

# Tunneling Current through Vertical Heterostructures Composed of Graphene and Atomically Thin MoS<sub>2</sub> Insulators

Nojoon Myoung<sup>1</sup>, Kyungchul Seo<sup>1</sup>, Seung Joo Lee<sup>2</sup>, Gukhyung Ihm<sup>1</sup>

<sup>1</sup> Department of Physics, Chungnam National University, Daejeon 305-764, Korea

<sup>2</sup> Quantum-functional Semiconductor Research Center, Dongguk University, Seoul 100-715, Korea  
[toughni@cnu.ac.kr](mailto:toughni@cnu.ac.kr)

## Abstract

Graphene has been considered to be a promising material for future electronics due to its extraordinary properties such as high carrier mobility[1], thermal conductivity[2], and strong break strength[3]. Although the extremely high electrical conductivity makes graphene a candidate for replacing silicon-based electronics, Klein tunneling causes that electrical transport of Dirac fermions is insensitive to electrostatic potentials, resulting low current on/off ratio of graphene based field-effect-transistors[4,5,6]. This is a serious problem for the prospect of graphene-based electronics. In order to increase the current on/off ratio, there have been many attempts to open a band gap by studying graphene nanoribbons (GNRs)[7,8,9], mechanically strained graphene[10], and bilayer graphene[11]. However, it has been revealed that, in those case, the electronic quality tends to be reduced compared to pristine graphene. Therefore, it is worthwhile to obtain high current on/off ratio in graphene-based devices without the reduction in the sample quality of graphene.

Very recently, increasing interest has been focused on an alternative graphene device structure by using quantum tunneling. In a graphene/silicon junction, large current on/off ratio was achieved by controlling Schottky barrier at the interface[12]. However, for graphene deposited on silicon substrate, carrier mobility is expected to decrease because of carrier inhomogeneity induced by the substrate[13]. Meanwhile, L. Britnell et al. reported the possibility of a graphene field-effect-transistor based on vertical heterostructures with atomically thin insulating barriers, hexagonal boron nitride (hBN) and molybdenum disulfide (MoS<sub>2</sub>)[14]. hBN has gained burgeoning interest as a material for use in graphene devices because the encapsulation of graphene by hBN maintains the high electronic quality of pristine graphene[15]. In spite of this advantage, the large band of hBN (~5.97 eV[16]) causes an insufficient current on/off ratio. The larger on/off ratio was observed in graphene heterostructures with MoS<sub>2</sub>, instead of hBN, owing to its smaller bandgap compared to hBN. Therefore, alongside the experimental observation of the significant on/off ratio in the graphene heterostructure with MoS<sub>2</sub>, it is natural to investigate possible functional devices utilizing its advantages for electronic applications.

Herein, calculations of the tunneling current density for graphene heterostructures with MoS<sub>2</sub> are presented. The purpose of this study is not only to enhance the performances of existing graphene field-effect-transistors based on the vertical heterostructure[14] with MoS<sub>2</sub> but also to add utilities to them. Our proposed structures consists of an atomically thin MoS<sub>2</sub> layer sandwiched by two graphene sheets as shown in Fig. 1. The MoS<sub>2</sub> layer in the heterostructure becomes a tunneling barrier for Dirac fermions in a graphene sheet, and both graphene sheets play the role of high-quality source and drain electrodes. Dirac fermions experience the direct bandgap near K-valley of the MoS<sub>2</sub> because of the momentum conservation in the lateral plane, neglecting electron-phonon scattering processes. The transmission probability through the barrier is calculated by using WKB approximation;

$$T(E) \sim \exp \left[ -\frac{2\sqrt{2m^*}}{\hbar} \int_{-d/2}^{+d/2} \sqrt{U(z) - E} dz \right], \quad (1)$$

Where  $d$  is the thickness of the barrier and  $U(z)$  is the potential energy of the barrier as a function of  $z$ . This approximation is valid for the direct tunneling regime, i.e.,  $E$  has to be less than  $U(z)$ . As Britnell et.al established[14], the tunnel barrier,  $U(z) = \Delta + (qV_b z/d)$ , is used, where  $\Delta$  is the barrier height for incident Dirac fermions. Based on it, the tunneling current through the MoS<sub>2</sub> insulating barrier can be obtained by

$$j(V_b, V_G) = j_0 \int_{-\infty}^{+\infty} D_S(E, V_b) D_D(E, V_b) T(E) [f_S(E, V_b, V_G) - f_D(E, V_b, V_G)] dE, \quad (2)$$

where  $j_0 = (qv_F)/(2\pi L_0^2)$  is the unit of current density with electric charge of carriers,  $q$ , and the characteristic length of the system  $L_0$ . Here,  $D_i$  and  $f_i$  are density of states of graphene and the Fermi-Dirac distribution for source ( $i = S$ ) and drain ( $i = D$ ) graphene electrodes on both sides of the MoS<sub>2</sub> layer, respectively, as shown in Fig. 1(a) and (b). The equilibrium chemical potential is defined as  $\mu_0 = \hbar v_F \sqrt{\pi |n|} = \hbar v_F \sqrt{\pi \alpha |V_G|}$ . Without a bias voltage,  $V_b$ , applied between the source and drain graphene electrodes, tunneling current from Eq. (2) must be zero.

The novel utility of our heterostructures, which is found in this study, is threefold. First, the distinct asymmetric current-voltage characteristics of graphene/MoS<sub>2</sub>/graphene implies that it could be used as a field-effect-diode which is operated by a gate voltage. Second, it is expected that the tunneling current exhibits interesting divergent behavior for a graphene/MoS<sub>2</sub>/GNR heterostructure. This result has great

potential for use of the divergent current peaks. Furthermore, the existent of magnetism in few-layer MoS2[17,18,19] leads to spin-polarized current in the graphene heterostructures. In this case, the graphene heterostructure could be a perfect spin-filter only for holes with the electron-hole asymmetric spin-splitting of magnetic MoS2[20]. Such tunneling phenomena may offer more potential applications in graphene-based electronics.

## References

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## Figures

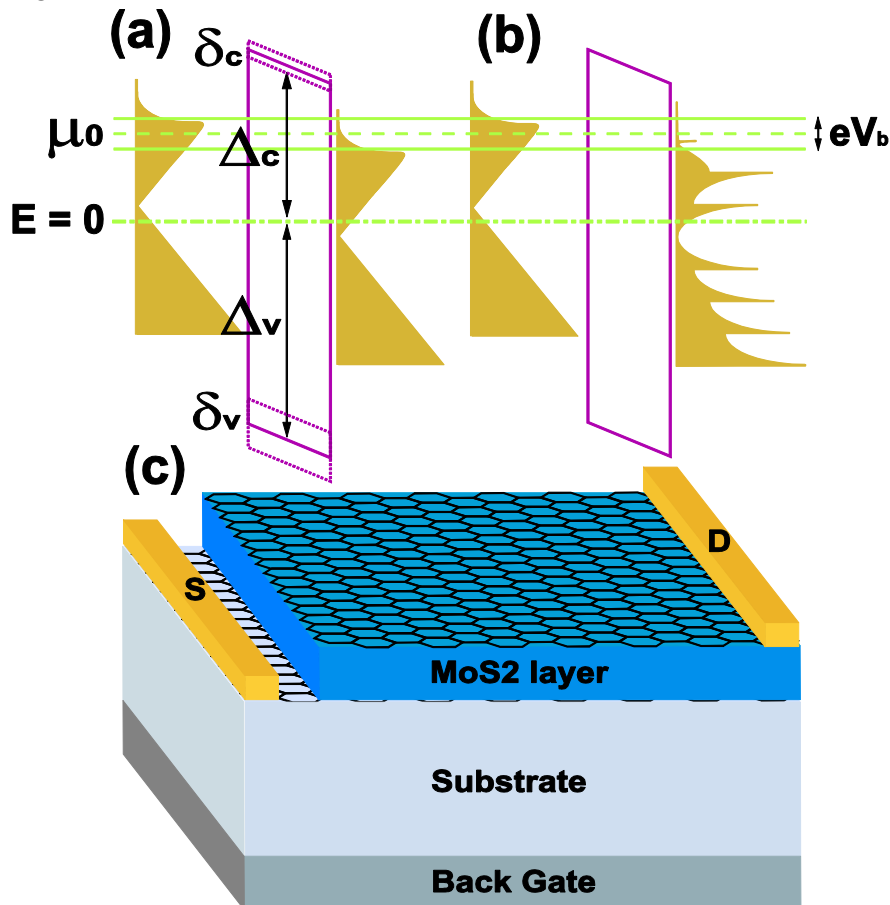


Fig. 1 Energetic diagrams of the systems considered in this study; (a) graphene/MoS2/graphene and (b) graphene/MoS2/AGNR. (c) Schematic diagram of the model fabrication.