بررسی ویژگی‌های اپتیکی مولیبدن دی سولفید تک‌لایه با روش تنگ بست

مریم نیری[۱]، مرتضی فتحی پور[۲] و آرش یزدان‌پناه گوهرریزی[۳]

[۱]دانشگاه آزاد اسلامی واحد علوم و تحقیقات،گروه مهندسی برق، تهران، ایران.

[۲]دانشگاه تهران، دانشکده مهندسی برق و کامپیوتر، تهران، ایران.

[۳]دانشگاه شهید بهشتی،گروه مهندسی برق، تهران، ایران.

چکیده –در پژوهش حاضر، ساختار نوار و شکاف نوار مولیبدن دی سولفید تک‌لایه با روش تنگ‌بست شبیه‌سازی گردید. .برای این منظور، اوربیتال‌های $d_{z^2}, d_{xy}, d_{x^2-y^2}$ از اتم مولیبدن و اوربیتال های p_x, p_y, p_z از اتم گوگرد در نظر گرفته شد تا بتوان حالات نزدیک نوار هدایت و ظرفیت را تشریح نمود. در این مدل با در نظر گرفتن تقریب نزدیکترین همسایه ها، شکاف نوار مستقیمی معادل ۱.۸۵ الکترون-ولت بدست آمد. با داشتن ماتریس هامیلتونین و در نظر گرفتن نظریه تابع اختلال، برای بررسی خواص نوری این ماده از روابط شبه کلاسیکی بهره گرفته شد. با انجام کد نویسی پارامترهای نوری از قبیل قسمت موهومی و حقیقی طیف دی الکتریک با بکارگیری معادلات کرامرز-کرونیگ و طیف تلف انرژی محاسبه و با نتایج اصول اولیه و حاصل از آزمایش مقایسه گردید. تحلیل عددی انجام شده در این مقاله از طریق کدنویسی در نرم افزار متلب صورت گرفته است. چنین مطالعاتی، به واسطه بکارگیری MoS_2 تک لایه در ادوات اپتو الکترونیک نظیر آشکارسازهای نوری و سلول های خورشیدی و دیودهای نورانی از اهمیت بسزایی برخوردار است.

کلید واژه- مولیبدن دی سولفید، خواص نوری، تابع دی الکتریک.

Study of Optical Properties of Single-layer Molybdenum disulfide by Tight Binding Method

Maryam Nayeri[1], Morteza Fathipour[2], and Arash Yazdanpanah Goharrizi[3]

[1]Department of Electrical Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

[2]School of Electrical and Computer Engineering, University of Tehran, Tehran, Iran.

[3]Faculty of Electrical Engineering, ShahidBeheshti University, Tehran, Iran.

Abstract- In this research, band structure and band gap energy of molybdenum disulfide is simulated by tight binding method. For this purpose, we assumed $d_{z^2}, d_{xy}, d_{x^2-y^2}$ orbitals of Mo atom and p_x, p_y, p_z orbitals of S atom to describe the near conductance and valence band states. The direct band gap, obtained by the nearest neighbor approximation, is equal to 1.85 eV. We used a semi classical approach by exploiting Hamiltonian matrix and perturbation theory to investigate the optical properties of single-layer MoS_2. Optical parameters such as imaginary and real part of dielectric function have been calculated via kramers-kronig transformation and the electron energy loss spectrum calculated and compared with experimental as well as first principle calculations. The numerical analysis in this paper has been carried out by coding in MATLAB. These studies are important since the monolayer MoS_2 has been envisaged for applications in the optoelectronic devices such as photo detectors, solar cells and light emitting diodes.

Keywords: Molybdenum disulfide, optical properties, dielectric function.

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Maryam Nayeri nayeri@iauyazd.ac.ir

Morteza Fathipour mfathi@ut.ac.ir

Arash Yazdanpanah Goharrizi ar_yazdanpanah@sbu.ac.ir

1 Introduction

The exfoliation of graphite in 2004 by Novoselov and Geim introduced a low-dimensional structure called graphene to which a wide range of applications has been assigned [1]. Two-dimensional structures such as black phosphorus, ZnO, silicene and Transition Metal Dichalcogenides (TMDCs) are focus of many researches today due to their unusual physical properties [2]. Among two-dimensional materials, extensive studies have been devoted graphene which has unique characteristics in terms of stability, thermal, electrical and optical conductivity [3]. Lack of band gap in pristine graphene degrades field-effect transistors performance which are made based on this material. This reduces the I_{on}/I_{off} and thus limits their suitability in digital circuits [4].

Recently TMDCs, a member of the family of two-dimensional materials, have attracted much attention due to its remarkable properties and its potentials in optoelectronics as well as nano-electronics. TMDCs are minerals with the chemical formula MX_2. M represents a transition metal of group 4 to 10 and X is a chalcogen. These materials have layered structure as X-M-X, i.e. the metal atoms have been sandwiched between two layers of chalcogenides [5]. Exfoliation mechanisms in these materials are similar to graphene. Molybdenum disulfide is a semiconductor TMDC that its exfoliation from bulk to single layer leads to transition from indirect band gap equal to 1.3 eV into direct band gap between 1.8-1.9 eV [6]. Relatively large and direct band gap provides for applications in optical electronics and digital circuits. Therefore, the study of this new material is important.

An atomic model for single-layer MoS_2 is shown in figure 1(a). The thickness of a single-layer MoS_2 is 6.5Å. The lattice constant for Mo-Mo and S-S is a=3.16Å [7].

In this paper, we report on optical properties of single-layer MoS_2. For this purpose, we obtain Hamiltonian matrix by tight binding approximate in section II. We will then calculate the gap energy and band structure. In section III, Using the Hamiltonian matrix, we represent optical properties. Finally in section IV a conclusion will be provided.

2 Methodology

To calculate the band structure and energy gap for single-layer MoS_2, we have employed tight binding approximation and MATLAB software. The considered unit cell for MoS_2 contains two S atoms and one Mo atom. Since MoS_2 has the D_{3h} symmetry point [8], one can only consider three orbitals $d_{z^2}, d_{xy}, d_{x^2-y^2}$ of Mo atom along with

three p-orbitals of S atoms to explain near valence and conductance band states.

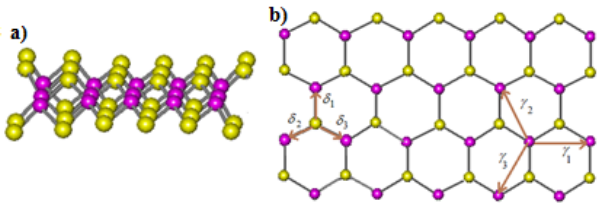

Figure 1: a) view of a single-layer MoS_2 structure. Mo and S are shown in violet and yellow, respectively. b) Hopping parameters used in the tight binding approximation.

To write the Hamiltonian matrix for single-layer MoS_2, the nearest neighbours between atoms should be considered namely Mo-Mo, S-S and Mo-S atoms. Hopping parameters between nearest neighbours of atoms are shown in figure 1(b). These parameters are calculated in terms of Slater-Koster [9]. The total Hamiltonian matrix is as follow:

$$H = H_{on-site} + H_{off-site} + H^{\dagger}_{off-site} \qquad (1)$$

Where diagonal elements in $H_{on\text{-}site}$ contains the on-site energy of d-orbitals of Mo atoms and p-orbitals of S atoms with inter layer hopping between p-orbitals of top and down S layers. Off-diagonal elements in this matrix are zero 3*3 matrices. Second term in Hamiltonian matrix (1) includes the hopping parameters between nearest neighbours for d-orbitals of Mo-Mo atoms ($\gamma_{1\text{-}3_{Mo}}$) and p-orbitals of S-S atoms ($\gamma_{1\text{-}3_{S}}$) and the nearest neighbours hopping parameters of Mo-S atoms ($\delta_{1\text{-}3}$).

After calculating of band structure, we want to determine the optical properties for single-layer MoS_2. The real part of the dielectric function can be calculated from [10].

$$\varepsilon_r(\omega) = 1 + \frac{4}{\pi}\wp\int_0^{\infty}\frac{\omega'\varepsilon_i(\omega')}{\omega'^2-\omega^2}d\omega' \qquad (2)$$

Where $\wp$ indicates the integral principle value. ε_i is the imaginary part of the dielectric function. It is obtained by using the Kramers-Kronig transformation [10].

Furthermore, the Electron Energy Loss Spectrum (EELS) can be obtain by $-\Im m\left[\varepsilon(\omega)^{-1}\right]$ [10], in which $\varepsilon(\omega)$ is the complex dielectric function and $\Im m$ denotes the imaginary part of the complex dielectric function.

3 Results and Discussion

In this section, we will calculate the band structure for single-layer MoS_2 by using tight binding method described in section II. This band structure is shown in figure 2 along directions of symmetry points Γ, K, M.

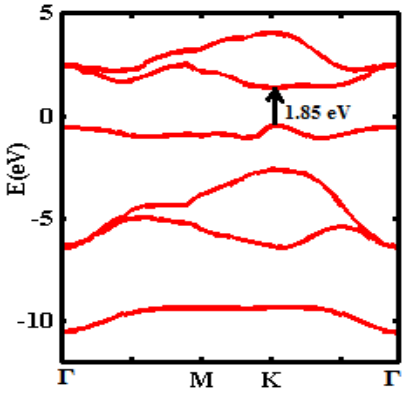

Figure 2: Band structure for single-layer MoS_2 along the directions of symmetry points.

The single-layer MoS_2 band diagram can be described near conduction as well as valence band by considering three orbitals of Mo and three orbitals of S atoms, within tight binding model.

The band structure in figure 2 shows a direct energy gap equal to 1.85eV in accordance with results reported in [11].

Utilizing Hamiltonian matrix optical spectra and other important optical properties can be described based on microscopic theory of the dielectric function. Figure 3 represents the dielectric function spectra in the energy ranges from 0 to 3eV.

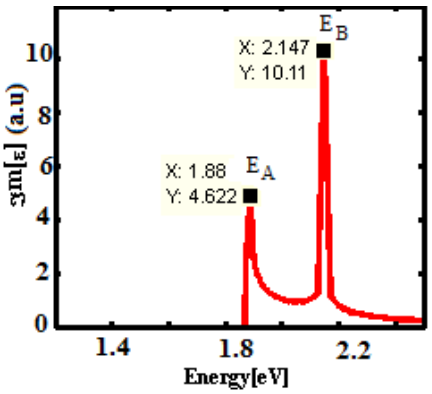

Figure 3: The imaginary part of dielectric function obtained by tight binding model.

Figure 3shows that the dielectric function spectrum has two exciton peaks at 1.88 eV and 2.15 eV, respectively. The presence of these two peaks indicates optical applicability in the visible regime. Table 1 shows position of the energy peaks in the range of 0 eV to 3 eV obtained by tight binding method (this work) and compares it with approximate exchange correlation method, namely

the Perdew-Burke-Ernzerhof (PBF), Van der Waals Lundqvist Langreth (vdW-DF) [12] and the experimental work reported in [13].

Table 1: The comparison of exciton energy in different method

Method [Ref]	E_A(eV)	E_B(eV)
Exp [13]	1.88	2.06
PBF [12]	1.93	2.32
vdW-DF [12]	1.94	2.33
TB (This work)	1.88	2.15

As shown in table 1, our result is in good agreement with the experimental results obtained by spectroscopic technique. Furthermore, EELS and the real part of dielectric function are obtained by the imaginary part of dielectric function, as shown in figure 4.

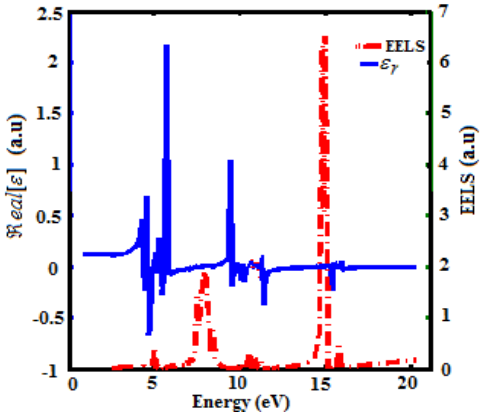

Figure 4: the electron energy loss spectrum (red color) and the real part of dielectric function (blue color).

4 Conclusion

The tight binding approximation has been employed for single-layer MoS_2 to obtain its band structure and analyze its optical properties. Simulations predict band gap equal to 1.85eV, in agreement with computations based on first principle. Optical properties of single-layer MoS_2 obtained by using the selection rules and momentum matrix element indicate two exciton peaks at 1.88 eV and 2.15 eV again in good agreement with spectroscopic techniques. Therefore, considering only 3-orbitals of Mo atom and 3-orbitals of S atom, is sufficient for investigation of electrical and optical properties of single-layer MoS_2 by tight binding approximation

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