# *Ab initio* study of $MoS_2$ nanostructures

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The atomic and electronic properties of molybdenum disurfide ($MoS_2$) nanostructures are investigated through density functional theory (DFT) calculations. We find that the band gap is indirect (about 1.79 eV) and direct (about 1.84 eV) in GGA for 2-dimensional $MoS_2$ in our calculations. On the other hand, 1-dimensional armchair nanoribbons have semiconductor properties (band gap is about 0.11 ~0.28 eV), while 1-dimensional zigzag nanoribbons are metallic.

## INTRODUCTION

The graphene has been expected to provide good performance due to its nano size effect and many interesting properties such as high electronic mobility and good transparency [1].

However, the zero band gap of graphene is main drawback for applications of electronic devices. The $MoS_2$ has a band gap compared to the graphene. In this regard, it was suggested that $MoS_2$ can be a complement to graphene for nano device applications [2]. Furthermore, its layered structure can also be obtained by mechanical exfoliation method similar to the graphene.

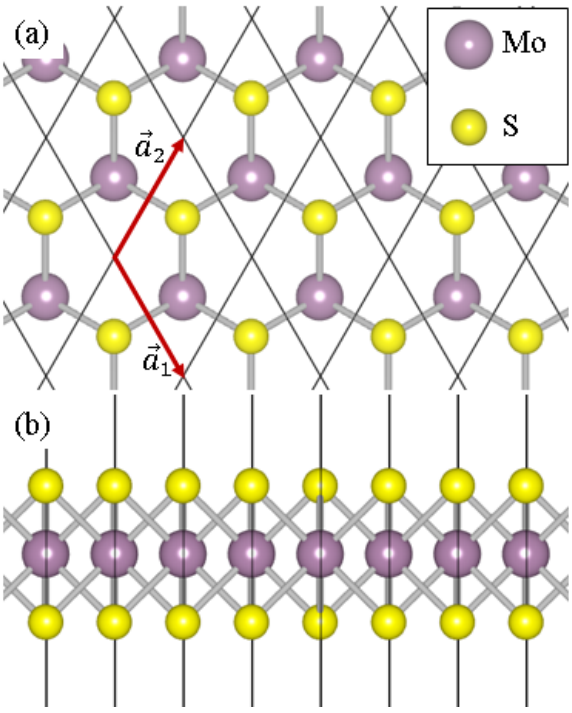


Fig 1. (a) top and (b) side views of atomic structure of 2-dimensional $MoS_2$. Light purple and yellow balls represent Mo and S atoms, respectively. Red arrows in (a) represent lattice vectors.

## SIMULATION METHODS

We have performed density functional theory (DFT) calculations to find atomic and electronic structure in generalized gradients approximation with SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) program on the EDISON (EDucation-research Integration through Simulation On the Net) web site [3]. The model structure is that infinite 2-dimentional sheet and 1-dimentional nanoribbon structures are considered for $MoS_2$ nanostructures, as shown in Figures 1 and 4. In the geometrical optimization, we use 3x3x1 and 5x1x1 k-points grid for 2-dimensional and 1-dimensional structures of $MoS_2$, respectively, in Monkhost-Pack scheme. In the band structure calculations, we use the 'Post

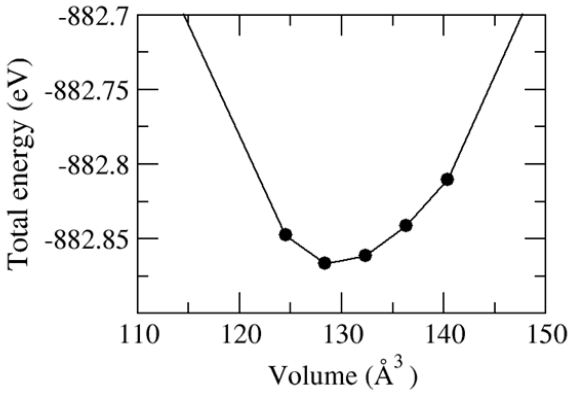


Fig 2. Total energy as a function of volume, which is used for calculation of lattice parameter.

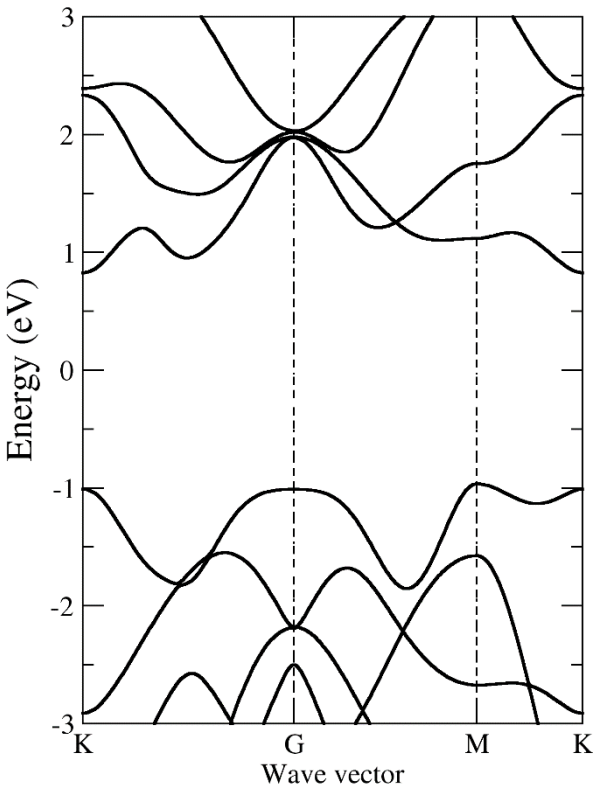


Fig 3. Calculated band structure of 2-dimensional $MoS_2$

processing' category in the EDISON web site for infinite 2-dimentional $MoS_2$, while 51x1x1 grid is used for 1-dimentional nanoribbon $MoS_2$ in Monkhost-Pack scheme.

The 2-dimensional $MoS_2$ sheet consists of 3 layered structures with 1 Mo atom and 2 S atoms in primitive unit cell. Figure 1 shows the optimized geometry of 2-dimensional $MoS_2$ structure with hexagonal planar lattice similar to graphene. The 2-dimensional $MoS_2$ sheet are placed on the xy-plane. The lattice vectors $\vec{a}_1$ and $\vec{a}_2$ have the same length with 120 degree interior angle. The vacuum region of about 10 Å is enough to neglect the inter layer interaction.

## RESULTS

We have performed the total energy calculation to find the optimized unit-cell with changing lattice constant. As a result, we find that the optimized lattice parameter is 3.22 Å at each lattice vectors. Consequently, the cell volume is 128.39 $Å^3$ ($a_3$= 15.0 Å), as shown in Figure 2.

Now, we have calculated electronic band structure of 2-dimensional $MoS_2$ using optimized lattice parameters, as mentioned above. In Figure 3,

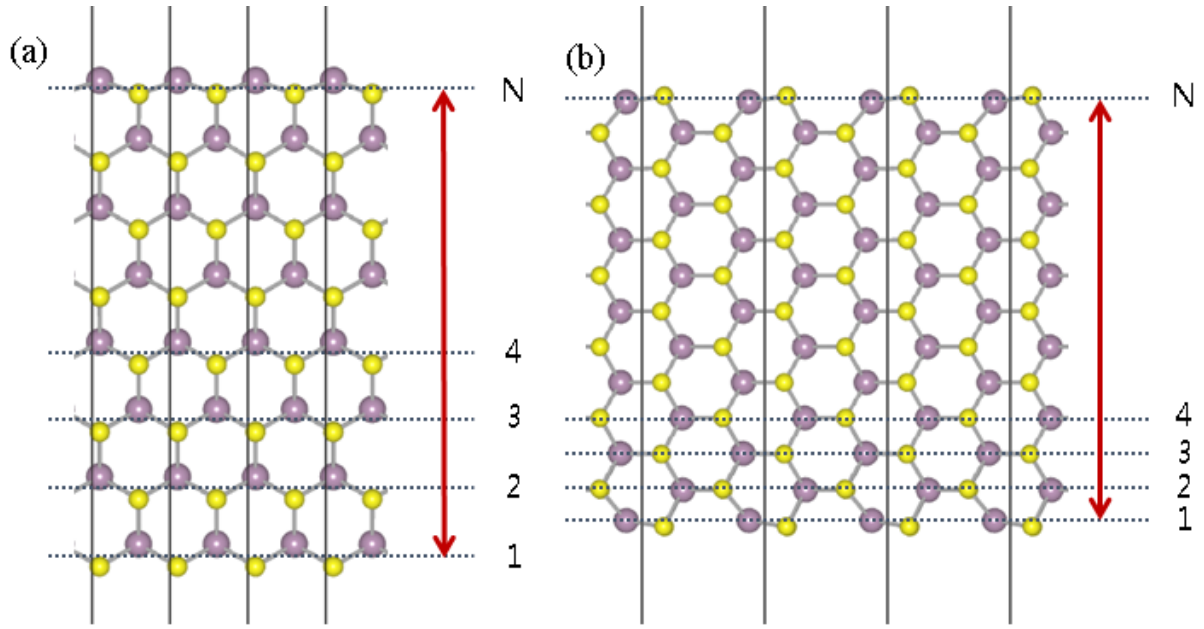


Fig 4. (a) Zigzag and (b) armchair nanoribbon $MoS_2$ structures.

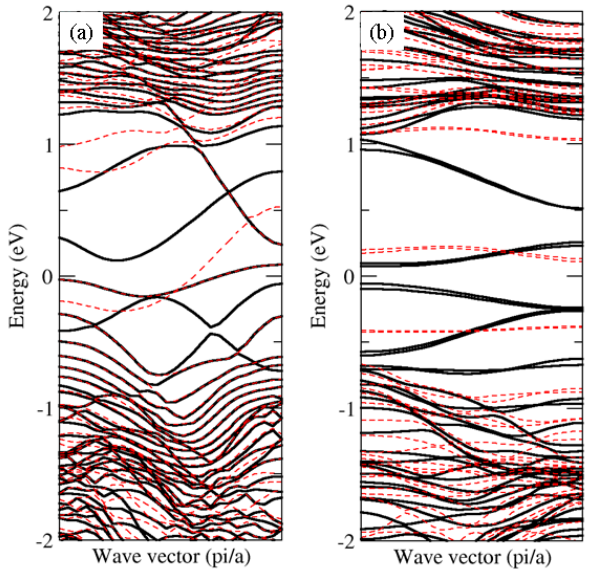


Fig 5. Electronic band structure of (a) zigzag and (b) armchair nanoribbon $MoS_2$. Black lines and red dotted lines represent spin-up and spin-down states, respectively.

the band gap is indirect (about 1.79 eV) and direct (about 1.84 eV) for 2-dimensional $MoS_2$, respectively. The difference between valence band maximum and conduction band minimum at the point K is direct band gap. The indirect band gap is from G to K.

We have already calculated the band structure of 2-dimensional $MoS_2$ using Vienna Ab-initio Simulation Package (VASP). The band structure is slightly different compared with the VASP results. This difference may come from the insufficient input parameters in this calculations. In order to get more accurate results, we need to use sufficient input parameters.

We finally consider two types of $MoS_2$ nanoribbon structures such as zigzag and armchair edge structures. Figures 4 (a) and (b) show the zigzag and armchair $MoS_2$ nanoribbon structures, respectively.

We find the band structure of zigzag and armchair nanoribbon $MoS_2$ as shown in Figures 5 (a) and (b). In the width corresponding to N=13, we find that the band gap is 0.28 eV in the armchair nanoribbon. On the contrary, the zigzag nanoribbon shows metallic properties. In the band structures shown in Figure 5, spin-up and spin-down states are represented by black line and red dotted lines. The band structures show that the nanoribbons have magnetic moments.

## CONCLUSION

In summary, we investigated atomic and electronic structure of 1-dimensional and 2-dimensional $MoS_2$ nanostructure. We found that the lattice constant of 2-dimensional $MoS_2$ is 3.22 Å. We obtained electronic band structure of 2-dimensional $MoS_2$ using optimized lattice parameters. The indirect band gap is about 1.79 eV and direct one is about 1.84 eV for 2-dimensional $MoS_2$. Also, we found that the zigzag $MoS_2$ nanoribbons are metallic, while armchair $MoS_2$ nanoribbons are semiconducting.

Thus, the $MoS_2$ can be a good candidate for the nano devices.

## ACKNOWLEDGEMENT

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