The 27th Iranian Conference on Optics and Photonics (ICOP 2021), and the 13th Iranian Conference on Photonics Engineering and Technology (ICPET 2021). University of Sistan and Baluchestan, Zahedan, Iran, Feb. 2-4, 2021

کد مقاله : ۲-۱۰۶۶-۱۰-A

بررسی محاسباتی اثر افزایش لایه ها در خواص الکترو-نوری ساختار دو بعدی MoS_2

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چکیده- در این مقاله با استفاده از روش محاسبات اصول اولیه پیاده سازی شده با روش تئوری تابع چگالی و در نظرگرفتن برهم-کنش‌های بین‌لایه‌ای واندروالس، خواص الکترو- نوری وابسته به فرکانس فوتون‌های نوری در یک ماده دو بعدی MoS_2 مورد مطالعه قرار می‌گیرد. به این منظور ابتدا ساختارهای بهینه تک/دو/سه-لایه استخراج می‌شوند و سپس تابع مختلط دی‌الکتریک، ضرایب جذب، شکست نور و میزان انعکاس در جهت های مختلف درون و برون صفحه ای استخراج می‌گردد. با توجه به نتایج، افزایش تعداد لایه‌ها موجب بیشتر شدن همسانی ساختار شده و بنابراین خواص نوری در جهت‌های مختلف هم‌سان‌تر می‌شود. افزایش تعداد لایه-ها از یک به دو عدد، ضرایب الکترونوری را افزایش می‌دهد در حالیکه بیشترکردن تعداد لایه‌ها مشخص می‌کند که لزوما رابطه مستقیمی مابین افزایش لایه و خواص الکترو-نوری وجود ندارد.

کلید واژه- مواد دو بعدی، MoS_2 تک/دو/سه-لایه، خواص الکترو-نوری، محاسبات تئوری تابع چگالی

Computational analysis of the effect of number of layers on the electro-optical properties of a two dimensional MoS_2

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Abstract- In this paper by first principle calculations implemented by density functional theory (DFT) and taking the van der Waals inter layer interactions into account, the optical photonic frequency depended electro-optical properties of two dimensional MoS_2, is investigated. For this purpose, first the optimized mono and multi-layer structures are extracted and then the complex dielectric function, the refractive index, absorption and the reflectivity coefficients along different in-plane and out-of-plane directions are obtained. According to the results, increasing the number of layers enhances the uniformity of the structure so the electro-optical properties become more isotropic. The increase of the number of layers from single to double gains the electro-optical coefficients significantly, whereas further increase of the number of layers, indicates that there is not necessarily a direct relationship between the number of layers and the electro-optical properties.

Keywords: two dimensional materials, mono/bi/tri-layer MoS_2, electro-optic properties, DFT calculations

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1. Introduction

The exceptional properties of the two-dimensional (2D) Molybdenum disulfide (MoS_2), as a typical transition metal dichalcogenide (TMDC) material is attracting notable attentions for wide studies related to electronic and optoelectronic applications [1, 2]. Electrical properties of MoS_2 such as its bandgap and carrier mobility can be engineered by the thickness and number of layers engendering MoS_2 as an applicable material in diverse electronic devices [3, 4]. Although, there are strong covalent bonding between the atoms of Molybdenum and Sulfur in each layer, there are very weak van der Waals interactions between adjacent multi layers which facilitate the MoS_2 thickness engineering. Mono or few layer MoS_2 can be produced by utilizing micro-mechanical cleavage technique and through anisotropic 2D growth by chemical vapor deposition [5]. In spite of various study on the electrical and optical characteristics of mono/bulk MoS_2 [3, 6], the electro-optical properties of a multi-layer MoS_2 structure at x/y/z-directions is not yet studied in detail. In this paper, regarding the effect of van der Waals inter layer interactions for the multi-layer MoS_2, we calculate the complex dielectric function as a basic description of light-matter interactions and an electrical property to investigate the optical properties. Then the optical properties including; absorption coefficients, refractive index and the reflectivity are obtained and discussed.

2. Theory and Methods

2.1 Density Functional Theory (DFT)

The first principle calculations to model the elctro-optical properties of mono/multi-layer MoS_2 are performed by density functional theory (DFT) as implemented in the Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA) code [7]. Generalized gradient approximation (GGA) based on Perdew-Burke-Ernzerhof (PBE) [8] with a 400eV cut-off energy is considered. D2 method of Grimme (DFT-D2) [9] is added, to the model the inter-layer van der Waals interactions for multi-layer structures. To simulate a quasi 2D structures and skipping the interactions along the out-of-plane direction a vacuum, fivefold thicker than the thickness of the structures is assumed. The optimized structure is obtained by allowing ions, cell shape and cell volume to get relaxed, so that the acting forces on atoms becomes less than 0.02eV/A˚. Also as the convergence criterion for relaxation, the total free energy, is set to be updated until the difference between two update steps becomes smaller than 10^{-7}eV.

2.2 Theory of electro optical properties

The imaginary part of the complex dielectric function ($\varepsilon(\omega)=\varepsilon_1(\omega)+j\varepsilon_2(\omega)$) is calculated from the joint density of states as:

$$\varepsilon_2(\omega)=\frac{4\pi^2e^2}{V}\lim_{q\to 0}\frac{1}{q^2}\sum_{c,\upsilon,K}2w_k\delta(E_{cK}-\omega) \qquad (1)$$

where in (1), q is the electron charge, ω is the frequency, δ is the infinitesimal value of energy, c,υ refer to conduction band and valence band states. E_{jK} is the single electron energy state of jth band with wave vector K. The real part of the dielectric function is computed by Kramers-Kronig transformation as:

$$\varepsilon_1(\omega)=1+\frac{2}{\pi}P\int_0^\infty\frac{\omega'\varepsilon_2(\omega')}{\omega'^2-\omega^2+i\eta}d\omega' \qquad (2)$$

where in (2), P is the principal value, η is an infinitesimal and ω' is the frequency over which equation (2) is integrated. The absorption coefficient is calculated by:

$$\alpha(\omega)=\frac{\sqrt{2}\omega}{c}[\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}-\varepsilon_1(\omega)]^{\frac{1}{2}} \qquad (3)$$

where in (3), c is the speed of light. The refractive index, $n(\omega)$ is calculated by:

$$n(\omega)=[\frac{|\varepsilon(\omega)|+\varepsilon_1(\omega)}{2}]^{\frac{1}{2}} \qquad (4)$$

and the reflectivity $R(\omega)$ will be:

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$$R(\omega)=\frac{(n-1)^2+k^2}{(n+1)^2+k^2} \quad (5)$$

where in (5) k is the extinction coefficient:

$$k(\omega)=[\frac{|\varepsilon(\omega)|-\varepsilon_1(\omega)}{2}]^{\frac{1}{2}} \quad (6)$$

3. Results and discussion

Fig. 1 illustrates the side view of MoS_2 mono/multi-layers, where the armchair, zigzag, and vertical direction are denoted as x, y, and z, respectively. $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ versus frequency are depicted in Fig. 2. The $\varepsilon_1(\omega)$ is more isotropic than $\varepsilon_2(\omega)$ along the in-plane direction especially for the energies below 2eV. Also the multilayer structures in comparison with mono-layer exhibit more dielectricity which might be related to the inter layer gap and the weak interlayer van der Waals interactions. For larger phonon energies, multi-layer MoS_2 has more isotropic dielectricity. Also the dielectric function arises from about 1.5eV which is attributed to the optical transition between the valance band maxima to conduction band minima. More number of layers slightly affects the dielectricity. Fig. 3 shows the absorption coefficient $\alpha(\omega)$ that describes the penetration depth of a light at a wavelength into a material before its complete absorption. Accordingly, similar to the dielectricity, the absorption edge arises from 1.5eV. Abrupt increase of absorption for the photon energy higher than about 1.5eV is a property of semiconductors and insulators. As can be seen in Fig. 3, the variation of absorption coefficient versus energy for tri-layer structure is slower. It is related to the bandgap narrowing. As the number of MoS_2 layers is increased, the bandgap decreases [3].

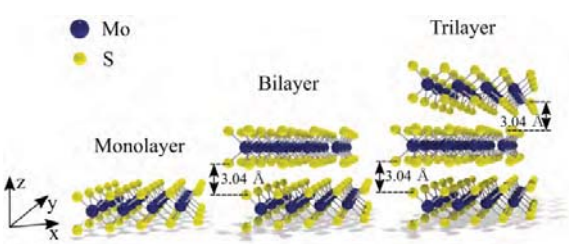

Fig. 1: side views mono-layer and AA' stacking mode bi/tri-layer MoS_2. Sulfur atoms are shown in yellow, and molybdenum atoms are shown in blue.

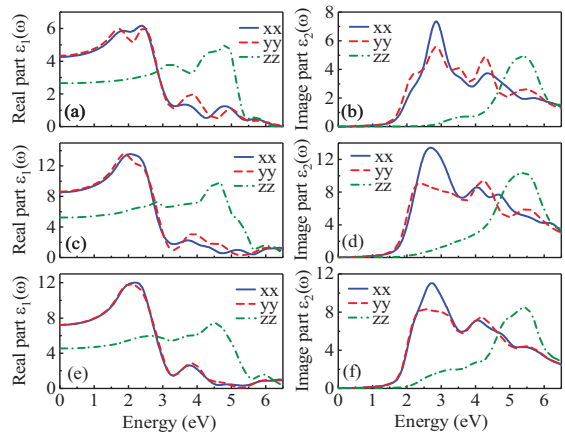

Fig. 2: (a, b), (c, d), (e, f) are the real and imaginary parts of dielectric function for mono, bi and tri-layer MoS_2 respectively.

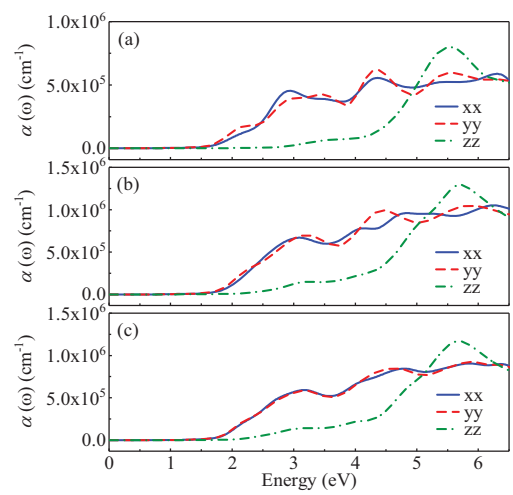

Fig. 3: (a), (b), (c) are the absorption coefficients versus photon energy for mono/ bi/ tri-layer MoS_2 along different directions.

On the other hand, it can be seen in Fig. 3 that the absorption coefficient enhances as the number of layers is increased. The interlayer space between the layers may increase the absorption coefficient of the multi-layer structures in comparison with mono-layer. The refractive index versus frequency is plotted in Fig.4. The refractive index as an important key factor for many opto-electronic applications is the ratio between the speed of light in free space and speed of light in a structure. The results indicate that for the energies larger than

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about 2.85eV (corresponding to the frequencies larger than 689THz), the in-plane refractive index of mono-layer MoS2 is between 1 and 2, so it performs as a transparent media. In this range, variation in the refractive index on the scale of the wavelength of light is negligible. The same structure along the out-of-plane direction except for 5eV, is always transparent. By increasing the number of layers, MoS2 becomes less transparent. Bi/tri-layer MoS2 are transparent along the in-plane direction for the energies larger than about 4.5eV and 4.3eV respectively and are transparent along the vertical direction for the energies larger than about 5.5eV. Finally the reflectivity is depicted in Fig. 5, revealing the fact that increasing the number of layer from bi to tri-layer, not only reduces the reflectivity, but also makes the in-plane reflectivity isotropic.

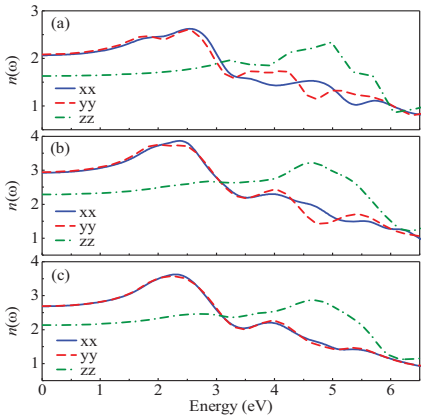

Fig. 4: (a), (b), (c) are the refractive index versus photon energy for mono, bi and tri-layer MoS_2 along different directions.

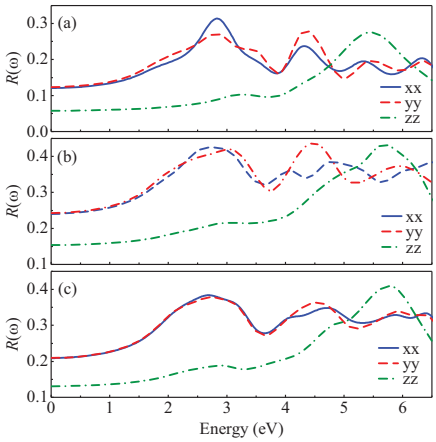

Fig. 5: (a), (b), (c) are the reflectivity versus photon energy for mono, bi and tri-layer MoS_2 along different directions.

4. Conclusion

The frequency dependent electro-optical properties of mono/bi/tri-layer MoS_2 along different directions were investigated by the first-principle DFT calculations. Then the effect of the increase of the number of layers on the obtained properties including; the complex dielectric function, absorption, refractive and reflectivity coefficients were studied. In multi-layer structure, the in-plane electro-optical properties of MoS_2 become more isotropic. This is attributed to more uniformity of the layered MoS_2. Also, unlike the increase of the electro-optical properties caused by doubling the number of layers, further increase of layers verifies the lack of a direct relationship between the number layers and the electro-optical properties.

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