the four spin-split energy branches (Fig.4)

$$E_{1,2}^+ = ((u + W_\pm)^2 + \Delta^2 + p_z^2)^{1/2} (4)$$

$$E_{1,2}^- = -((u + W_\pm)^2 + \Delta^2 + p_z^2)^{1/2},$$

$$\text{where } W_\pm = \pm(L^2 + p_\perp^2)^{1/2}.$$

Using the ansatz of the supersymmetric quantum mechanics we obtain the following solution of the TIS

$$E = \mp \left\{ (u_0 V_0 - \Delta_0 (u_0^2 + \Delta_0^2 - V_0^2)^{1/2}) (\Delta_0^2 + u_0^2)^{-1} \right\} \times (p_{\perp}^2 + L^2)^{1/2}, (5)$$

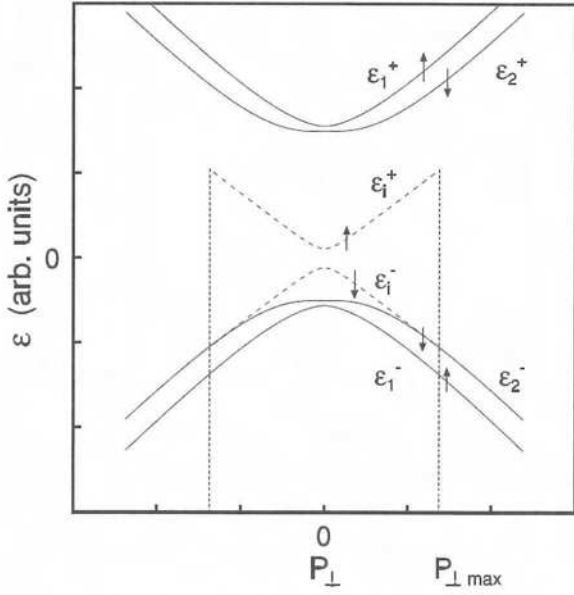


Fig.4 Energy spectrum of topological interface states in the heterostructure with antiferromagnetic ordering and electrical polarization.

The developed low-energy Hamiltonian (1) for bulk Bi2Te3 is adequate to highlight TIS on the cylindrical surface. The TIS forming inside the bulk gap (Fig.5) corresponds to one dimensional bands indexed by total angular momentum. For nanowire or nanopore of radius R, the wavefunction to vanish at the boundary $r = R$ is required, which is automatically ensured by expanding in the orthonormal set of radial Bessel functions J_m or Y_m with integer m .

In comparison with gapless character of TSS of flat surface all TIS modes of cylindrical surface have a finite gap described qualitatively by relations $E_{gs} \sim v/R$ (Fig.5). In results nanowire and nanopore composites of TI have distinct peculiarities from layered ones and offer new opportunities in tailoring the properties of nanostructures.

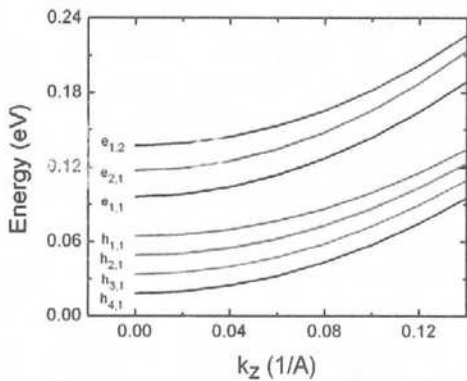


Fig.5. Electronic structure of TI Bi2Te3 nanowire with a radius of 10 nm.

Figure 6 describes the electronic structure of the TI Bi2Te3 nanotube with an external radius of 60 nm and internal radius of 10 nm. Here, the first 3 (4) electron (hole) modes $e_{1,1}$, $e_{2,1}$, and $e_{3,1}$ ($h_{1,1}$, $h_{2,1}$, $h_{3,1}$, and $h_{4,1}$), corresponding to different values of angular momentum quantum number and radial quantum number being equal to 1, are presented.

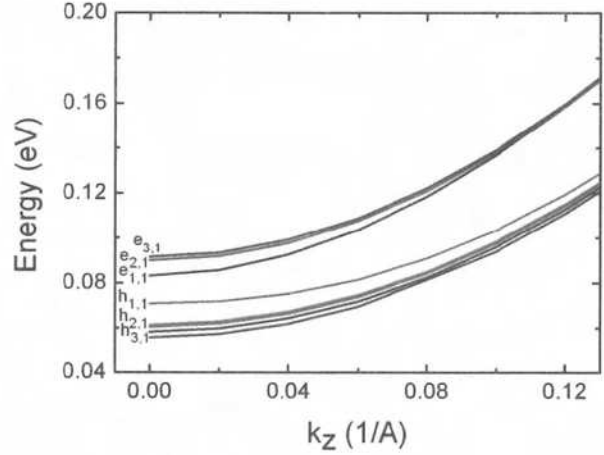


Fig.6. Electronic structure of TIS Bi2Te3 nanotube with an external radius of 60 nm and internal radius of 10 nm. The origin is at the Γ point.

IV. Topological Insulator Nanodevices

Perhaps most importantly, the surfaces of topological insulators enable the transport of spin-polarized electrons while preventing the "scattering" typically associated with power consumption, in which electrons deviate from their trajectory, resulting in dissipation. Because of such characteristics, these materials hold great potential for use in future transistors, memory devices and magnetic sensors that are highly energy efficient and require less power. Bismuth telluride and selenide are well known as a thermoelectric material, but recently was also establish to be a three-dimensional topological insulator with robust and unique surface states [6,7]. Recent experiments with bismuth telluride bulk materials have also suggested two-dimensional conduction channels originating from the surface states. But it has been a great challenge to modify surface conduction, because of dominant bulk contribution due to impurities and thermal excitations in such small-band-gap semiconductors. Experimental evidence for the modulation of such surface states by using a gate voltage was tested in Bi2Te3 nanoribbons [8]. The nanoribbon acts as the channel in the device and is connected to electrodes made of titanium and gold (Fig. 1). In such a device, the gate voltage controls the Fermi level, and therefore the carrier density, of the material. If the Fermi level is moved into the gap between the bulk conduction and valence bands, then the transport properties of the FET are completely governed by the surface states and

can be clearly seen. The new findings shed light on the controllability of the surface spin states in topological insulator nanoribbons and demonstrate significant progress toward high surface electric conditions for practical device applications.

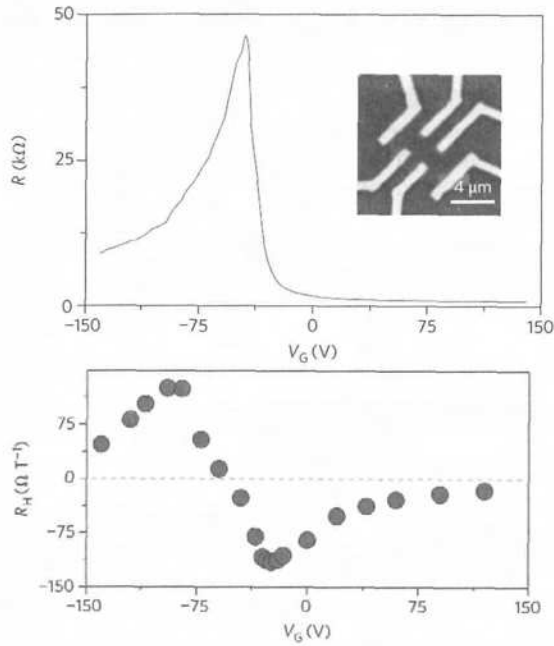


Fig. 7 Ambipolar field effect in ultrathin nanoplates of $(\text{Bi}_x\text{Sb}_{1-x})_2\text{Te}_3$

New memory device concept on the TI was proposed using the intrinsic TI attribute- Berry curvature [10]. The basis for proposed device is the Hall effect mediated by the k -space Berry curvature in the presence of spin-orbit coupling. In TI-based magnetic memory cell a bit is stored via the exchange coupling of the TI surface states. The magnetism induces a finite k -space Berry curvature in the surface states, thereby driving the Hall effect (Fig.8). The readout (Hall) voltage of the cell is related directly to the Hall conductivity, which is highly sensitive to the magnetization of the surface (i.e., the stored bit) but which is insensitive to weak disorder, cell imperfections, and cell geometry. The memory cell is illustrated in Fig. 8, based on a 3D TI block (e.g., Bi_2Te_3 , Bi_2Sb_3 , Sb_2Te_3). In memory cell, a bit is stored by the magnetization M of the FM-doped TI surface, with, say, a “1” (“0”) being stored by an upward (downward) pointing M . Writing to the cell would require a writing field whose field strength exceeds the magnetic coercivity of the surface.

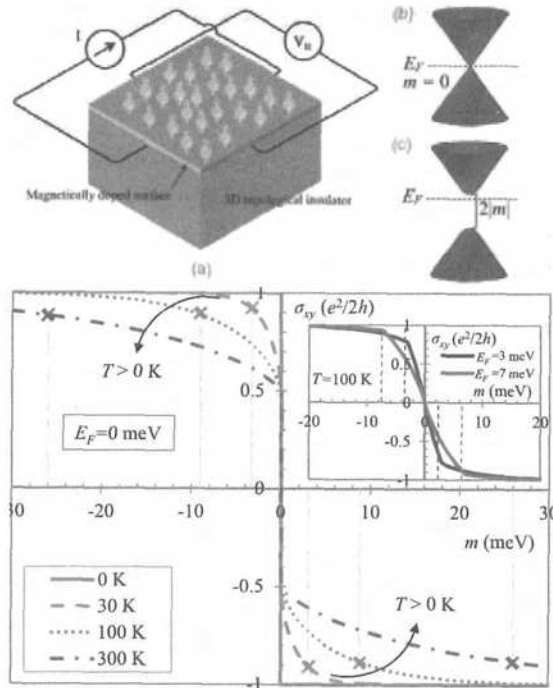


Fig. 8. Structure of proposed memory cell, based on a TI block with a magnetically doped surface (left) and Hall conductivity as a function of magnetization for various temperatures.

References

- [1] Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, *Nat Phys* 5 (6), 398 (2009)
- [2] M.Z. Hasan, C.L. Kane. *Reviews of Modern Physics* 82, 3045–3067 (2010).
- [3] B. A. Bernevig, T. L. Hughes, and S. C. Zhang, *Science*, vol. 314, pp. 1757, 2006.
- [4] Kantser V., Malkova N, *PhysRevB*.56,p.2004, (1997)
- [5] Ryuji Takahashi and Shuichi Murakami. *Phys. Rev. Lett.* 107, 166805, 2011
- [6] Vadim M. Apalkov, Tapash Chakraborty. *cond-mat-1203.5761*
- [7] Christophe De Beule, Bart Partoens. *cond-mat-1302.3359*
- [8] M. S. Miao_ Q. Yan, C. G. Van de Walle, W. K. Lou, L. L. Li, and K. Chang. *cond-mat -1205.2912*
- [9] I. Bejenari and V. Kantser *PHYSICAL REVIEW B* 78, 115322 2008