Edge Roughness Effects on the Optical Properties of Zigzag Graphene Nanoribbons: A First Principles Study

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Introduction

Graphene based devices have attracted much attention due to their excellent electronic, optical, and thermal properties [1]. Very recently graphene has been successfully employed at high speed communications [2]. Graphene is a gapless material. To induce an energy gap graphene sheets can be patterned into nanoribbons. The electronic and optical properties of graphene nanoribbons (GNRs) strongly depend on the orientation of the edges. GNRs can have edges with zigzag shapes, armchair shapes, or combination of these two. However, in reality edges are not perfect and irrigularities are observed [3]. The role of roughness on the properties of armchair GNRs has been studied before [4]. In this work by imploying first principle methods we investigate the role of roughness on the electronic and the optical properties of zigzag GNRs. Fig. 1 compares the goemetry of zigzag GNRs with perfect edges and with Klein defects [5].

Model and Method

For first principle calculations the SIESTA package has been employed [6]. We use a double-ζ basis set with additional orbitals of polarization for total energies and electronic band structures, the generalized gradient approximation, Perdew-Burke-Ernzerhof (PBE) as the exchange-correlation function, and the Troullier-Martins scheme for the norm-conserving pseudopotential. Furthermore, spin polarized effects are considered in our calculations.

Results and Discussion

Fig. 2 compares the imaginary part of the dielectric function, which is an indication of the rate of photon absorption for a particular material, and the electronic dispersion relation for the structures of Fig. 1 . The optical polarization vector is assumed to be along the transport direction. In the energy range $\hbar\omega < 5$ eV photon absorption decreases as the roughness periodicity increases. The band structures shown in the insets of Fig. 2 indicate that the band gaps decrease as the roughness increases. Therefore, the absorbtion peaks shift to low energies of the optical spectrum.

The spin effects in these structures are investigated in addition. The first peak of the dielectric function shifts to higher energies whereas other peaks are only weakly affected. Optical transitions in ZGNRs with perfect edges occur only between subbands with the same parity (odd to odd and even to even) [7]. However, transitions between subbands with different parities are observed by considering spin polarization (See Fig. 2-b). The spin effect decays as the roughness periodicity increases (See Fig. 3). Roughness structures affect the optical properties of ZGNRs. Depending on the periodicity of the edge roughness the peaks in the optical spectrum shift. Our results indicate that for optimizing the performance of GNR based photodetectors the role of roughness and spin need to be carefully studied.

Acknowledgment

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References

[1] P. Avouris *et al.*, Nature Photonics **2**, 341 (2008).
[2] T. Mueller *et al.*, Nature Photonics **4**, 297 (2010).
[3] C. Tao *et al.*, Nature Phys. **7**, 616 (2011).
[4] A. Y. Goharrizi *et al.*, **58**, 3725 (2011).
[5] A. Cresti *et al.*, **11**, 095004 (12pp) (2009).
[6] J. M. Soler *et al.*, J. Phys.: Condens. Matter **14**, 2745 (2002).
[7] H. Hsu *et al.*, **76**, 045418 (5pp) (2007).

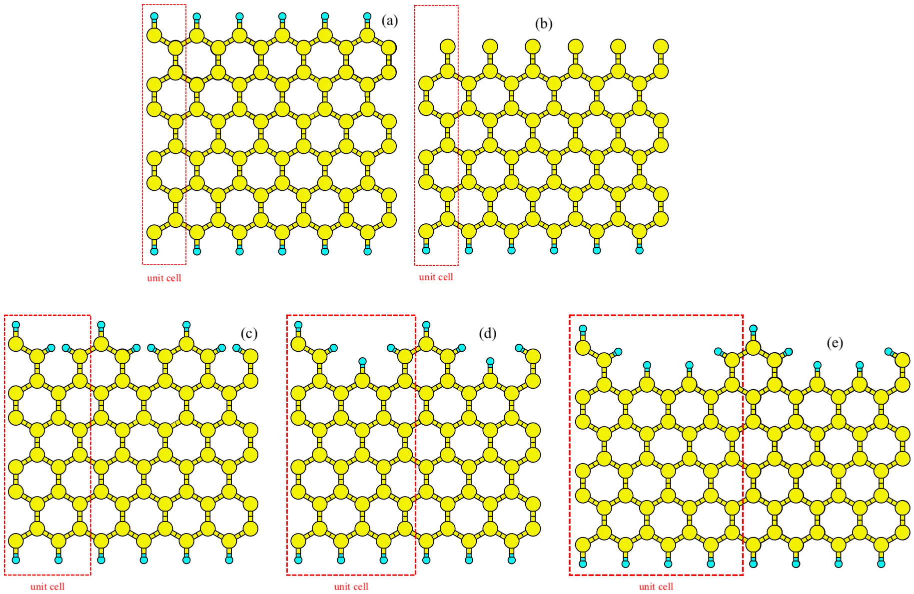

Fig. 1. (a) A perfect 6-ZGNR and (b) a 6-ZGNR with Klein defect. (c)-(e) 6-ZGNRs with different roughness periodicity.

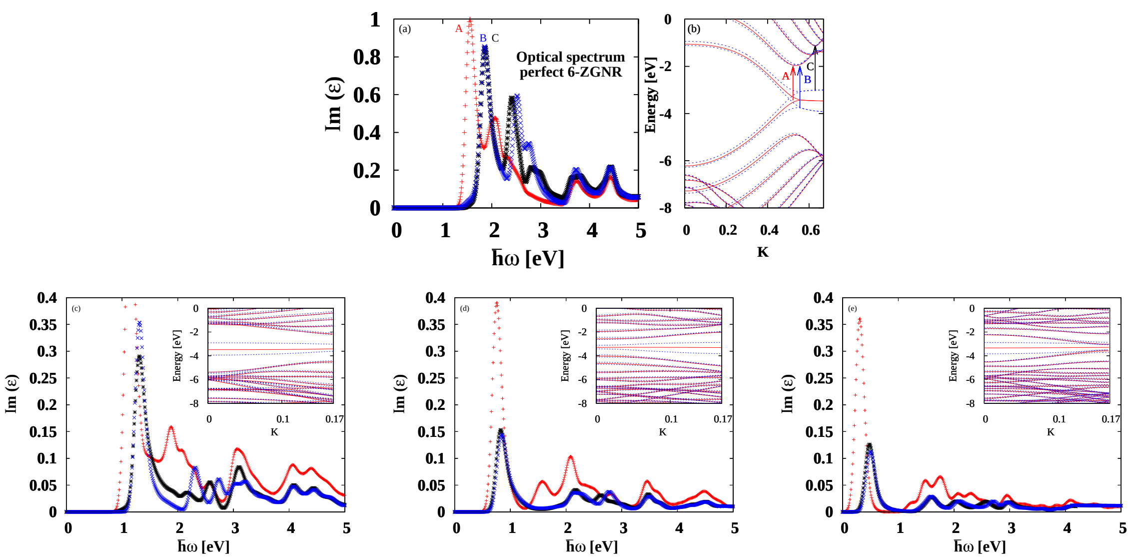

Fig. 2. (a) The imaginary part of the dielectric function and (b) the energy dispersion relation without (red plus symbol) and with (blue crosses and black stars) spin consideration for a 6-ZGNR. (c)-(d) The imaginary part of the dielectric function and the energy dispersion relation for the structures shown in Fig. 1-c, Fig. 1-d, and Fig. 1-e, respectively.

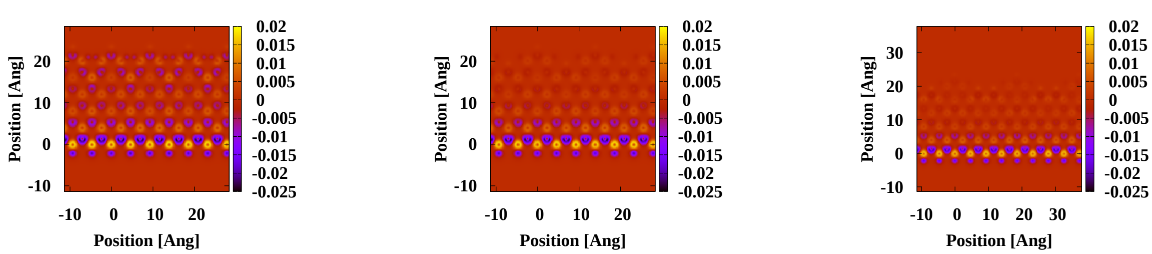

Fig. 3. The self-consistent charge density difference between the spin up and spin down for the structures shown in Fig. 1-c, Fig. 1-d, and Fig. 1-e, respectively.