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تحلیل اثر نقص استون-ولز روی خواص نوری نانونوار گرافنی با لبه آرمچیر

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چکیده- در این مقاله، اثر اعمال نقص استون-ولز روی هدایت نوری و طیف جذب آشکارساز نوری ساخته شده از نانونوار گرافن آرمچیر بررسی شده است. با استفاده از روش تقریب تنگ‌بست و با در نظر گرفتن همسایه اول، ساختار انرژی نانونوارها محاسبه شده است. با استفاده از ساختار انرژی بدست آمده، چگالی حالت‌های دوگانه را محاسبه کرده و با استفاده از محاسبات فوق و با بکارگیری قانون طلایی فرمی، هدایت نوری نانونوار آرمچیر محاسبه شده است. طیف جذب و هدایت نوری نانونوارها در حالت‌های مختلف بررسی و مقایسه شده است. نتایج حاصل از تحلیل‌های عددی نشان می‌دهد که اعمال نقص به نانونوارهای گرافن فلزی با لبه آرمچیر می‌تواند باعث افزایش تعداد گذرهای مجاز و در نتیجه وسیع‌تر شدن طیف جذب نوری و همچنین افزایش هدایت نوری آشکارساز نوری در گستره انرژی‌های تابشی فروسرخ شود.

کلید واژه-**تقریب تنگ‌بست، چگالی حالت‌های دوگانه، نانونوار گرافنی، نقص استون-ولز، هدایت نوری**

The Role of Stone-Wales Defect on the Optical Properties of Armchair Graphene Nanoribbon

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Abstract-In this study, the effect of Stone-Wales defect on the optical properties of the armchair graphene nanoribbon (GNR) including joint density of states and optical absorption spectra is investigated. By using the tight binding approximation,the energy band structure of nanoribbon is computed byconsidering the first neighbor sites. Using the energy band structure, the joint density of states calculated by Fermi's golden rule and band energy structures. By calculating the optical matrix elements and interband transition rule, the optical conductivity of the GNR is calculated. optical conductivity of nanoribbon is analyzed in the presence of Stone-Wales defects within different locations in GNR structure and compared with GNR with no defect state. The numerical result shows that by applying defect to the metallic type of the armchair GNR, the number of allowed optical interband transitions can be increased resulting in a broader range of optical absorption and also increasing the optical conductivity in the infrared range of incident energies.

Keywords: Graphene nanoribbon, Tight-binding, Stone-Wales Defect, Joint density of state, optical conductivity

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1. Introduction

Graphite and its derivatives havereceived extensive research attention due to theirunique electrical, optical and mechanical properties. Among them, grapheneshows promising in the area of electronic and photonics [1]. The excellent electrical conductivity, ultra-high mobility of massless fermions, and flexibility make graphenethe ideal material to potentially use in various material/device applications, including optical waveguide [2], field effect transistors [3-4], and sensors [5-6]. Graphene is a gapless material with a linear dispersion relationship showing metallic like behavior with unique transport properties. However, it cannot be used in pristine form for semiconductor photonic and nano-electronic applications. Therefore, it is crucial to create a finite gap in the energy dispersion at the Dirac point.Graphene nanoribbon (GNR) is a popular form of monolayer material which shows extraordinary electronic and optical properties depending on the edge of the GNR [7]. GNRs with armchair edge can be semiconductor or metallic depending on the width of the ribbons.

The optical properties of carbon nanotubes and GNRshave been investigated with armchair edges, and the inter-band transition rules for these nanoribbons arecalculated [8]. The optical conductivity of graphene nanoribbon with zigzag edges and carbon nanotubes has been calculated using tight-binding approximation and it has beenproven that although these two carbon-based materialspossess the same atomic structure, theirelectronic structure,andeigenstates symmetryare quite different. Hence, this leads to the different optical responses of these carbon-based materials.In this paper,we study the effect of the Stone-Wales lattice defect on the optical properties of armchair GNR.The tight-binding method has been employed to calculate the electronic band-structure and optical responses, including the joint density of states and optical conductivity of GNR.

2.Material and Methods

To model the electronic structure, the tight-binding approximation has been widely used. The tight-binding Hamiltonian H is written as [9]

$$H = \sum_i \varepsilon_i \left(c_i c_i^{\dagger}\right) + \sum_{i,j} t_{ij} \left(c_i c_j^{\dagger} + c_j c_i^{\dagger}\right) \quad (1)$$

where$c_i\left(c_i^{\dagger}\right)$ denotes the creation (annihilation) operators of an electron at site i, and indices i and j, include all atoms in the unit cell. ε_i is the in-suitepotential and t_{ij} is the hoping parameter between the carbon atoms.By applying the defect to graphene nanoribbons, the position of the atoms in the network and energy bands structure will changerelative to the perfect atomic state leading to a variation in the selection transition rule and optical response. Stone-Wales defects (5-7-7-5)are formed by linking two 5-7 defects [10]. The length of atomic bonds between carbon atoms will change due to the displacement and relaxation of the atoms. Using Quantum Espresso software, the length of the new bonds between atomsis obtained in the network after relaxation. By changing the bond length between the carbon atoms, the hoping parameter is varied between neighboring atoms. The hoping parameter for different lengths can be obtained from:

$$\gamma(l) = \gamma_0 e^{-3.37\left(\frac{l}{a_0}-1\right)} \quad (2)$$

In Figure (1) theStone-Wales defect is shown and the length of the atomic bonds around the defect is calculatedin the GNR plane after relaxation process.

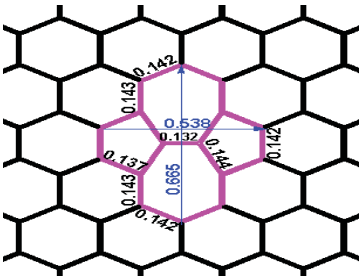

Figure 1: The bonds' length between the atoms around defect Stone-Wales after the relaxation of atoms. The atomic lengths are in nanometers.

To study the optical excitation properties of graphene nanoribbons which have been affected by the incident radiation from an external source two quantities are important:The joint density of states ($D_j(\omega)$) and the optical conductivity ($\sigma(\omega)$).

The joint density of states (JDOS) can be obtained from the nanoribbon band structure as [8],

$$D_j(\omega) = \frac{2}{W}\sum_{n,n',k}\left[f\left(E_{n,k}\right) - f\left(E_{n',k}\right)\right] \times \delta\left(E_{n',k} - E_{n,k} - \hbar\omega\right) \quad (3)$$

where$W$is the width of nanoribbon, ω is the frequency of photons which, n and n ' are the index of sub-bands for the valence and the conduction bands respectively, and f ($E_{n,k}$) is the function of the Fermi-Dirac distribution.The real part of the

optical conductivity is directly related to the absorption of the incident photon energyand determinedusing perturbation theory in the weak electric field as [8],

$$\sigma_1(\omega) = \frac{2\pi e^2}{{m_0}^2 \omega W} \sum_{n,n',k} \left[f(E_{n,k}) - f(E_{n',k})\right] \times |\langle n,k|P_x|n',k\rangle|^2 \delta(E_{n',k} - E_{n,k} - \hbar\omega) \quad (4)$$

wherem_0 and e is the electron mass and charge, respectively.⟨n,k | P_x | n',k⟩ is the optical matrix elements.

3. Results

We consider armchair nanoribbon with N_0=17 atoms in width and analyze different cases in terms of the frequency and location of the defects. Since the armchair nanoribbons by N_0=17 is metallic, the energy bandgap is zero.According to this Figure by applying the defect,abandgap is created in the energy band structure of nano-ribbons and also increases the number of spectral peaks in the JDOS and optical conductivity. The size of the gap for different conditions of applying the defects is presented in Table 1.

Table(1): Energy bandgaps for different defect states.

Defect	
One defect in width	
Two defects at center	
Two defects at edge	
Two defects in width	

By considering the case with two defect states in GNR, if the lateral distance between the defects is decreased, the energy gap will increase. The maximum bandgap is achieved for the GNR with two defects connected at the centre of ribbon. By applying defect, the number of allowedinterband optical transitions is increased, therefore,the optical conductivityspectrum is broadened, and the absorption peak is decreased to the lower energy ranges, as seen in Fig. 2d. The optical conductivity in the infrared region of the spectrum increases due to the increased JDOSthrough the applying defects. As can be observedin Fig. 2, in the case of one defect in the nanoribbon, the second peak in optical conductivityappears at $\hbar\omega$=1.24eV (corresponding to the energy difference between the valance band with energy 0.5eV and the conduction band with energy 0.74eV at k_x=0).This peak, compared to the first peak of the GNR with no defect, is appeared for an incident photon with lower energy and shows higher photoabsorptionintensity. Also, due to applying the defect and opening the bandgap in the energy range $\hbar\omega$< 0.75eV, the JDOS of the GNR is increased, compared to that without any defect state. (Fig. 2c)).By applying two defect states in the GNR network, two peaks can be observed at higher photon energy range, compared to that of with one defect at centre of GNR. This results from higher energy bandgap of the GNR structures with two defect states.

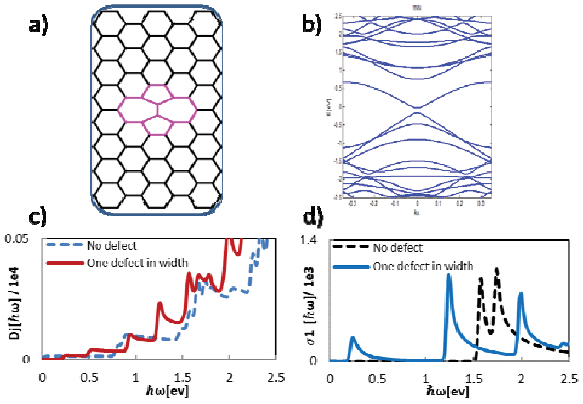

Figure 2: a) Armchair GNR17with asymmetrical defect inthe middle. b) The energyband structure, c) Joint density of states, and d)Real part of the optical conductivity of the GNR. Dashed lines indicate the GNR with no defect.

For example, for the GNRwith two defectssymmetricallyspaced from the GNR edge two peaks in the JDOSin energy range $\hbar\omega$< 0.8eVappear, as seen in Fig. 3b-d.Also, twopeaksin the optical conductivity at energy $\hbar\omega$=0.52eV (corresponding to the energy difference between the first valance band with energy -0.18eV and the first conduction band with energy 0.34eV at k_x= 0) and $\hbar\omega$=0.96eVappear.

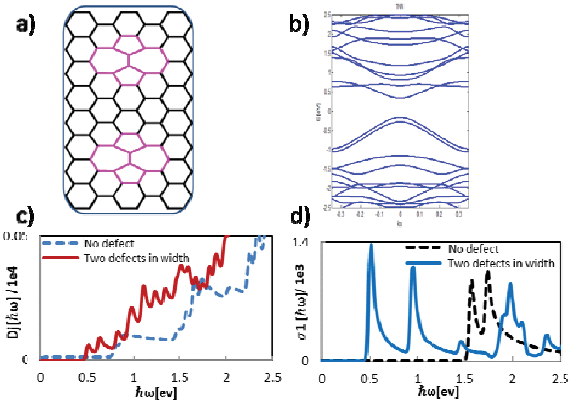

Figure 2: a) Armchair GNR17 with two symmetrical defectsin the middle with the same distance from the edges. b) The energy band structure, c) Joint density of states, and d) Real part of the optical conductivity of the GNR.

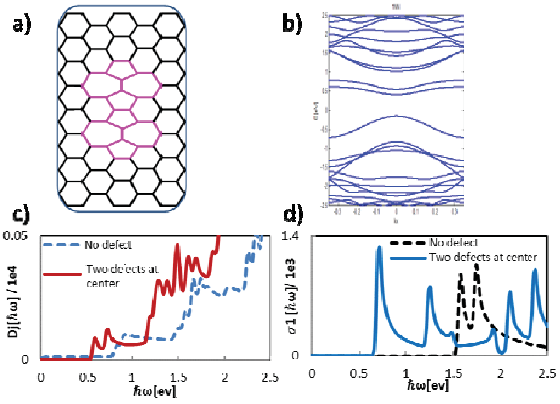

Figure 3: a) Armchair GNR17 with two symmetrical defectsat the center of GNR. b) The energy band structure, c) Joint density of states, and d) Real part of the optical conductivity of the GNR.

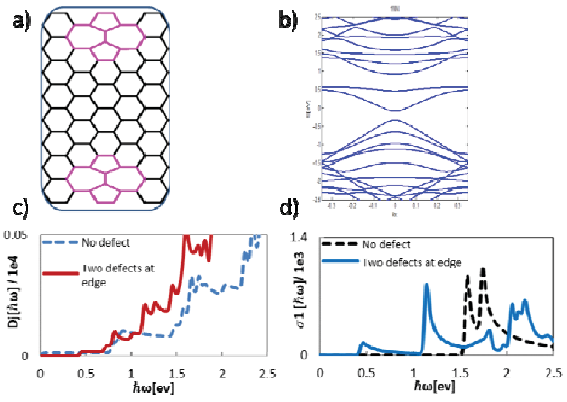

Figure 4: a) Armchair GNR17 with two symmetrical defectsat the edges. b) The energy band structure, c) Joint density of states, and d) Real part of the optical conductivity of the GNR.

Compared to the first two peaks in the GNR with no defect and GNRs with one and two defect states within the width of the ribbon, the intensity of both peaks is increased, which results fromthe higherJDOS in the energy range of $\hbar\omega$< 1eV (Fig. 3c). The same analysis can be done for the GNRs with two defects at the center (Fig. 3) and at the edge of the ribbons (Fig. 4).

4. Conclusion

In this paper, the effect of Stone-Wales defect on the energy band structure, joint density of states, and the optical conductivity of armchair graphene nanoribbon (GNR) was investigated using the tight binding approximationapproach.Results showed thatby applying defect to nanoribbon the absorption peaks intensity in the optical conductivity spectrum can be increasedin low incident energy range (infrared energy region) and photon absorption arises in a broader incident energy range. Due to bandgap opening of the GNR in the presence of defect states the interband transition events move toward the infrared energy range.

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