Quantum conductance of MoS$_2$ armchair nanoribbons

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Molybdenum disulfide (MoS$_2$) is layered transition-metal dichalcogenide (TMDC), which in its monolayer form, has the direct bandgap of 1.8 eV. We investigated the effect of width and strain on quantum transport for MoS$_2$ armchair nanoribbons. That indicates MoS$_2$ armchair nanoribbons are a good candidate for transistors even with strain.

I. INTRODUCTION

In recent decades, one-dimensional (1D) nanostructures have been extensively investigated because of their interesting properties and their mesoscopic physics. Among them, carbon nanostructures are well-studied, theoretically and experimentally. On the other hand, carbon-based nanostructures are not suitable for some applications because of their small bandgap.

Fortunately, a good alternative to carbon-based systems is a class of inorganic layered materials which exhibit different properties and also could be synthesized in the form of nanotubes and nanoribbons. These systems could use in a large variety of applications of one-dimensional systems. Molybdenum disulfide (MoS$_2$) is layered transition-metal di-calcogenide (TMDC) semiconductor that has attracted considerable interest because of its properties. In its bulk structure, an indirect bandgap of about 1.2 eV is observed, while in monolayer form, the bandgap increases to 1.8 eV with a transition to direct bandgap, which makes it useful for some applications in electronics, optoelectronics, and photovoltaic devices.

It has already been shown that monolayer of MoS$_2$ is an ideal material for valleytronics. This fact is due to the inversion-symmetry breaking together with spin-orbit coupling leads to coupled spin and valley degree of freedoms in a monolayer of MoS$_2$ and other group-VI dichalcogenides. It means that it is possible to control both spin and valley in these 2D materials. It has been shown that Mo and W dichalcogenides can exhibit two thermodynamically stable hexagonal (H) and tetragonal (T) structural phases which provide opportunities for flexible, low power and transparent electronic devices.

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II. COMPUTATIONAL DETAILS

The first-principle calculations are performed utilizing the projector augmented wave (PAW) pseudopotentials in the framework of density functional theory (DFT), as implemented in the Quantum-Espresso package. The exchange-correlation effects are evaluated using the generalized gradient approximation as proposed by Perdew-Bruke-Ernzerhof (PBE-GGA). The Monkhoest-Pack scheme of k-point sampling is used for integration over the first Brillouin zone. For monolayer and nanoribbons structures, $7 \times 7 \times 1$ and $1 \times 7 \times 1$ k-point meshes are used, respectively. The energy and the wave-function cut-offs are set to 400 Ry and 35 Ry, respectively. We set all vacuum at least to 12 Å. The wannierization is obtained by Marzari and Vanderbilt’s method using the WANNIER90 code. In the case of entangled energy, we used Souza, Marzari, and Vanderbilt approach.

III. RESULTS AND DISCUSSION

Electronic Properties:

Firstly, we investigated the electronic structure of MoS$_2$ monolayer. The optimized lattice constant was 3.16 Å and the band gap obtained 1.76 eV, in good agreement with the previous calculation. Then we investigated MLWF (Maximally Localized Wannier Function) of the monolayer. We chose d orbital of Mo atom and p orbital of S atoms for initial projections in wannierization and we obtained MLWF for monolayer, in coincident with the previous results.

After monolayer, we investigated MoS$_2$ nanoribbons. Such as geraphene nanoribbons, MoS$_2$ nanoribbons also can be described with 2 integer indices. So the chiral vector is $\vec{C}_h = n\vec{a} + m\vec{b}$ that causes we have 2 types
of nanoribbons: zigzag for \( n \neq 0, m = 0 \) and armchair for \( m = n \). From previous calculations, we know that zigzag nanoribbons are metallic and magnetic and armchair nanoribbons are semiconductor and nonmagnetic. Since our purpose is how to make a transistor, we chose armchair nanoribbons. After cutting monolayer and building armchair nanoribbons, we optimized lattice constant. Then the electronic spectrum of relaxed structures extracted from band structure calculation (see Fig. 3 and Fig. 4(a)). Others also reported the same results.

Then we modulated our structures with O and H atoms. Based on Zhang et. al paper, if each edge S atom is saturated by one H atom and each edge Mo atom is saturated by one O atom. As shown in Fig. 1 and Fig. 2 in the case of ANR-bare the edge atoms after relaxation are more displaced than the case of ANR-passivated so passivation cause order in structure. We can see the bandgap of AMoS\(_2\)NR-H-Os converges to 1.4 eV that closer to the bandgap of monolayer compare to bare-nanoribbons (see Fig. 2), and then similarity to bare-nanoribbons we obtained band structure of passivated nanoribbons.

Then binding energy per atom has been defined as:

\[
E_{\text{Binding energy}} = (E_H - O - E_{\text{bare}} - mE_H - nE_O)/(n+m)
\]  
(1)

and computed for each width. In table (I) you can see bond length for edge atom and binding energies for every width. You can see our results for 3-AMoS\(_2\)NR to 8-AMoS\(_2\)NR (see Fig. 4(a)). Our result is in good agreement with the previous result. The bandgap is oscillating like the previous study but there is an interesting point in 4-ANR.

For optimization lattice constant of nanoribbons we should obtain the relation between total energy and lattice constant. Because our structure is periodic in the y-direction we plotted total energy in terms of lattice constant in the y-direction. For all structure, we get one minimum in the plot but for 4-AMoS\(_2\)NR-bare we got two minima. Of course, the global minima was right and was in good agreement with other works. But there was another minimum that should be investigated (Fig. 8). As you saw in Fig. 4(a), the graph of an increasing/decreasing of bandgap after passivation remains as the same in bare one except for 4-AMoS\(_2\)NR. We investigate this little subject in the app. A.

**MLWF and quantum transport:**

After that, we should obtain MLWF for each nanoribbon. It should be noted that choosing some appropriate begin projections for wannierization lead to meaningful localized orbitals. After obtaining MLWF of each nanoribbon we can investigate the quantum transport of our systems. You can see our results in Fig. 4(b), as you see with increasing width of the AMoS\(_2\)NR-H-Os number of passing channel is increased and the value of G (the quantum transport for each energy) is increased too.

It should be noted that only electrons at the \( E_f \) (Fermi energy) playing a role in the quantum conductance. At finite temperature, every sub-band near the \( E_f \) can contribute to the quantum conductance. The current, for a finite bias voltage (\( V \)), is given by

\[
X = \frac{X_\Gamma}{X_0}
\]

**Figure 1.** Optimized structure of a MoS\(_2\) 8-ANR, where the gray atoms in background indicate the atomic positions before relaxation. The structure is periodic along the y direction.

**Figure 2.** Optimized structure of a MoS\(_2\) 8-ANR-passivated, where the gray atoms in background indicate the atomic positions before relaxation. The structure is periodic along the y direction.

**Figure 3.** Band structure, density of state and conductance of a the nanoribbons with 8 layer.
Table I. Bond Distances (Å) at the Edge of Nanoribbons, Binding Energies \( E_b \) (eV), and Band Gaps \( E_g \) (eV) of Different AMoS\( -2\)NRs

| W  | \( d_{Mo-O} \) Å | \( d_{S-H} \) Å | \( d_{S-Mo} \) Å | \( E_b \) (eV) | \( E_{g(bare)} \) (eV) | \( E_{g(passivated)} \) (eV) |
|----|-----------------|-----------------|-----------------|-------------|-----------------|-----------------|
| 3  | 1.70            | 1.36            | 2.56            | -3.99       | 0.40            | 1.40            |
| 4  | 1.70            | 1.35            | 2.37            | -4.11       | 0.15            | 1.56            |
| 5  | 1.71            | 1.36            | 2.56            | -4.10       | 0.55            | 1.32            |
| 6  | 1.71            | 1.36            | 2.37            | -4.11       | 0.44            | 1.29            |
| 7  | 1.71            | 1.36            | 2.56            | -4.10       | 0.59            | 1.45            |
| 8  | 1.71            | 2.57            | 2.37            | -4.10       | 0.53            | 1.41            |

Figure 4. a) Energy band gap as a function of the ribbon width \( w \) with \( 3 \leq w \leq 8 \) for AMoS\( 2\)NR-bare and AMoS\( 2\)NR-H-O. b) The Landauer quantum conductance of an AMoS\( 2\)NR-H-O in the y direction for \( w = 3 \rightarrow 8 \)

\[ I = \int_0^\infty \frac{d\epsilon}{e} \left[ f(\epsilon + \mu) - f(\epsilon) \right] G(\epsilon) \]

\[ \simeq \int_0^\infty d\epsilon \mu \frac{\partial f}{\partial \epsilon} G(\epsilon) \]

\[ = V \int_0^\infty d\epsilon \frac{\partial f}{\partial \epsilon} G(\epsilon) \]

\[ \text{where} \ f \ \text{is the Fermi-Dirac distribution function and} \ \mu \ \text{is the chemical potential.} \]

\[ \text{At a finite temperature} \ \mu \frac{\partial f}{\partial \epsilon} \ \text{has a Gaussian peak that at} \ T = 0 \ \text{K becomes a Dirac delta function. We can estimate that at room temperature the current can be approximated by integrating over} \ \epsilon \in [-0.3, 0.3] \ \text{eV}^{27} \ \text{and compute conductance room temperature.} \]

Because of bandgap presence in AMoS\( 2\)NR-H-O, we can use them in transistors. As a result, we should check how the quantum transport change if the system influence by various gate voltage (see Fig. 7 a) As you see all of the nanoribbons are good for transistors because of their high ratio of On/Off in different gate voltages. But one should choose a proper gate voltage for transistors. For example, if you want to use 8-AMoS\( 2\)NR-H-O for the transistor using 0.8 V and 1.1 V to 1.5 V value for gate voltage is recommended.

Response of AMoS\( 2\)NR-H-Os to strain:

We investigated the effect of strain on AMoS\( 2\)NR-H-O. According to previous works\( ^{16} \) we know that there are two typical families of AMoS\( 2\)NR-H-O, symmetric for odd width and asymmetric for even width. As a result, AMoS\( 2\)NR-H-O with widths \( w = 7 \) and 8 was chosen to represent two typical families of AMoS\( 2\)NR-H-O. Now we want to extract band structure in various strain and you can see our result in fig(5), with both positive and negative strain bandgap is decreased for both symmetric and asymmetric nanoribbons. With increasing or decreasing strain the number of passing channel for electrons is increased. Figure 6 shows the quantum transport of the 7-,8-AMoS\( 2\)NR-H-O under various induced strain at \( T = 0 \) K.

In room temperature, we can use Eq. 2 for computing quantum conductance in various strain for the 7-,8-AMoS\( 2\)NR-H-O as you see in Fig. 7. With increasing or decreasing strain the number of passing channel for electrons is increased, but as you see in Fig. 7 in room temperature 7-,8-AMoS\( 2\)NR-H-O have low conductance, as a result, you can use them for the transistor in high strain. Also if there is for example 1 V gate voltage you can use these nanoribbons as strain sensors.
IV. CONCLUSION

Density functional studies of nanoribbons width and strain effects on the electrical transport properties of the AMoS$_2$NR-H-O are presented. By applying a uniaxial tensile strain in the y-direction, the electronic properties of the AMoS$_2$NR-H-O nanoribbons were studied. Using the Wannier functions, the band structure and density of states were calculated for different strains from -15% to +15%. It is observed that AMoS$_2$NR-H-O in different width and strain are a good candidate for using in the transistor. In addition, you can use them for strain sensors.

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Discussions with ... about various choices of methods are appreciated.

Appendix A: ANR-4-bare

We guessed that maybe there is a bond that reinforced in the second minimum in compare with maximum, so we checked that and we saw that (Fig. 8). But there was no bond that approves this guess. Then we investigate that if one of this minimum or maximum has magnetic structure, and the value of total magnetization is zero. We plot band structure for these 3 that you can see in Figs. (9).

We have seen that in the case of 4-AMoS$_2$NR-bare for lattice parameter 5.4 the bandgap is 0.15 eV (indirect) that is in good agreement with the previous result, and in the case of 4-AMoS$_2$NR-bare for lattice parameter 5.7,6.0 the band gap is 0.32eV (indirect) and 0.67eV (direct in $\Gamma$ point) respectively.

Figure 7. a) Conductance of AMoS$_2$NR-H-Os for various gate voltage b) Conductance of 7-AMoS$_2$NR-H-Os for various strain and gate voltage

Figure 8. Total energy in terms of lattice constant for 4-AMoS$_2$NR-bare
Figure 9. Band structure of 4-AMoS$_2$NR-bare for lattice parameter 5.4, 5.7, and 6.0 respectively Å

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