ISSN: 2997-8440 www.aristonpubs.com/matsci-express https://doi.org/10.69626/mse.2024.0043

RESEARCH ARTICLE

A CrO_2 and Out-of-Plane Silicene based Sub-10nm MTJ with perfect spin filtering efficiency and high tunnel magnetoresistance

Gul Faroz Ahmad Malik[1*], **Mubashir Ahmad**[1], **Farooq Ahmad Khanday**[1], **Feroz Ahmad Najar**[2], **Sparsh Mittal**[3] **and M.Tariq Banday**[1]

ABSTRACT: In this paper, properties of spin transport for MTJs (magnetic tunnel junction) consisting of CrO_2 Half Metallic Ferromagnetic (HMF) electrodes with out of plane silicene sheet as scattering region are analyzed. The transport phenomena in the proposed structure are purely tunneling due to the absence of transmission states near the Fermi level. This is contrary to the in plane structures where transmission states exist near the Fermi level. The proposed device shows the highest value (100%) of magneto-resistance. Spin-filtering efficiency reported in out-of-plane silicene-based MTJ is also increased because of silicene acting as a perfect barrier, results in feeble spin down current in both parallel and anti-parallel configurations. The proposed device has dimensions below 10-nm. Due to the use of silicene sheet as a scattering region, it is also likely to integrate well with the already existing silicon technology. It can be used for high-performance memory applications similar to MRAMs.

Keywords: Spintronics, Spin-FET, TMR, Spin Devices, MTJ, Spin Valve.

Received: 14 January 2024; Revised: 07 February 2024; Accepted: 13 March 2024; Published Online: 15 March 2024

1. INTRODUCTION

Among the different fundamental properties of an electron, spin is one of its essential properties. Conventional electronics consider the charge of an electron for transport. In “spin electronic” or spintronics, the spin of an electron is used for the information. The spintronics field emerged with the discovery of GMR (giant magneto-resistance) [1]. The conventional CMOS-based devices do not scale well and also have low energy efficiency. Spintronic devices such as magnetic tunnel junctions (MTJ) offer an excellent scaling capability and high energy efficiency. Hence, MTJ is considered a viable alternative for conventional CMOS-based devices [2].

In the field of spintronics, MTJ has played a pivotal role. In this structure, there exists three layers, wherein an insulating or a non-magnetic layer is placed in two FM (ferromagnetic like cobalt, iron, nickel etc.) or between two half-metallic ferromagnetic (like chromium dioxide, CrO_2) layers. The two FM electrodes or HMF layers act as drain and source, while the non-magnetic or insulating layer acts as a scattering region [3-7]. The MTJs have potentially infinite endurance, provide scaling capabilities and, most importantly, consume lower power than the conventional memories. MTJs can be used in memory devices and analog to digital converters because they turn off without data loss, resulting in energy saving. As far as the performance parameters like endurance and energy efficiency are concerned, MTJ based memories show superior performance. The effect of tunnel magneto-resistance (TMR) was observed in MTJs with thin-film growth in device fabrication technology. Due to their high TMR values, MTJs catch interest from the devices like MRAM (magnetic random access memory) and magnetic field sensors for ICs of nanoscale range. The read heads made using MTJs have not only been fabricated but have also been commercialized. TMR can be calculated in either a pessimistic way and or an optimistic way. In the pessimistic approach, TMR goes maximum up to 100%.

---

[1] Department of Electronics and Instrumentation Technology University of Kashmir, Hazratbal, Srinagar, 190006, Jammu and Kashmir, India
[2] Department of Physics, Central University of Kashmir, Ganderbal, J&K, India
[3] Department of Electronics and Communications Engineering, Indian Institute of Technology, Roorkee, India
*Author to whom correspondence should be addressed: gfarozam@gmail.com (G. F. A. Malik)

This is already claimed by several researchers [8].

The MTJ has two states; high resistance and low resistance states. When the comparative orientation of magnetic moments is the same in two FM electrodes, it is called a parallel configuration. The spin-polarized electrons coming from a ferromagnetic source get into the scattering region, where the spin polarization does not get processed. The electrons enter directly into the drain electrode. In this state, the current is maximum, and hence, this state acts as a low-resistance state or ON-state. On the other hand, when the relative alignment of magnetic moments is different in source and drain electrodes, it is called an anti-parallel configuration. The electrons which are spin-polarized by the source electrode have different magnetization than the drain electrode. Hence, these electrons are not accepted by the drain electrode. The current in this state is minimum, due to which it acts as a high resistance state or OFF-state. Recently, researchers have focused on MTJs based on 2D materials [9-16]. For example, graphene, silicene, germanene, metal chalcogenides and phosphorene are used as non-magnetic (scattering) layers in MTJs. These MTJs have shown extraordinary properties.

In this paper, MTJ consisting of CrO_2 HMF electrodes with an out-of-plane silicene sheet as a scattering region has been proposed. For comparison purposes, the same device has been simulated with an in-plane silicene scattering region. The structure referred to as "out-of-plane Silicene" means that the Silicene layer is oriented perpendicular to the plane of the electrodes, while "in-plane Silicene" implies that the Silicene layer lies parallel to the plane of the electrodes. The width and thickness of the structures were chosen based on typical dimensions used in similar studies and to ensure compatibility with sub-10nm device requirements. These experiments prove the superiority of the proposed device. The transport phenomenon in the proposed structure is purely tunneling due to the fact that near the Fermi level, the transmission states does not exist. This is contrary to in-plane structures, as transmission states exist nearby to the Fermi level. The proposed device has the dimensions less than 10 nm, thus resolving the conventional devices' scaling issues. The I-V curves for both the configurations (parallel as well as anti-parallel) have been calculated. The proposed device offers ~100% magneto-resistance and ~100% spin filtering efficiency, which is extraordinary and has been reported for the first time in open literature as per the authors' best knowledge. The continuing portion of the paper has been ordered as follows: Section II presents the models and methods used to simulate the proposed device. In Section III, the obtained results of device simulation and discussion are presented. The conclusion is presented in Section IV.

2. EXPERIMENTAL DETAILS

Quantum Atomistix Toolkit (ATK) software has been used to simulate the proposed device. The DFT (density functional theory) coupled with NEGF (non-equilibrium Green's function) is used for calculations. The generalized gradient approximation (GGA) parameterized by Purdew-Burke-Ernzerh (PBE) formula has been used to calculate correlational interactions. The moderation of the atomic positions and the lattice constants without any symmetry is done until the maximum force is less than 0.01 eV/Å. A vacuum space of 20 Å is chosen to avoid any spurious interactions between the periodic images. For taking care of the expansion, a double zeta-basis has been chosen. The density mesh cut off is fixed to be 150 RY. 5 × 5 × 125 Monkhorst-Pack K-points grid has been selected for sampling. LBFGS (Limited-memory Broyden Fletcher Goldfarb Shanno) algorithm has been used to optimize the device's geometry.

The two HMF electrodes made of CrO_2 and a central scattering region comprising of silicene nanoribbon forms the proposed device. The proposed device's model is shown in Figure 1 (a), and its 3D model is shown in Fig. 1 (b). Fig. 1(a) shows the front view or what we can call a 2D-view while as the Fig. 1(b) shows the 3D-view. The red atom represents chromium, blue atom represents oxygen and the golden colored atoms represent atoms of silicon in a sheet form of silicene. The spin current employing transmission coefficients is evaluated by using eq. (1). Eq. (1) relates the current to the transmission coefficient, which describes the probability of electron transmission through the scattering region. This is a well-known Landauer-Büttiker formula. The formalism stands as a pivotal tool in comprehending the conductive behaviors of small quantum coherent systems. It constitutes a fundamental contribution to condensed matter physics, notably within the realm of quantum transport in mesoscopic systems.

The Fermi-Dirac distribution function accounts for the distribution of electrons with respect to energy levels at a given temperature. The temperature used in our calculations was room temperature (300 K), which is a common assumption in similar studies.

$$I\uparrow(\downarrow) = \frac{e}{h}\int T\uparrow(\downarrow)(E,V_{BIAS})[F_L(E,V_{BIAS}) - F_R(E,V_{BIAS})]dE \qquad (1)$$

Where, $T\uparrow(\downarrow)\ (E, V_{BIAS})$ is the spin up (↑) and spin down (↓) transmission coefficient states at a bias voltage V_{BIAS} and energy $E, F_L(E, V_{BIAS})$ being the Fermi-Dirac distribution function for (L) left and $E, F_R(E, V_{BIAS})$ for R (right) electrodes, e and h are electronic charge and Planck's constant respectively.

3. RESULTS AND DISCUSSION

The I-V curves for both configuration (P and AP) of the device have been calculated. The bias voltage has been varied from 0 up to the maximum value of 1.2 V. For parallel configuration, it has been observed that the current increases as the bias voltage is increased. A comparison of the proposed device has been made with the in-plane silicene scattering region-based MTJ.

The increase in the current with bias voltage occurs in both configuration and it is the direct consequence of the increase in conduction states near the Fermi-level.

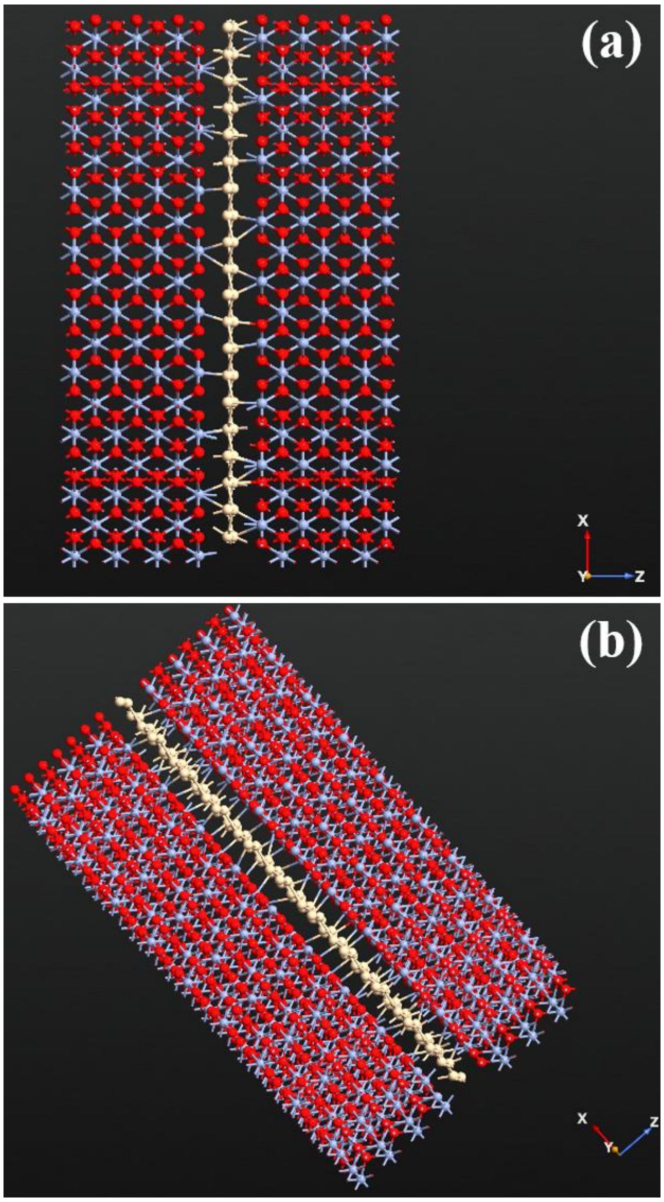

Fig. 1. Proposed device model (a) front view, (b) 3D-view.

At the same time, the suppression of conduction orbitals causes NDR at some voltage [17].

Figure 2(a) and 2(b) shows the spin-up and spin-down current for parallel configuration respectively. For parallel configuration, it has been observed that the spin up current is much greater in magnitude than the spin down current. The magnitude of spin-up and spin-down currents vary with applied bias voltage. Here again, the simultaneous comparison is made with the in-plane silicene-based device. It could be observed that the magnitude of the current is much higher in the case of out-of-plane silicene-based device as compared to the in plane spin based device. Accordingly, the same analysis is done for the antiparallel configuration. The spin up and spin down current for anti-parallel configuration is shown in Figure 3(a) and 3(b). For antiparallel configuration, the spin-up current is almost equal or slightly greater than the spin down current. This is well supported by the literature [3].

Regions of Current Independence: The regions where the current remains independent of voltage, particularly in Figure 3 (b) and 4 (a), can be attributed to saturation effects. In electronic devices, saturation occurs when the device reaches its maximum achievable current under a given bias voltage. In this state, further increases in voltage do not result in a proportional increase in current due to limitations such as carrier mobility saturation, band bending, or other device-specific factors. Thus, the observed plateau in current can be explained by the device operating in a saturated regime, where the current remains relatively constant despite changes in applied voltage.

Decrease in Current at Higher Bias Voltages: The observed decrease in current as the bias voltage increases above 2.5 V, particularly in Figure 4(b), can be attributed to the interplay of spin polarization and spin flip of electrons within the scattering region of the device. As the bias voltage exceeds a certain threshold, the energy levels within the scattering region may become conducive to spin flip processes, where electrons with one spin orientation flip to the opposite spin orientation. This spin flip process can lead to a reduction in the net spin current flowing through the device, resulting in a decrease in the overall current observed at higher bias voltages.

The observed behaviors in Figures 3(b) and 4(a) are indicative of saturation effects and spin-related phenomena inherent to the operation of the proposed device. We appreciate the opportunity to clarify these points and provide deeper insights into the underlying physical mechanisms governing the device behavior.

In our specific study, the focus was primarily on theoretical modeling and simulation of the electronic device, rather than experimental measurements. As such, the data presented in the V-I graph were obtained through computational simulations, where uncertainties typically arise from factors such as model parameters, numerical approximations, and computational methods. While error bars are commonly used in experimental studies to represent measurement uncertainties but not in simulation-based research.

Furthermore, the dependencies of current on bias voltage (I-V curves) are influenced by various factors such as the density of states, band structure, and scattering mechanisms. The divergence of curves at higher bias voltages is attributed to non-linear transport effects and/or breakdown of certain approximations in the theoretical model.

The value of magneto-resistance (MR) can be calculated by Eqn. (2),

$$MR = \frac{I_{PC} - I_{APC}}{I_{PC}} \times 100\% \qquad (2)$$

Where, I_{PC} is the spin-current for parallel configuration, and I_{APC} is the spin-current for antiparallel configuration.

Figure 5 shows the graph for the variation of magneto-resistance with the bias voltage applied for parallel configuration. From Figure 5, the least and the top values of the magneto-resistance for out-of-plane silicene-based MTJ is between 95% to 100%. For in-plane silicene, the least and the top value of the magneto-resistance is between 60% to 70% at bias voltages between 0 to 1.2 V. Furthermore, as shown in Fig. 5, for out-of-plane silicene, the value of magneto-resistance is ~100% as the bias voltage is varied from 0 V up to 1.2 V. Furthermore, the value of magneto-resistance is less for in-plane silicene-based MTJ and hence, cannot be used for efficient applications. On the contrary, it can be observed that the value of magneto-resistance remains almost fixed throughout the bias voltage range. This makes the proposed design a viable choice for circuit application beyond CMOS technology.

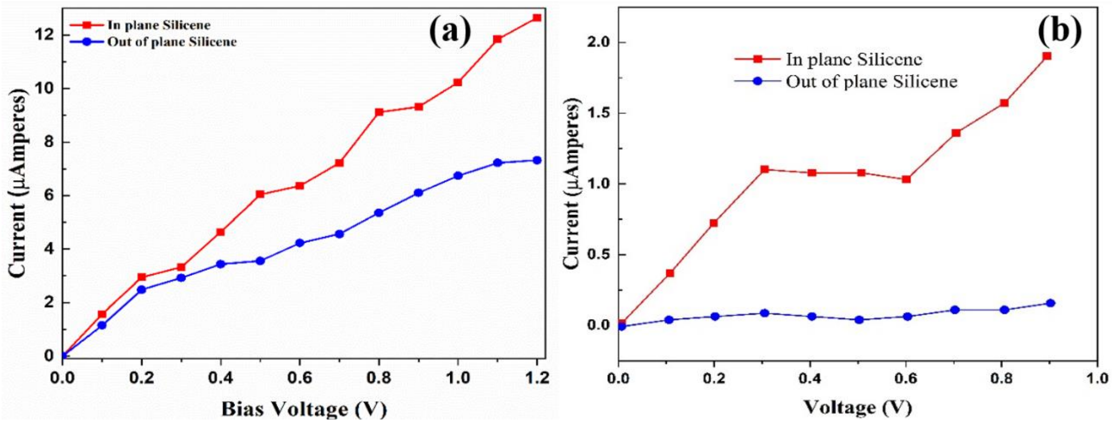

Fig. 2. I-V characteristics of net (spin up + spin down current) for: (a) parallel configuration, (b) anti-parallel configuration.

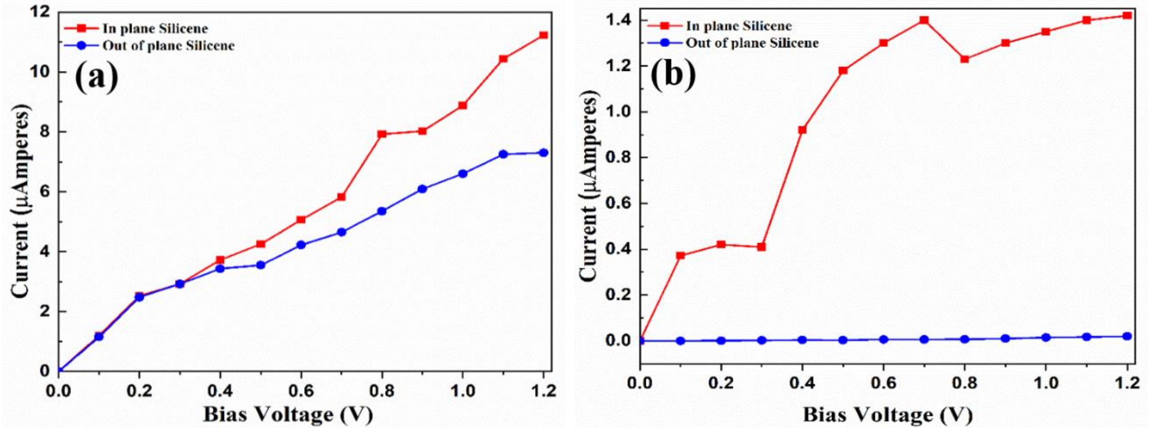

Fig. 3. I-V characteristics of parallel configuration; (a) spin up current, (b) spin down current.

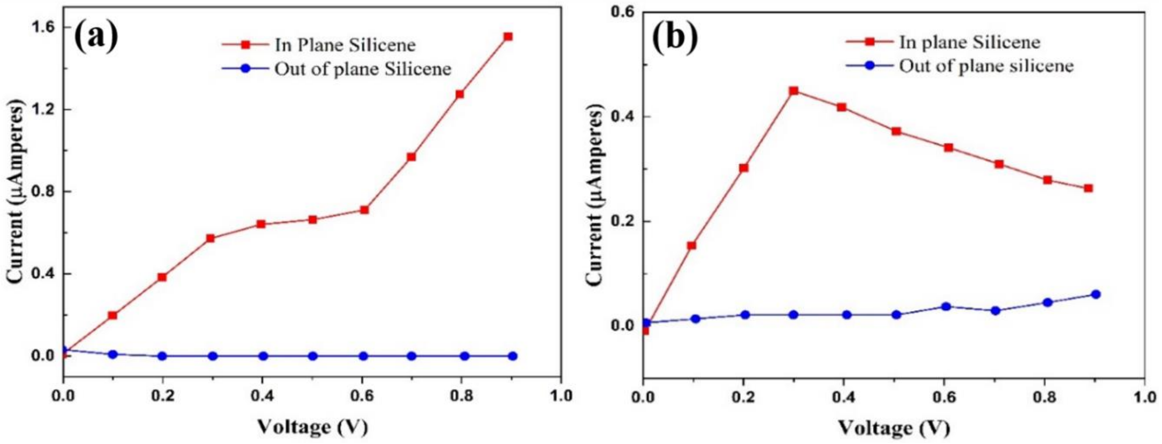

Fig. 4. I-V characteristics of anti-parallel configuration; (a) spin-up current, (b) spin-down current.

Theoretically, the out-of-plane silicene offers ~100% magneto-resistance. Although various research papers have claimed this value, the added advantage of the proposed device is that it utilizes silicene as its scattering region. Hence, it ensures smooth integration with the existing platform. Use of novel materials other than silicon presents high integration overheads into the existing silicon-based ecosystems. By contrast, our proposed device uses silicon as its material, which adds to its advantage.

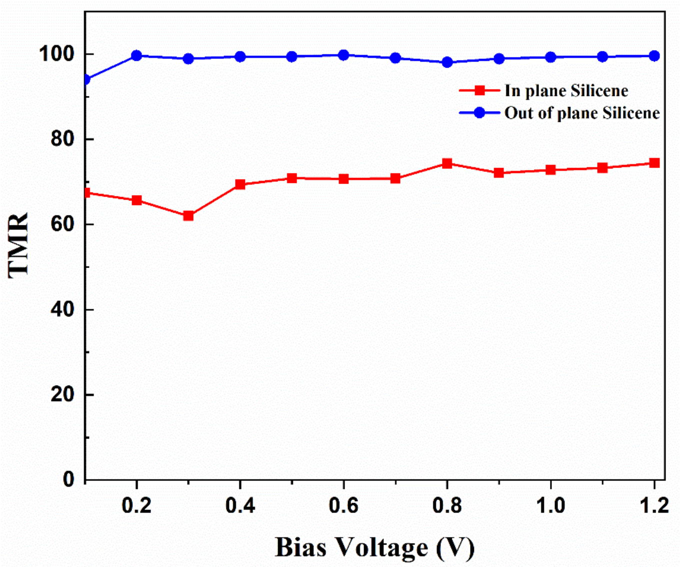

Fig. 5. Magneto-resistance vs. bias voltage.

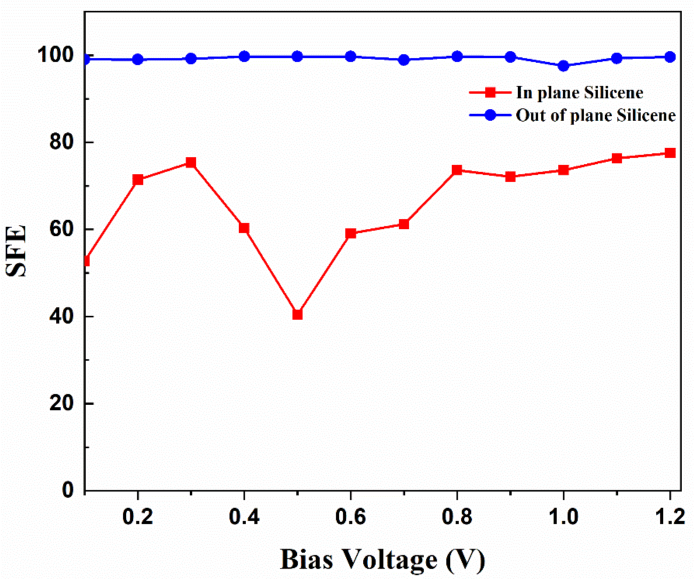

Fig. 6. Spin filtering efficiency vs. bias voltage.

Another critical parameter of spintronic devices is SFE (spin filtering efficiency). Using obtained I-V characteristics, the SFE of the device is calculated as:

$$\eta = \frac{I_{up} - I_{down}}{I_{up} + I_{down}} \quad (3)$$

Where I_{up} is the total spin up and I_{down} is the net spin down current. The graphs for variation of SFE with respect to applied bias voltage for parallel configuration is shown in Figure 6. It can be observed the maximum value of SFE achieved in in-plane silicene-based MTJ is around 80%, while for the out-of-plane silicene-based MTJ, it is ~100%. Half metallic electrodes (CrO_2) based electrodes improve SFE., but using CrO_2 electrodes with out of plane silicene scattering region-based MTJ improves it further. Thereby, it can be concluded that using an out-of-plane silicene scattering region in MTJ improves the spin filtering efficiency in MTJ. Hence, it allows only one type of spin current to propagate through the device. Given the novelty of our proposed device configuration, direct comparisons with existing TMR structures may be limited.

4. CONCLUSIONS

In this paper, the spin-transport properties of CrO_2-Silicene-CrO_2 MTJ have been carried using NEGF, coupled with the DFT. From the I-V characteristics, the values magneto-resistance and SFE have been calculated. In the proposed device, the scattering region has been placed in out-of-plane geometry, and results have been compared with the in-plane geometry. The transport phenomena in the proposed device are purely tunneling due to the non-existence of transmission states near the Fermi level, which is totally opposite to that of in-plane geometry. The proposed device shows maximum magneto-resistance of ~100%. As the silicene acts as perfect barrier in out of plane configuration, the value of SFE reported in this configuration of MTJ increases. Due to this the spin-down current in both; parallel as well as antiparallel is negligible. The proposed device has dimensions below 10-nm, and due to the usage of silicene sheet as a scattering region, it also has expected integration with already existing silicon technology. The device can also be used for high-performance memory applications like MRAM, which are universal memories and use MTJ as their basic building block.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests.

REFERENCES

[1] Lei, M., Peng, T., Zhou, F., Yu, J., Liang, S., Liu, J. and Li, L., **2022.** Optimal design and implementation of tunneling magnetoresistance based small current sensor with temperature compensation. *Energy Reports*, *8*, pp.137-146.

[2] Joshi, V.K., Barla, P., Bhat, S. and Kaushik, B.K., **2020.** From MTJ device to hybrid CMOS/MTJ circuits: A review. *IEEE Access*, *8*, pp.194105-194146.

[3] Kharadi, M.A., Malik, G.F.A., Khanday, F.A. and Shah, K.A., **2020.** Hydrogenated silicene based magnetic junction with improved tunneling magnetoresistance and

spin-filtering efficiency. *Physics Letters A*, *384*(32), p.126826.

[4] Datta, S. and Das, B., **1990.** Electronic analog of the electro-optic modulator. *Applied Physics Letters*, *56*(7), pp.665-667.

[5] Malik, G.F.A., Kharadi, M.A. and Khanday, F.A., **2019.** Electrically reconfigurable logic design using multi-gate spin Field Effect Transistors. *Microelectronics Journal*, *90*, pp.278-284.

[6] Malik, G.F.A., Kharadi, M.A., Parveen, N. and Khanday, F.A., **2020.** Modelling for triple gate spin-FET and design of triple gate spin-FET-based binary adder. *IET Circuits, Devices & Systems*, *14*(4), pp.464-470.

[7] Malik, G.F.A., Kharadi, M.A., Khanday, F.A. and Shah, K.A., **2020.** Performance analysis of indium phosphide channel based sub-10 nm double gate spin field effect transistor. *Physics Letters A*, *384*(19), p.126498.

[8] Yoshikawa, M., Kitagawa, E., Nagase, T., Daibou, T., Nagamine, M., Nishiyama, K., Kishi, T. and Yoda, H., **2008.** Tunnel Magnetoresistance Over 100% in MgO-Based Magnetic Tunnel Junction Films With Perpendicular Magnetic $L1_0$-FePt Electrodes. *IEEE Transactions on Magnetics*, *44*(11), pp.2573-2576.

[9] Choudhary, S. and Jalu, S., **2015.** First-principles study of spin transport in Fe–SiCNT–Fe magnetic tunnel junction. *Physics Letters A*, *379*(28-29), pp.1661-1665.

[10] Han, J., Shen, J. and Gao, G., **2019.** CrO_2-based heterostructure and magnetic tunnel junction: perfect spin filtering effect, spin diode effect and high tunnel magnetoresistance. *RSC advances*, *9*(7), pp.3550-3557.

[11] Zeng, J., Chen, K.Q., He, J., Zhang, X.J. and Sun, C.Q., **2011.** Edge hydrogenation-induced spin-filtering and rectifying behaviors in the graphene nanoribbon heterojunctions. *The Journal of Physical Chemistry C*, *115*(50), pp.25072-25076.

[12] Zeng, J. and Chen, K.Q., **2013.** Spin filtering, magnetic and electronic switching behaviors in manganese porphyrin-based spintronic devices. *Journal of Materials Chemistry C*, *1*(25), pp.4014-4019.

[13] Tang, G.P., Zhou, J.C., Zhang, Z.H., Deng, X.Q. and Fan, Z.Q., **2013.** A theoretical investigation on the possible improvement of spin-filter effects by an electric field for a zigzag graphene nanoribbon with a line defect. *Carbon*, *60*, pp.94-101.

[14] Kum, H., **2012.** *Spin Injection, Transport, and Modulation in III-V Semiconductors* (Doctoral dissertation). University of Michigan, 2012.

[15] Kang, J., Chang, K.J. and Katayama-Yoshida, H., **2005.** First-principles study of ferromagnetism in Mn-doped GaN. *Journal of superconductivity*, *18*, pp.55-60.

[16] Yao, K.L., Min, Y., Liu, Z.L., Cheng, H.G., Zhu, S.C. and Gao, G.Y., **2008.** First-principles study of transport of V doped boron nitride nanotube. *Physics Letters A*, *372*(34), pp.5609-5613.

[17] Fan, Z.Q. and Chen, K.Q., **2010.** Negative differential resistance and rectifying behaviors in phenalenyl molecular device with different contact geometries. *Applied Physics Letters*, *96*(5).

[18] Slaughter, J.M., **2009.** Materials for magnetoresistive random access memory. *Annual Review of Materials Research*, *39*, pp.277-296.