Physical mechanism of layer-dependent strong and weak coupling with electromagnetic wave in 2H-MoS$_2$

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Abstract

In this work, we use the first-principles calculation method to theoretically study the strong and weak coupling between the layer-dependent MoS$_2$ and electromagnetic waves. Through the calculation of the electronic structure and the analysis and fitting of Van Hove singularity (VHS), the differences between the strong coupling and weak coupling mechanisms are discussed. The exponential law of electronic structure parameters with the number of layers is explained. Finally, combined with cavity quantum electrodynamics (QED), it is revealed that the physical mechanism of strong coupling and weak coupling is related to the transition dipole moment. Strong coupling is dominated by inter-band transitions and weak coupling is dominated by in-band transitions.

1. Introduction

Low-dimensional materials are an emerging material system [1–5]. This low-dimensional material has important application potential in many fields due to its various novel properties that are different from other materials [6, 7]. Low-dimensional materials have novel physical properties mainly because their electronic states are different from traditional bulk materials. Early low-dimensional materials consisted mainly of graphene and hexagonal boron nitride [8–11]. Graphene has the characteristics of zero band gap, and Dirac cone exists in its energy band. Hexagonal boron nitride is a wide bandgap semiconductor, and its optical absorption is in the ultraviolet region [12]. In recent years, a series of new two-dimensional materials have been developed [13, 14]. The first of these is transition metal dichalcogenides (TMDs). This series of materials has two different phases that show metallic and semiconductor properties, respectively. The most representative material in the TMDs series is MoS$_2$. MoS$_2$ has many excellent properties, such as topology and charge density waves. The optical properties of MoS$_2$ should not be ignored. It has a good exciton effect in the long wavelength region. This exciton can be coupled to the surface plasmon to increase the hot electron lifetime of the plasmon [15]. Improve photocatalytic reaction efficiency. After two-dimensional materials are stacked in a direction perpendicular to the material plane, their properties will change regularly, and this law is very important for the study of MoS$_2$ [16, 17]. The reason is firstly that it is difficult to control the exact number of layers in the experimental preparation process, and secondly that the optical properties of the material can be adjusted by the number of layers for better application [6]. The research on twisted bilayer graphene in recent years also indicates that the research of multilayer two-dimensional materials is very valuable.

The properties of multilayer MoS$_2$ are related to the interaction between layers. And this kind of interlayer interaction will have regular influence on the electronic structure and optical properties. In other words, the optical property is the interaction between electromagnetic waves and multilayer MoS$_2$ [3], and this interaction will change regularly with the number of layers. But this change is not a simple linear relationship. Therefore, a quantitative study of this law is needed. On the other hand, the interaction between electromagnetic waves and the system can be divided into strong coupling and weak coupling [18]. The strong coupling includes surface
plasmons and rabbis splitting. The weak coupling includes exciton and Purcell effect. Therefore, it is appropriate to explore this regular change through the study of strong and weak electromagnetic coupling of MoS2. This is because there are both plasmon and exciton effects in MoS2. The interaction between electromagnetic waves and matter has both propagation and local behavior, which involves the transition of quantum states. Therefore, it is necessary to discuss this effect from the perspective of cavity quantum dot dynamics (QED) [19]. In this work, we use density functional theory to calculate the optical properties, band structure, density of states, and Van Hove singularities (VHS) of multilayer MoS2. Then, by fitting the band gap and the effective mass, the exponential law of the electronic structure is explained as the number of layers changes. Finally, the physical nature of strong coupling and weak coupling was analyzed using the view of cavity QED.

2. Method

In this work, the different layers MoS2 are perform as calculation model by density functional theory (DFT) [20]. A vacuum layer of 15 Å is present in the direction perpendicular to the plane of MoS2. The atomic central basis set [21] and the GGA-PBE functional [22, 23] with DFT-1/2 pseudo-potential are calculated using the QuantumATK-2019.03-SP1 software package [24]. All of optimization (cell and position) of the atomic geometry is performed until all the components of the residual forces are less than 0.05 eV Å\(^{-1}\) and the total energy converges within \(1.0 \times 10^{-6}\) eV. The \(k\)-mesh is \(7 \times 7 \times 1\) and the cut-off energy is 1200 eV [25]. Using the same cut-off energy in the optical property calculations, the \(k\)-mesh increases to \(15 \times 15 \times 1\), and the self-consistent field convergence limit increases to \(1.0 \times 10^{-8}\) eV.

3. Results and discussion

3.1. Structure of different layers MoS2

we carried out theoretical research on 2H phase MoS2 with different layers. As the number of layers increases, the crystal structure of MoS2 does not change in a direction parallel to the plane of MoS2. Therefore, its Brillouin zone \(k\)-space path are also constant, that is, the Brillouin zone he hexagonal crystal system, see figure 1(a). The layer-dependent optical properties are set by setting MoS2 cells with different layers, see figure 1(b). Because there are van der Waals interactions between the layers of MoS2, which is also called dispersion force. This interaction is related to the exchange of electrons. Therefore, Grimme’s DFT-D3 correction method is always accompanied in the calculation and geometric optimization.

3.2. Strong and weak interaction with electromagnetic wave in different layers MoS2

When the system interacts with electromagnetic waves, from the perspective of classical physics, electromagnetic waves will be absorbed or reflected by the system. But from a QED perspective, this process is much more complicated [26]. The strength of interaction is divided into strong coupling and weak coupling. Although it appears to be an absorption process in the macroscopic spectrum, its physical nature is different. First, strong coupling is generally thought of as the existence of plasmons and rabi oscillations [27, 28]. There are certain conditions for the generation of surface plasmons at the interface. If the dielectric function of the

![Figure 1. Brillouin zone and k-space path (a) and lattice structure (b) of number of layers in two dimensional 2H-phase MoS2.](image-url)
medium is written in the form of a complex dielectric function [26]:

$$\epsilon(\omega) = \epsilon'(\omega) + i\epsilon''(\omega)$$  \hspace{1cm} (1)

where the $\omega$ is the frequency of electromagnetic wave. Then the $\epsilon'(\omega)$ and $\epsilon''(\omega)$ are the real and imaginary part of dielectric function, respectively.

The imaginary part of the dielectric function generally represents the loss of the medium, in other words the absorption effect of the system on electromagnetic waves. The complex dielectric function determines the conditions under which the plasmon appears. Usually, the real part of the dielectric function of the interface is less than zero, which presents $\epsilon'(\omega) < 0$ at special frequencies [18, 26]. But if you want to ensure that plasmons appear, you also need the imaginary part of the dielectric function to be greater than zero, which is $\epsilon''(\omega) < 0$. Although it looks macro, this is an absorption process. In fact, due to the condition of the real part of the dielectric function, electromagnetic waves are not absorbed, but exist on the interface in the form of evanescent waves. This is the surface plasmon at classical physical views. In this work, we calculated the complex dielectric functions of MoS$_2$ with different layers and shown them in figure 2(a). It can be seen from the figure that at 400 ~ 500 nm, there is a strong imaginary part of the dielectric function. This shows that the small layer of MoS$_2$ has a strong absorption of electromagnetic waves in this frequency range. In the longer wavelength region, the imaginary part of the dielectric function also has multiple peaks. However, the real part of the dielectric function in the long wavelength region is positive, so there is no strong coupling effect. According to the foregoing description, the frequency range in which the dielectric function satisfies the conditions for generating a plasmon is shown in figure 2(b). The green translucent area in the figure is the area that satisfies the existence of the surface plasmon described above. Although it appears from a macro perspective, the dielectric functions in these frequency regions satisfy the conditions for generating surface plasmons, and as the number of layers increases, the imaginary part of the dielectric function increases continuously, while the real part of the dielectric function gradually decreases. But the detail changes in this part don’t look very smooth. For the imaginary part of the dielectric function, the values of MoS$_2$ from two to six layers increase steadily, but the increase between the monolayer MoS$_2$ and the bilayer is relatively large.

In addition to the strong coupling in the short wavelength region, there are also four distinct peaks in the imaginary part of the dielectric function in the long wavelength region. As mentioned above, since the real part
of the dielectric function is greater than zero in the long wavelength region (500 ~ 1000 nm), see figure 2(c). Therefore, in this frequency range, the coupling between the system and electromagnetic waves is weak [18, 29–31]. The law of the four weakly coupled peaks also increases with the number of layers. However, the gap between the single layer and other small layers is large. In summary, no matter the strong coupling or the weak coupling, the change law of the absorption spectrum is basically the same. The main absorption peaks are shown in figure 2(d). It can be clearly seen from the line chart that the absorption coefficient changes between the single layer and the double layer are relatively steep, while the absorption coefficient between the subsequent few layers of MoS2 changes smoothly. This phenomenon is usually interpreted as a smooth change due to interlayer interactions [32]. Interlayer interactions do not exist in single-layer systems. This interlayer interaction is also often demonstrated as interlayer charge transfer [33]. But no matter what form of interaction, its physical nature is always related to the electronic structure, especially VHS in DOS.

3.3. Electronic structure of different layers MoS2

In order to study the physical mechanism leading to strong coupling and weak coupling, the band structure and DOS of different layers MoS2 are calculated, see figure 3. In general, the form of the band structure is similar, but due to the increase in the number of layers, the number of atoms in the unit cell increases, which in turn leads to an increase in the number of electrons. Therefore, the number of energy bands in the energy band diagram also increases. Of course, the absolute value of DOS has also increased. Although, the increase in the number of bands is normal. However, an increase in the number of energy bands will cause an overlap between the energy bands. This overlap often creates new VHS [24–36]. Figure 3 shows the band structure of MoS2 with different layers. Whereas, the position pointed by the green arrow in the figure does not overlap with the band structure in a single layer, and the band overlap degree becomes larger as the number of layers increases. This is due to the increase in the number of energy bands. Between the G and M points, the d orbital of Mo and the p orbital of S become closer and closer as the number of layers increases. This overlap will cause new VHS to appear. The green circle in figure 3 shows the new VHS due to band overlap. In other words, a new spike appears in the red DOS curve. The emergence of this new VHS is the main reason for the change in the intensity of the interaction between electromagnetic waves and the system.

As the number of layers and the number of energy bands increase, the band gap and effective mass also change, see figure 4. The effective mass is related to the curvature of the energy band. The energy band curvature will change due to overlapping energy bands, so the effective masses of electrons and holes also change regularly. From the line chart, whether it is a direct band gap or an indirect band gap, it decreases exponentially with the increase of the number of layers, and it tends to converge to a constant value, see figure 4(a). From a physical point of view, this is also reasonable, because with the increase of the number of layers, the properties of the two-dimensional system are closer to the properties of the bulk phase. Therefore, this convergent value is the value of the bulk phase [37, 38]. As shown in figure 4(d), the effective mass of electrons and holes decreases and increases with the number of layers, respectively. This shows that as the number of layers increases, the curvature of the conduction band increases, while the curvature of the valence band decreases. Regardless of band gap or effective mass, the law is close to exponential change. Therefore, the data points are fitted in an exponentially decaying form, see figures 4(b), (c), (e), and (f):

\[ y = Ae^{-n/t} + B \]  \hspace{1cm} (2)

where the \( A \) and \( t \) are exponential factor and coefficient, respectively. The \( n \) is the number of layers of MoS2. The \( y \) can be a direct band gap, an indirect band gap, an electron effective mass or a hole effective mass.

Fit coefficients and mean square deviations (R-square) are shown in table 1. The MSD values in the table show that this fit is precise. As shown in table 1, the exponential factor of direct gap is smaller than indirect gap. Therefore, the decrease rate of the direct band gap with the number of layers is greater than the indirect band gap. This shows that the energy band at point K varies greatly, because the effect of interlayer stacking on point K is greater than that at \( \Gamma \). But for effective masses the rate of change of holes is greater than electrons. This shows that the effect of interlayer stacking on the valence band is greater than the conduction band. This is because as the number of energy bands increases, the orbit is occupied, that is, the valence band energy bands overlap more. If the change between the single layer and the double layer is analyzed separately, this change is significantly larger than that of the other layers. This is consistent with the previous discussion. This is because the interlayer interaction forces also obey the exponential relationship [19].

3.4. Strong coupling and weak coupling analysis with cavity QED

In fact, plasmons are the interaction between materials and light. Its essence can be explained by quantum electrodynamics (QED). From the viewpoint of cavity QED, the Hamiltonian of the plasmon emission process can be defined by the electric field \( \vec{E}(\vec{k}) \) and the transition dipole moment \( \vec{T} \) as:
where the $\sigma_x$ is the optical electric conductive. Since the plasmon is a propagation behavior, the Green’s function method can be used to express the plasmon intensity as \[ | \langle \mathbf{P} \rangle \rangle | \langle \mathbf{P} \rangle \rangle = \int g_{\mathbf{r}}(\omega, \mathbf{k}, \mathbf{k}) \mathbf{G}(\omega, \mathbf{k}, \mathbf{k})^\ast d^2r^* \] where the $\mathbf{G}(\omega, \mathbf{k}, \mathbf{k})$ is the Green’s function of plasmon, which is defined by:

$$
\text{Im} \mathbf{G}(\omega, \mathbf{k}, \mathbf{k}) = \frac{\omega^2}{\mathbf{c}^2} \int d^2r^* \epsilon^\prime(\mathbf{k}, \omega) \langle \mathbf{k} \rangle \mathbf{G}(\omega, \mathbf{k}, \mathbf{k})^\ast (\omega, \mathbf{k}, \mathbf{k})$$

From the analysis of the formula, the imaginary part of the Green’s function and the imaginary part of the dielectric function have a positive correlation. Therefore, the surface plasmon intensity, that is, the coupling strength, has a great relationship with the imaginary part of the dielectric function. Of course, this conclusion has already been discussed in the previous article. However, according to equation (3), the coupling strength is not only related to the Green’s function, but also closely related to the transition dipole moment. First, in the high-energy region of the dielectric function, that is, the short-wavelength region, the corresponding absorption spectrum energy appears as an inter-band transition in the energy band. The transition dipole moment of the inter-band transition is significantly larger than the in-band transition. This is because there are more vacant

$H_{\text{int}} = -\sigma_x \mathbf{T} \cdot \mathbf{E}(\mathbf{k})$  \hspace{1cm} (3)

$|g(\omega)|^2 = \frac{1}{\hbar \epsilon_0} \frac{\omega^2}{\mathbf{c}^2} \text{Im} \mathbf{G}(\omega, \mathbf{k}, \mathbf{k})^\ast$  \hspace{1cm} (4)

$\text{Im} \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) = \frac{\omega^2}{\mathbf{c}^2} \int d^2r^* \epsilon^\prime(\mathbf{k}, \omega) \langle \mathbf{k} \rangle \mathbf{G}(\omega, \mathbf{k}, \mathbf{k})^\ast (\omega, \mathbf{k}, \mathbf{k})$  \hspace{1cm} (5)
states in the conduction band. Secondly, as the number of energy bands increases, more density of states appears in the occupied orbit, or valence band. Even new VHS appeared due to band overlap. VHS can significantly increase the transition dipole moment of the inter-band transition. Therefore, strong coupling occurs in the high energy region. The transition dipole moment in the low energy region is very small, because the transition

Figure 4. The direct and indirect energy band gap (a) and their fitting results (b) and (c), and the electronic and hole effective mass (d) and their fitting curves (e) and (f).

| Table 1. The exponential fitting coefficients of energy band gaps and effective masses. |
|---------------------------------|----------------|----------------|----------------|----------------|
|                                 | Constant term (B) | Exponential factor (A) | Exponential coefficient (t) | R-square |
| Direct gap (eV)                | 1.362 ± 0.032    | 0.120 ± 0.013    | 0.902 ± 0.087    | 0.9962 |
| Indirect gap (eV)              | 0.605 ± 0.013    | 1.287 ± 0.195    | 0.909 ± 0.125    | 0.9925 |
| Effective mass of electron     | 0.386 ± 0.001    | 0.047 ± 0.019    | 0.882 ± 0.310    | 0.9578 |
| Effective mass of hole         | −0.883 ± 0.009   | −2.286 ± 0.142   | −0.900 ± 0.050   | 0.9987 |
dipole moment is defined as:

\[ \bar{T} = \langle \hat{k}_e | \hat{p} | \hat{k}_s \rangle \] (6)

This definition requires that there must be enough electrons in both the excited initial and final states to have a higher transition dipole moment. So this also explains that the inter-band transition is the cause of the strong coupling, and the in-band transition is the main contribution of the weak coupling.

4. Conclusion

In this work, the strong-coupling and weak-coupling properties of MoS2 and electromagnetic waves with a small number of layers are studied by first-principles calculations. The physical nature of strong coupling and weak coupling is analyzed by cavity QED theory. First, through first-principles calculations, it was found that as the number of layers increased, the band overlap in the conduction band of the MoS2 with fewer layers became more and more significant, and a new Van Hove singularity (VHS) appeared in the overlapping portion. As the number of layers and band overlap increase, the changes between the single layer and the double layer are greatest, including the band gap and effective mass. Secondly, by analyzing the optical properties of MoS2 with few layers, it is found that there is strong coupling in the high energy region and weak coupling in the low energy region. The coupling strength, that is, the law that the absorption spectrum strength increases with the number of layers, is consistent with the energy band. It is also a large change in the single layer and the double layer, and then the change converges to the body phase value through an exponential relationship. Finally, through the conclusion analysis of cavity QED, the physical mechanism of strong coupling is the inter-band transition, while the weak coupling is the in-band transition. Both strong coupling and weak coupling have huge application potential in MoS2 surface plasmon or exciton devices. Especially in the surface plasmon-exciton hybrid photocatalytic reaction or the surface plasmon-exciton coupled waveguide device, a reliable theoretical rule is needed to design a new high-performance device.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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