Calculation Study of Electric Properties on Molybdenum Disulfide By Using Density Functional Theory

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Abstract. Molybdenum disulfide (MoS₂) has some unique properties such as symmetry properties in honeycomb structure. In this work, we investigate the electronic properties of different number of layer by using first-principles calculation based on density functional theory (DFT) with calculation using PHASE/0. The Generalized Gradient Approximation (GGA) and ultrasoft pseudopotential method were used. In this study, we compare between monolayer and multilayer of MoS₂, and we investigate the effects of layer number on their electronic properties such as showing direct and indirect bandgap. The properties is important for applications in material devices and energy saving applications.

1. Introduction

The human need for energy growing increased, especially in the field of electrical energy. Electricity invented by Thomas Edison is very beneficial for people around the world. At the moment very growing use Light Emitting Diode (LEDs). LEDs has several advantages compared to ordinary bulbs such as more energy efficient and LEDs does not emit heat. However, LEDs lights also have shortcomings that led prices more expensive than regular bulbs. Molybdenum disulfide is one of material main to make a LEDs. Several studies investigating the use of semiconducting MoS₂ as a host material so as to emit light in multiple colors include red, green and blue. The use of LEDs produced from MoS₂ can provide high levels of efficiency and excellent savings in energy and costs. In previous theoretical research results using algorithms and computing power are predicting that indirect bandgap in bulk MoS2 into direct bandgap when molded into monolayer MoS₂ [1].

The purpose of the present study is to observe the electronic structure of MoS₂. We carry out first-principles calculation to investigate the electronic structure of monolayer and bilayer MoS₂ by using first-principles calculation based on density functional theory (DFT). The results of first-principles calculations are based on density functional theory (DFT) by comparing with the reference as a validation results of the calculation. One approach that is popular in the field of quantum mechanics is the DFT [2]. DFT is a calculation involving first-principles calculations on the effect of the interaction of materials or molecules that applying the local approach and density functional semilocal [3].

2. Model

We carry out first-principles calculation based on density functional theory. We have performed density functional theory (DFT) with exchange-correlation by generalized gradient approximation (GGA). The generalized gradient approximation (GGA) method more accurate than local density
approximation to calculation many electronic properties. We apply ultrasoft in pseudopotential method.

Figure 1. The crystal structure of monolayer MoS$_2$

The crystal structure of monolayer MoS$_2$ composed one atom of moybdenum's (Mo) and two atoms of sulphur (S). And also crystal structure bilayer MoS$_2$ composed two atoms Mo and four atoms of S. In this calculation, monolayer MoS$_2$ obtained the bond length between Mo-S atoms is 2.4219 Å. In this result almost similar with experimental value is 2.383 Å [4]. Figure 2 show that bilayer MoS$_2$ has the bond length between Mo and S is 5.8963 Å. The result calculation almost close with experimental value is 6.0 Å [5].

We use the k-sampling 6x6x1 with mesh method and primitive unit cell with lattice constant, a = 3.16 Å [4] and c = 20 Å and 30 Å for monolayer and bilayer, respectively. We performed from four atoms in each layer is the rectangular lattice. We use cutoff energies of 25 rydberg and 250 rydberg for wave function and charge density grid, respectively. In optimization value of the kinetic energy cut off are wave function and charge density with a total value of state energy calculation result tend to convergence. In this calculation, self-consistent field (SCF) used limits the energy value convergence is 1.0 e-05 Hartree/Bohr.

3. Result and Discussion

3.1 Monolayer MoS$_2$

The cutoff wave function and charge density has been used in our calculation. After optimization, we find that the cutoff of kinetic energy to wave function and charge density are 25 rydberg and 250 rydberg, respectively. Due to the value of the kinetic energy of the charge density multiplied by 9 in accordance with tutorials on PHASE/0 manual. And also, the monolayer MoS$_2$ obtained k-point is 6x6x1. The lattice constant of MoS$_2$ has been used in our calculations. The calculation of the minimum value of cell unit in MoS$_2$ is done by varying lattice parameter of lattice constant (a). We find that the lattice constant of monolayer MoS$_2$ is 3.2183 Å. The result of our calculation is almost close to the experimental value is 3.16 Å [4].
Figure 3. (a), (b), and (c) are relation between total energy and cutoff, k-point, and lattice constant, respectively.

Figure 4 is band structure and density of state (DOS) of monolayer MoS$_2$. Monolayer MoS$_2$ has a direct bandgap energy located at K$\rightarrow$K of k-point with the different in value gap is 1.63 eV. The result of our calculation is almost close to the experimental value is 1.79 eV [4].

Figure 4. The band structure and density of state (DOS) of monolayer MoS$_2$
In this calculation, the pattern on the electronic structure of monolayer MoS$_2$ show that crystal structure of monolayer MoS$_2$ has a direct bandgap, there may be mentioned monolayer MoS$_2$ a direct bandgap of the semiconductor [4].

3.2 Bilayer MoS$_2$

![Figure 5](image.png)

Figure 5. (a), (b), and (c) are relation between total energy and cutoff, k-point, and lattice constant of bilayer MoS$_2$, respectively.

Figure 5 show that the value of k-point approach convergent is $8 \times 8 \times 1$, the value cutoff wave function approaching convergence by 30 Rydberg then cutoff the charge density to 270 Rydberg had reached a value of convergence. Bilayer structure of MoS2 lattice constant achieves minimum energy at 3.26 Å. Optimization is considered complete when lattice constant has reached the minimum energy at a certain value. After optimization on all obtained the parameters for further calculations can be done.

Figure 6 show explain that structure of the left image is a band structure and the right of the image is the image density of states (DOS) in bilayer MoS$_2$. In the image, the band structure is the top and bottom of the conduction band is the valence band. The bilayer MoS$_2$ has an indirect bandgap that point $A \rightarrow \Gamma$ with the difference in the value of 1.38 eV. The difference band structure within the conduction band and valence band become smaller. Due to the distance between atoms in the layer MoS$_2$ greater. In this calculation, the conduction band produced fewer than the valence band. The difference in input a few parameters in this calculation greatly affects the energy gap of MoS$_2$. The
pattern of the electronic structure of the result of this calculation indicates that the material MoS$_2$ with a bilayer structure has the energy band gap properties that are not direct (indirect bandgap).

Figure 6. The band structure and density of state (DOS) of bilayer MoS$_2$

4. Conclusion
In this study, we compare between monolayer and bilayer of MoS$_2$, and we investigate the effects of layer number on their electronic properties such as showing direct and indirect bandgap. The properties is important for applications in material devices and energy saving applications.

References
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