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Spin-dependent transport in Normal/Ferromagnetic/Normal monolayer zigzag molybdenum disulfide nanoribbon junction

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Abstract. In this paper, with the three-band tight-binding model, we investigate spin transport in Normal/Ferromagnetic/Normal monolayer zigzag molybdenum disulfide nanoribbon junction with double electric barriers using Green's function technique. We discuss the influence of the height of the double electric barrier on spin transport. The results demonstrate that spin conductance has relatively large dependence on electric field modulation. We can obtain large spin polarization in low energy region which may be applied as a spin filter**.** In addition, we study the effect of magnetic field, and we find that we can obtain a larger spin polarization area which may provide a theoretical basis for spin filter application.

1. Introduction

After graphene [1,2] was discovered, two-dimensional materials have attracted a lot of attention due to the potential application in nano-electronics and opto-electronics. However, due to the weak spin-orbit coupling effect and zero band gap in graphene [3] system, which makes their application in spintronics limited extremely. Recently, with the successful preparation of the monolayer (ML) transition metal dichalcogenides, especially ML molybdenum disulfide (MoS_2) [4], the research of spintronics has developed to a new height. ML MoS_2 has comparatively large direct band gap (~1.8eV) [5]. Meanwhile, ML MoS_2 has a very strong spin-orbit coupling (SOC), which is originated from the d orbital of heavy metal atoms along with the inversion symmetry, providing a possibility for controlling the spin-dependent electron transport in the ML MoS_2-based structures. In earlier works involving spin transport on graphene and silicene nanoribbons [6–9], the modulations of electric field and magnetic field are widely used. Here, we propose a Normal/Ferromagnetic/Normal monolayer zigzag MoS_2 nanoribbon junction where a double electric barriers structure is applied in normal MoS_2 region, which is connected to the two semi-infinite monolayer MoS_2 nanoribbon. In this system, we mainly study the influences of electric field and magnetic field on spin transport in ML MoS_2 nanoribbon and obtain great spin filtering effect.

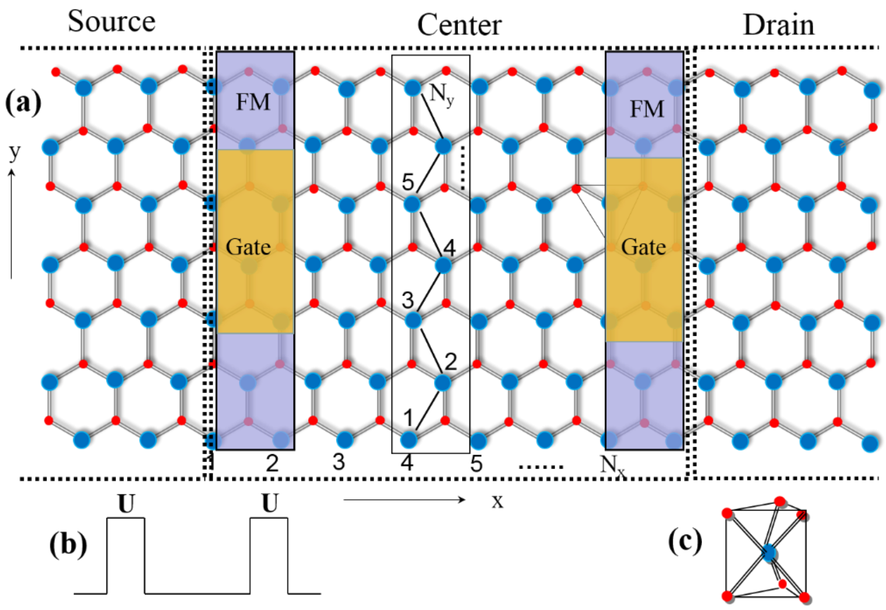

Fig. 1 (a) Schematic diagram for the N/F/N zigzag MoS2 nanoribbon junction with source and drain electrodes shows semi-finite MoS2 nanoribbon. Nx is the length of center part and Ny is the width. The blue sphere is Mo and the red sphere is S. Gate electrode is applied on the ferromagnetic strips regions. (b) is the double electric barriers structure which originates from the gate electrodes. (c) Schematic diagram for the structure of trigonal prismatic coordination, corresponding to the black triangle in (a) (color online).

2. Theory and Formula

Only involving the nearest-neighbor Mo-Mo hopping, the Hamiltonian of the system is given in detail by the three-band tight-binding model which is developed by Yao [10]. Therefore, the total Hamiltonian of the system can be described by

$$H_{total} = H_S + H_D + H_C \tag{1}$$

Here, H_S is the Hamiltonian of source electrode, H_D is the Hamiltonian of drain electrode, H_C is the Hamiltonian of center region.

$$H_C = H_{LN} + H_{CF} + H_{RN} \tag{2}$$

Here, H_{LN} and H_{RN} are the Hamiltonian of left and right normal regions with voltage gates, H_{CF} is the Hamiltonian of ferromagnetic section in center region. Because H_S and H_D are the Hamiltonian of the source and drain electrodes, they can be written as

$$\begin{aligned} H_N(k_x) =& \sum_{k_x, n=1,\cdots,N_y} c^+_{\alpha,\sigma}(k_x,n) \begin{pmatrix} h_1 & 0 \\ 0 & h_1 \end{pmatrix} c_{\beta,\sigma}(k_x,n) \\ &+ \sum_{k_x, n=2,\cdots,N_y} c^+_{\alpha,\sigma}(k_x,n-1) \begin{pmatrix} h_2 & 0 \\ 0 & h_2 \end{pmatrix} c_{\beta,\sigma}(k_x,n) + \sum_{k_x, n=1,\cdots,N_y-1} c^+_{\alpha,\sigma}(k_x,n+1) \begin{pmatrix} h_2^+ & 0 \\ 0 & h_2^+ \end{pmatrix} c_{\beta,\sigma}(k_x,n) \end{aligned} \tag{3}$$

For H_{LN} and H_{RN}, owing to the existence of double electric barriers U, they can be expressed by

$$H_{L(R)N}(k_x)=\sum_{k_x,n=1,\cdots,N_y} c^{+}_{\alpha,\sigma}(k_x,n)\begin{pmatrix} h_1+h_4 & 0 \\ 0 & h_1+h_4 \end{pmatrix} c_{\beta,\sigma}(k_x,n)$$
$$+\sum_{k_x,n=2,\cdots,N_y} c^{+}_{\alpha,\sigma}(k_x,n-1)\begin{pmatrix} h_2 & 0 \\ 0 & h_2 \end{pmatrix} c_{\beta,\sigma}(k_x,n)+\sum_{k_x,n=1,\cdots,N_y-1} c^{+}_{\alpha,\sigma}(k_x,n+1)\begin{pmatrix} h_2^{+} & 0 \\ 0 & h_2^{+} \end{pmatrix} c_{\beta,\sigma}(k_x,n) \tag{4}$$

H_{CF} is the ferromagnetic region, the Hamiltonian is

$$H_{CF}(k_x)=\sum_{k_x,n=1,\cdots,N_y} c^{+}_{\alpha,\sigma}(k_x,n)\begin{pmatrix} h_1+h_3 & 0 \\ 0 & h_1+h_3 \end{pmatrix} c_{\beta,\sigma}(k_x,n)$$
$$+\sum_{k_x,n=2,\cdots,N_y} c^{+}_{\alpha,\sigma}(k_x,n-1)\begin{pmatrix} h_2 & 0 \\ 0 & h_2 \end{pmatrix} c_{\beta,\sigma}(k_x,n)+\sum_{k_x,n=1,\cdots,N_y-1} c^{+}_{\alpha,\sigma}(k_x,n+1)\begin{pmatrix} h_2^{+} & 0 \\ 0 & h_2^{+} \end{pmatrix} c_{\beta,\sigma}(k_x,n) \tag{5}$$

Here, k_x is the momentum in the *x* direction, $C^{+}_{\alpha,\sigma}(C_{\beta,\sigma})$ creates (annihilates) an electron on site $\alpha(\beta)$ with spin σ ($\sigma=\uparrow,\downarrow$). Here, the d_{z^2}, d_{xy}, and $d_{x^2-y^2}$ orbitals of Mo atom are separately labeled by *l*, *m*, and *n* which are dominant components for conduction and valence bands.

$$h_1=\begin{pmatrix} 2t_0\cos k_x+E_1 & 2it_1\sin k_x & 2t_2\cos k_x \\ -2it_1\sin k_x & 2t_{11}\cos k_x+E_2 & 2it_{12}\sin k_x \\ 2t_2\cos k_x & -2it_{12}\sin k_x & 2t_{22}\cos k_x+E_2 \end{pmatrix} \tag{6}$$

$$h_2=\begin{pmatrix} 2t_0\cos\frac{k_x}{2} & i\sin\frac{k_x}{2}\left(3^{1/2}t_2+t_1\right) & \left(-t_2+3^{1/2}t_1\right)\cos\frac{k_x}{2} \\ i\left(3^{1/2}t_2-t_1\right)\sin\frac{k_x}{2} & \frac{t_{11}+3t_{22}}{2}\cos\frac{k_x}{2} & \left(\frac{3^{1/2}}{2}t_{22}-\frac{3^{1/2}}{2}t_{11}-2it_{12}\right)\sin\frac{k_x}{2} \\ \left(-t_2-3^{1/2}t_1\right)\cos\frac{k_x}{2} & \left(\frac{3^{1/2}}{2}t_{22}-\frac{3^{1/2}}{2}t_{11}+2it_{12}\right)\sin\frac{k_x}{2} & \frac{3t_{11}+t_{22}}{2}\cos\frac{k_x}{2} \end{pmatrix} \tag{7}$$

$$h_3=\begin{pmatrix} U & 0 & 0 \\ 0 & U & 0 \\ 0 & 0 & U \end{pmatrix} \tag{8}$$

$$h_4=\begin{pmatrix} \sigma M & 0 & 0 \\ 0 & \sigma M & 0 \\ 0 & 0 & \sigma M \end{pmatrix} \tag{9}$$

U is the height of the double electric barriers, $\sigma=\pm1$ for (spin up/spin down), M is the intensity of the exchange field, ϵ_j is the on-site energy corresponding to the atomic orbital j, $t_0=E_{ll}(R_1)$, $t_1=E_{lm}(R_1)$, $t_2=E_{\ln}(R_1)$, $t_{11}=E_{mm}(R_1)$, $t_{12}=E_{mm}(R_1)$; $t_{22}=E_{nn}(R_1)$; $E_{jj'}=<\phi_{j(r)}\left|\hat{H}\right|\phi_j(r-R)>$ is the hopping integral between the atomic orbital j at 0 and j' at lattice vector R. Confined by the symmetry of the system, the nine parameters E_1, E_2, t_0, t_1, t_2, t_{11}, t_{12}, t_{22} are independent.

Next, we investigate the spin transport properties of zigzag MoS_2 nanoribbon by Green's function technique and Landauer-Buttiker formula [11]. Hence the spin conductance of the system is

$$G^{\sigma}=\frac{2e^{2}}{h}Tr\left(\Gamma_{S}^{\sigma}G_{C}^{r,\sigma}\Gamma_{D}^{\sigma}G_{C}^{\alpha,\sigma}\right) \tag{10}$$

Here, $\Gamma_{S(D)}^{\sigma}=i\{\Sigma_{S(D)}^{r,\sigma}-[\Sigma_{S(D)}^{r\sigma}]^{+}\}$ are the linewidth functions $G_{C}^{r,\sigma}=[G_{C}^{a,\sigma}]^{+}=(EI-H_{C}-\Sigma_{S}^{r,\sigma}-\Sigma_{D}^{r,\sigma})$ is the retarded Green's function with the Hamiltonian in the center region H_{C}. $\Sigma_{S(D)}^{\sigma}$ is the retarded self-energy term due to the conductor coupling with source (drain) electrode.

3. Results and Discussion

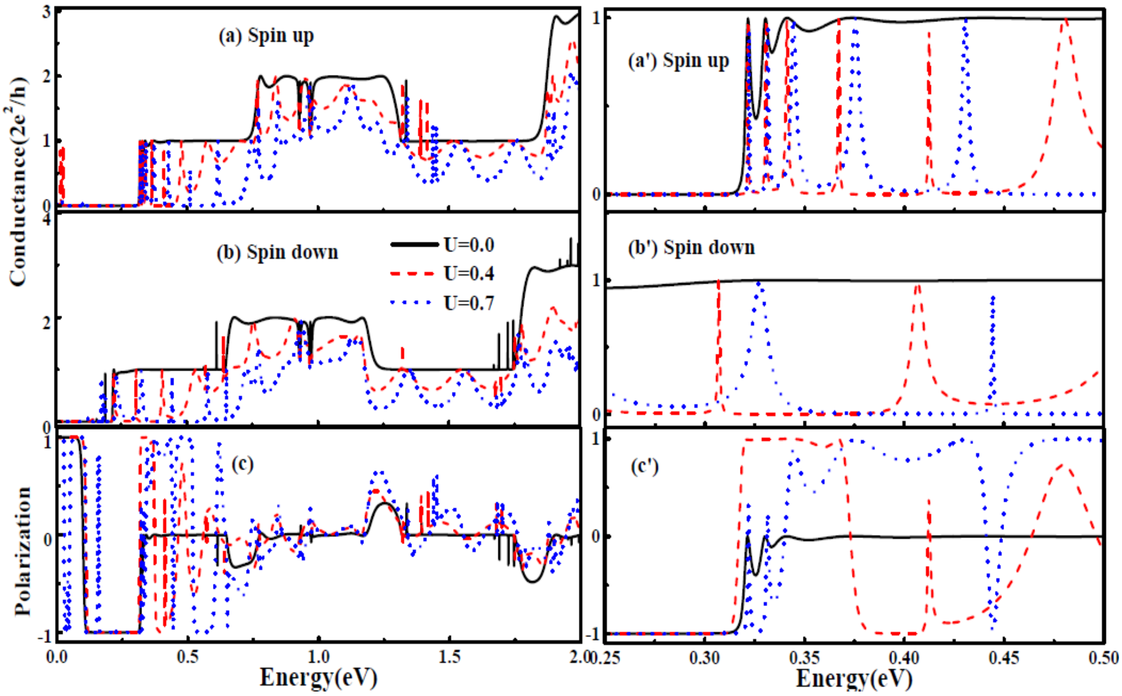

Fig. 2 (a) Spin-up conductance, (b) spin-down conductance and (c) spin polarization versus the energy for a variety of the heights of double electric barriers. The length of the center part N_x = 14, the width Ny=8, the width of the double electric barriers is set to be Nx=1, namely, a 1-12-1 unit-cell-layer double electric barriers structure is imposed on this device, the intensity of the exchange field M = 0.1eV and the heights of double electric barriers are set at U = 0.0; U = 0.4eV; U = 0.7eV. The right panel is the local enlarged diagram.

First, we consider the influence of the heights of the double electric barriers on spin transport in MoS_2 nanoribbon which can be seen from Figure 2. Here, the nanoribbon length of the center part Nx=14, the width is set to be Ny=8. The width of barriers is Nx=1, namely, a 1-12-1 unit-cell-layer barriers structure is imposed in this MoS_2 nanoribbon device. The intensity of the exchange field M = 0.1eV. Without the double electric barriers, both the spin-up and spin-down conductances are close to the staircase. When we increase the barrier height of the double electric barriers to U= 0.4eV, conductance steps are destroyed and evolved into resonant tunneling conductance as shown in Fig. 2(a) and (b). Once the barrier height is raised enough to U= 0.7eV, the oscillating peaks are enhanced, which is originated from the energy level splitting, and conductance is reduced accordingly. Moreover, the position of resonant tunneling peaks shift to the higher energy. Hence, we can obtain 100% spin polarization at the energy from 0.45 eV to 0.6 eV [see Fig.2(c)] which can be a potential application for spin filter.

Further, in order to demonstrate the modulation of the external field convincingly, we study the effect of the exchange field on spin transport in MoS_2 nanoribbon. As shown in Fig. 3(a), with the intensity of the exchange field enhanced, the spin-up conductances shift to the higher energy and oscillating peaks increase. Comparing Fig. 3 (a) and Fig. 3 (b), the change of the spin-down conductances [see Fig. 3 (b)] is not greatly. Therefore, Within the range from 0.25 eV to 0.75 eV in Fig. 3 (c), we can obtain a broadened 100% spin polarization when the intensity of the exchange field is raised to M=0.5eV, which may be used as a perfect spin filter application.

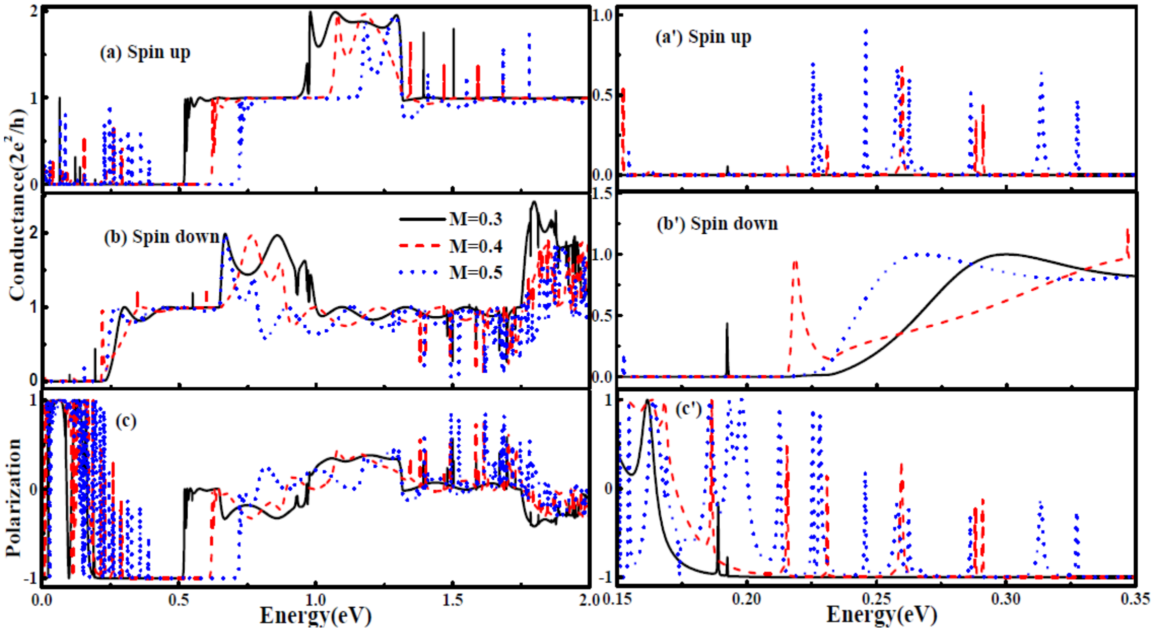

Fig. 3 (a) Spin-up conductance, (b) spin-down conductance and (c) spin polarization as a function of the energy for a variety of the intensity of exchange field. The length of the center part N_x = 14, the width N_y = 8. A 1-12-1 unit-cell-layer double electric barriers structure with barriers height U = 0.1eV is imposed on this device, the intensity of the exchange field are M = 0.3eV, M = 0.4eV, M = 0.5eV. The right panel is the local enlarged diagram.

4. Conclusions

In conclusion, we have explored spin transport properties in Normal/Ferromagnetic/Normal ML zigzag MoS2 nanoribbon junction with double electric barriers. Our results show that in zigzag MoS2 nanoribbon, the height of the double electric barriers and the intensity of the exchange field effectively control the spin transport in proposed structure. Hence, we can obtain 100% spin polarization in a large area. This structure may make MoS2 as a promising candidate for future spintronics, valleytronics devices.

Acknowledgments

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