Charge Effect on Current-Voltage Characteristics of MoS₂ Nanoribbon

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Abstract. Charge effect on I-V characteristics of single layer zigzag nanoribbon MoS₂ (Z-NR-MoS₂) have been studied using first-principles quantum transport calculations. We show that the internal electric polarization is strongly dependent on dominating edge atoms; hence, two structures with different edge atoms are investigated. Our calculations show that due to this internal polarization a large negative differential resistance (NDR) has been observed.

1. Introduction
In recent years, low dimensional nanomaterials have drawn many attentions due to their physical, mechanical and chemical properties. Among them graphene is one of the most investigated one with its diverse applications in electronics[1], but the existence of an indirect band-gap in pristine graphene turned focuses on alternative materials such as boron nitride, tungsten disulfide, molybdenum disulfide (MoS₂), and others.

Molybdenum disulfide, a transition metal dichalcogenide, consists of three layers which are bounded by weak Van der Waals forces, though covalently interacting internally. In bulk form, MoS₂ is a semiconductor with an indirect band gap of 1.2 eV, however, there is a transition to 1.9 eV direct band gap in monolayer form. There have been reports about some unusual electronic and magnetic properties: the zigzag nanoribbon was ferromagnetic and metallic, while the armchair nanoribbon was nonmagnetic and semiconducting with a width-dependent band gap. Both experiment and theory show that the zigzag MoS₂ nanoribbons are generally more stable than the armchair MoS₂. Absorption and defects may also affect their physical properties [2].

An important requirement in material applications is the control of electronic and magnet properties by means of an external force in a given material. Therefore, effects of an external field on the electronic structures of graphene nanoribbon has been studied [3]. This result also can be applied to the modulation of MoS₂ nanoribbon. It has been shown that the electronic properties of zigzag MoS₂ nanoribbon are also sensitive to electric field [4], which stem from the energy level shifts induced by an internal electric polarization and the competing covalent/ionic interactions.

In present work, we report a first principles study of transmission properties of Zigzag Molybdenum disulfide nanoribbon passivated by Hydrogen (Z-MoS2-NR-H). Our results on electronic properties of the compound show promising functionalities for future FETs.

2. Computational method
First-principles calculations based on the Density functional theory (DFT) have been performed using SIESTA/TRANSIESTA package [5] with pseudopotentials implemented in the SIESTA code.
The generalized gradient approximation (GGA) in the form of the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional is implemented. $1 \times 1 \times 12$ Monkhorst-Pack k-point grids are used in the structural optimizations and energy calculation. A mesh-cutoff of 300 Ry is chosen and all atoms are relaxed to a force of $<0.02$ eV/Å. To isolate the nanoribbons a vacuum of 4 nm and 5 nm is chosen in Z and Y directions respectively. Results are consistent with previous works on MoS$_2$ nanoribbon, hence ensuring their validity [6].

Unit cell is extracted from a sheet of MoS$_2$ nanoribbon then the structure is made by repeating it in Z direction, both sides are passivated by hydrogen to eliminate dangling bonds. As shown in figure 1 dashed lines show electrodes.

![Figure 1](image1.png)

**Figure 1.** Two structures with different edges, (a) Zigzag MoS$_2$ nanoribbon with one edge dominated by Mo and the other dominated by S (Z-MoS$_2$-SM), (b) a Zigzag MoS$_2$ nanoribbon with both edges dominated by S (Z-MoS$_2$-SS)

### 3. Results

Previous studies on Zigzag MoS$_2$ nanoribbon showed that it has an internal electric dipole due to the asymmetrical edges [4]. In order to investigate the effects of internal electric dipole we used two types of structures, first a Zigzag MoS$_2$ nanoribbon with one edge dominated by Mo and the other dominated by S (Z-MoS$_2$-SM), second structure is a Zigzag MoS$_2$ nanoribbon with both edges dominated by S (Z-MoS$_2$-SS).

![Figure 2](image2.png)

**Figure 2.** Band structure, Density of states and Transmission spectrum for (a) (Z-MoS$_2$-SM) and (b) (Z-MoS$_2$-SS).

8 rows of atoms are used for scattering region, any more than that had little effect on transmission spectrum. Band structure calculations are done using a unit cell with boundary conditions in Z direction.

Figure 2 shows the band structure of a metal with two bands crossing the Fermi level ($E_f$) which is consistent with density of states (DOS) for both structures. We also calculated transmission spectrum of the system at 0 Voltage, near $E_f$ there are two transmission channels (two bands crossing $E_f$), it indicates that these channels contribute most to the current.
As can be seen from figure 3, by increasing Voltage, most contributing channels stay near Fermi level while the higher level channels move away from it.

![Figure 3](image)

**Figure 3.** Transmission spectrum for (a) (Z-MoS2-SM) and (b) (Z-MoS2-SS), colors indicate different Bias Voltages ranging from 0 to 1.3 V.

In this figure 3, it is observed that the transmission channel near $E_f$ vary dramatically after 0.5V, as for the other structure, It’s transmission near $E_f$ decreases gradually with increasing voltage (figure 3b). As a result of these variations one observes negative differential resistance (NDR) effect around 0.5 V in the I-V characteristics (figure 4). We believe, observed NDR is caused by an internal electric dipole which strongly depends on edge atoms. This can be evidence from comparison of internal electric dipoles: internal electric dipole for Z-MoS2-SM is almost 7 times stronger than that of Z-MoS2-SS. Notice that for Z-MoS2-SM an increase in the current is observable after 1V which suggests the saturation of transmission channels, hence showing ohmic behavior in the diagram. Furthermore, I-V characteristics revealed larger number of transmission channels for Z-MoS2-SS which in return means larger conductivity in this configuration.

![Figure 4](image)

**Figure 4.** Current-Voltage diagram for (Z-MoS2-SM) and (Z-MoS2-SS).
4. Conclusion
Charge effect on current-voltage characteristics of MoS$_2$ were investigated using TRANSIESTA package, findings suggest that Internal electric dipole created by edge atoms, plays an important role in electron transmission and hence its overall conductivity. A negative differential resistance effect has been observed. The origin of this effect has been discussed.

References
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