

PAPER • OPEN ACCESS

Band gap control of bilayer zigzag graphene nanoribbon by direction of magnetic moment

To cite this article: T B Prayitno *et al* 2019 *J. Phys.: Conf. Ser.* **1402** 044106

View the [article online](#) for updates and enhancements.

You may also like

- [Fano Factor in Strained Graphene Nanoribbon Nanodevices](#)
Walid Soliman, Mina D. Asham and Adel H. Phillips
- [Efficacy evaluation of an *in situ* forming tissue adhesive hydrogel as sealant for lung and vascular injury](#)
Biji Balakrishnan, Umashanker Payanam, Alexandre Laurent et al.
- [Dispersive hybrid states and bandgap in zigzag graphene/BN heterostructures](#)
Van-Truong Tran, Jérôme Saint-Martin and Philippe Dollfus



ECS
The
Electrochemical
Society
Advancing solid state &
electrochemical science & technology

DISCOVER
how sustainability
intersects with
electrochemistry & solid
state science research

Band gap control of bilayer zigzag graphene nanoribbon by direction of magnetic moment

T B Prayitno*, E Budi and R Fahdiran

Department of Physics, Faculty of Mathematics and Natural Science, Universitas Negeri Jakarta, Kampus A Jl. Rawamangun Muka, Jakarta Timur 13220, Indonesia

*teguh-budi@unj.ac.id

Abstract. We have demonstrated the first-principles calculation to tune the band gap of the bilayer zigzag graphene nanoribbon by arranging the direction of the magnetic moments of carbon atoms at the edges. These directions were specified by the polar angle, as defined in the spherical coordinates. From the ferromagnetic configuration to the antiferromagnetic configuration, as the polar angle increases, the band gap increases. We also showed that the ferromagnetic configuration leads to the metallic system while the others lead to the insulator, in a good agreement with the previous calculations. These results indicated that the bilayer zigzag graphene nanoribbon is potential for the spintronics devices.

1. Introduction

A thorough observation on the graphene, which has been found a few years ago [1-3], triggered many scientists to exploit the properties, such as strength, high electron mobility, or high conductivity, for the nanotechnology [4-7]. However, the theoretical studies proved that the graphene has no band gap. This means that the graphene is not suitable for the spintronics devices.

Before the graphene was found, Fujita *et al.* has proposed a theoretical model of the ribbon material [8], which can be used for the spintronics devices. By adopting this model, a new model of the graphene can be successfully achieved by cutting an infinite sheet of the graphene to be finite. This leads to the so-called graphene nanoribbon. Regarding the cutting form, the graphene can be divided into two types, i.e., the zigzag graphene nanoribbon (ZGNR) and the armchair graphene nanoribbon (AGNR).

In this paper, we concern the ZGNR, in which the band gap can be generated by arranging the directions of the magnetic moments of carbon atoms at the edges. This treatment has been successfully conducted in the case of a monolayer ZGNR for the noncollinear calculations [9,10]. Interestingly, this treatment also succeeded to calculate the spin stiffness in the monolayer ZGNR [11-13]. This spin stiffness can be considered as an important indicator in the spintronics applications for the ZGNR. Here, we extend the discussion by considering the bilayer ZGNR. We prove that the same treatment also works for the bilayer ZGNR. Here, we prefer to choose the ZGNR rather than the AGNR because the interesting properties of magnetism in the ZGNR were explored more significantly than that in the AGNR.

Our model of the bilayer ZGNR will be given in section 2. We also draw the directions of the magnetic moments of carbon atoms at the edges. The computational details, as well as the results, will be discussed in section 3. The conclusion will be given in section 4.



2. Method and materials

We gave the illustration of the bilayer ZGNR with the available directions of the magnetic moments of the carbon atoms at the edges in Fig. 1. These configurations lead to the collinear ferromagnetic ($\theta = 0^\circ$)-noncollinear magnetic ($0^\circ < \theta < 180^\circ$)-collinear antiferromagnetic ($\theta = 180^\circ$), as shown in Fig. 1. In the noncollinear calculation, we exploited a constraint scheme to establish the fixed directions of the magnetic moments of the carbon atoms at the edges [14,15]. Here, θ , which is varied from 0° to 180° , is the angle of the magnetic moment, which is defined as usual in the spherical coordinates. So, θ will be fixed by implementing the constraint scheme when the noncollinear calculations at $0^\circ < \theta < 180^\circ$ are performed. In the realistic experiment, the arrangements of the magnetic moments can be done by applying the external magnetic field.

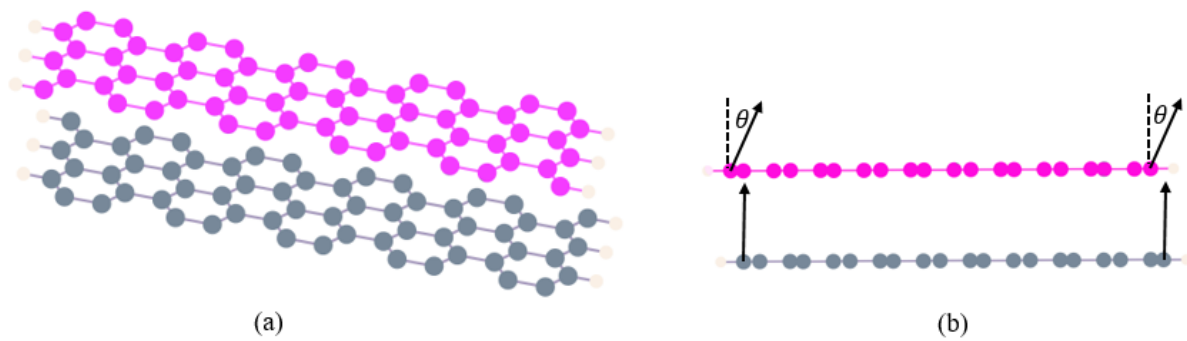


Figure 1. Structure model of bilayer ZGNR from top view (a) and side view (b). The carbon and hydrogen atoms are indicated by the large and small filled circles, respectively.

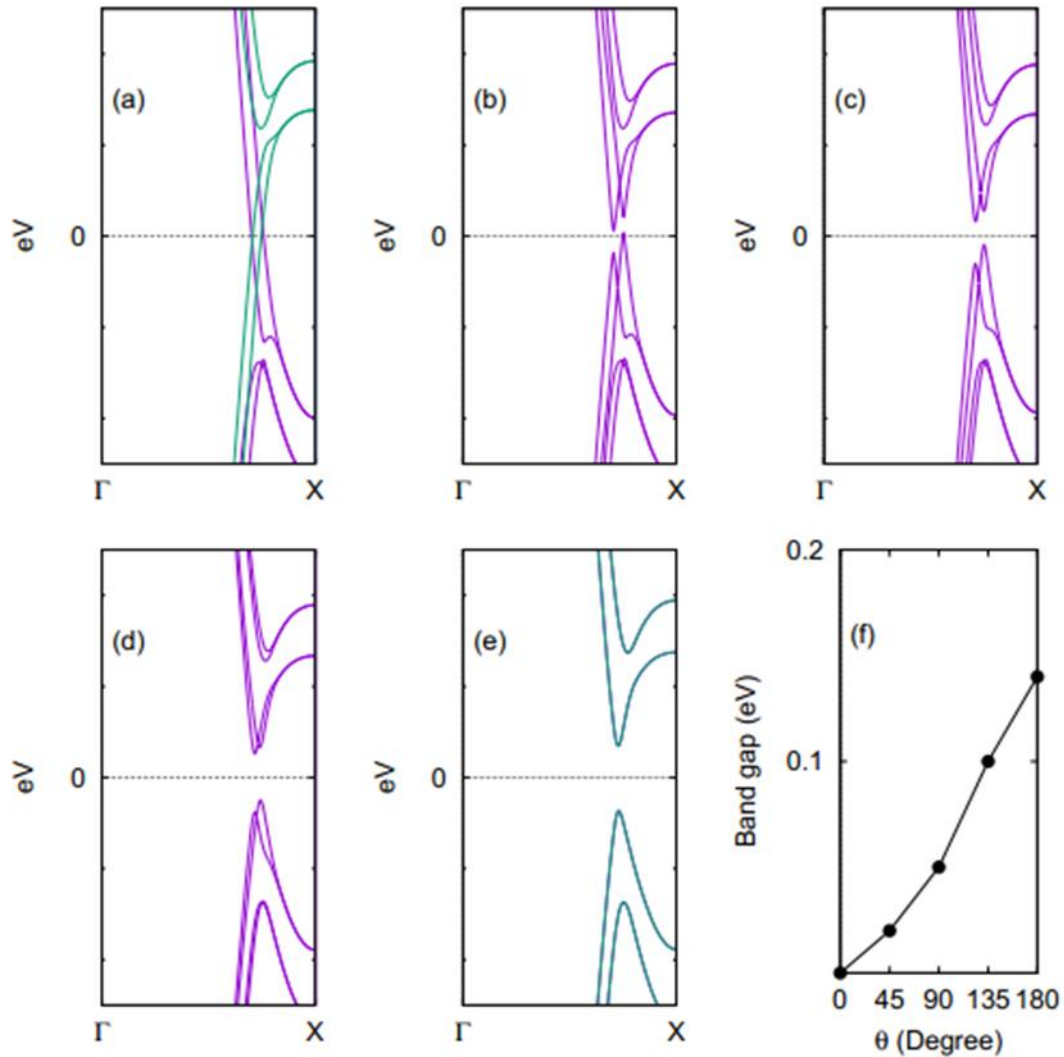
We carried out the computational details by using the OpenMX code [16], which exploits the localized basis set via the confinement scheme [17,18] and the norm-conserving pseudopotentials [19]. In this calculation, we used the cutoff energy of 200 Ryd, the generalized gradient approximation (GGA) for the electron-electron interaction [20], and a $65 \times 1 \times 1$ k-point mesh. Two s and two p orbitals are assigned for the C atoms with the cutoff radius of 6.0 a.u. while two s and one p orbitals are assigned for the H atoms with the cutoff radius of 6.0 a.u. We also used the lattice constant of 2.46 Å and the vacuum region of 30 Å. Here, the used lattice constant was adopted from the experimental result of graphite. For the brief demonstration, we took the ribbon width of ten, which is symbolized by 10-ZGNR.

3. Results and discussions

We observe that the band gap increases as θ increases, as shown in Fig 2. Figure 2 shows the band structures of the bilayer 10-ZGNR for all the calculations. This situation is similar to the previous results in the monolayer case [9], which achieved the increase of the band gap by increasing θ . The metallic state appears in the collinear FM without the band gap, while others show the insulator with the band gap. So, we deduce that the collinear AFM gives the highest band gap, in a good agreement with Ref. [21]. The tendency of band gap is shown in table 1. Since the band gap determines the quality of the spintronics devices, we claim that the results give the important information of how to obtain the wished band gap.

Table 1. Calculated band gap for the bilayer 10-ZGNR with respect to θ .

θ (Degree)	0°	45°	90°	135°	180°
Band gap (eV)	0	0.02	0.05	0.1	0.14

**Figure 2.** Band dispersions of 10-ZGNR with $\theta = 0^\circ$ (ferromagnetic) (a), $\theta = 45^\circ$ (b), $\theta = 90^\circ$ (c), $\theta = 135^\circ$, and $\theta = 180^\circ$ (antiferromagnetic) (e), while the increase of band gap with respect to θ is given in (f).

Note that the highest band gap in the ZGNR can only be found for the collinear antiferromagnetic structure both in the monolayer and bilayer ZGNRs. In Ref. (21), the authors also confirmed that one of the antiferromagnetic states has the highest band gap. Unlike the monolayer case, the bilayer ZGNR has many possibilities to create several collinear structures, such as the ferromagnetic, antiferromagnetic, and ferrimagnetic states, see Ref. (21). Therefore, if one wishes to investigate the band gap in the bilayer ZGNR for the noncollinear structure, we suggest to set $\theta = 90^\circ$ by choosing the azimuthal angles $\varphi = 0^\circ$ or/and $\varphi = 90^\circ$. This treatment can give the different band gap with the interesting phenomena, such as the phase transition or the spin stiffness.

Here, would like to give some comments on the theoretical aspect of the obtained band gap. The highest band gap in the antiferromagnetic state is closely related to the stability of the structure. As θ increases the energy decreases (see table 1), which means that the antiferromagnetic state is the most stable state. The band gap will gradually increase until the system reaches the most stable state. Therefore, the highest band gap in the antiferromagnetic state is a consequence to get the most stable condition.

4. Conclusions

We observe that the change of the band gap is influenced by the polar angle θ . The band gap increases as θ increases from 0° to 180° rotation. Therefore, we can manipulate the band gap by varying θ , which represents the directions of the magnetic moments of the carbon atoms at the edges. We also show that $\theta = 0^\circ$ and $\theta = 180^\circ$ refer to the metallic and insulator systems while the others become only the insulator. Although the calculations at $0^\circ < \theta < 180^\circ$ and $\theta = 180^\circ$ give the band gap, the noncollinear calculations strongly need a constraint method to fix the magnetic moment while the collinear calculations does not.

Acknowledgements

All the detailed computations were performed by using the high computer at the Universitas Negeri Jakarta. This work was funded by a research grant "Penelitian Unggulan Universitas 2019 No. 15/KOMP-UNJ/LPPM-UNJ/V/2019" at the Universitas Negeri Jakarta.

References

- [1] Novoselov KS, Geim AK, Morozov SV, Jiang D, Zhang Y, Dubonos SV, Grigorieva IV, Firsov AA 2004 *Science* 306: 666
- [2] Novoselov KS, Geim AK, Morozov SV, Jiang D, Katsnelson MI, Grigorieva IV, Dubonos SV, Firsov AA. 2005 *Nature* 438: 197
- [3] Geim AK, Novoselov KS 2007 *Nature Mater* 6: 183
- [4] Wang F, Zhang Y, Tian C, Girit C, Zetti A, Crommie M, Shen YR 2008 *Science* 320: 206
- [5] Liao L, Lin YC, Bao M, Cheng R, Bai J, Liu Y, Qu Y, Wang KL, Huang Y, Duan X 2010 *Nature*. 467 305
- [6] Bonaccorso F, Sun Z, Hasan T, Ferrari AC 2010 *Nature Photonics* 4: 611
- [7] Schwierz F 2010 *Nature Nanotech* 5: 487
- [8] Fujita M, Wakabayashi K, Nakada K, Kusakabe K 1996 *J. Phys. Soc. Jpn* 65: 1920
- [9] Sawada K, Ishii F, Saito M 2008 *Appl. Phys. Express* 1: 064004
- [10] Sawada K, Ishii F, Saito M, Okada S, Kawai T 2009 *Nano Lett* 9: 269
- [11] Yazyev OV and Katsnelson MI 2008 *Phys. Rev. Lett* 100: 047209
- [12] Prayitno TB, Ishii F. *J. Phys. Soc. Jpn.* 2018; 87: 114709
- [13] Prayitno TB, Ishii F 2019 *J. Phys.: Condens. Matter* in press
- [14] Gebauer R, Baroni S 2000 *Phys. Rev. B* 61: R6459
- [15] Kurz P, Förster F, Nordström L, Bihlmayer G, Blügel S 2004 *Phys. Rev. B* 69: 024415
- [16] Ozaki T, Kino H, Yu J, Han MJ, Kobayashi N, Ohfuti M, Ishii F, Ohwaki T, Weng H, Terakura K OPENMX website, Available from: <http://www.openmx-square.org>
- [17] Ozaki T 2003 *Phys. Rev. B* 67: 155108
- [18] Ozaki T, Kino H 2004 *Phys. Rev. B* 69: 195113
- [19] Troullier N, Martins JL 1991 *Phys. Rev. B* 43: 1993
- [20] Perdew JP, Burke K, Ernzerhof M 1996 *Phys. Rev. Lett* 77: 3865
- [21] Sawada K, Ishii F, Saito M 2014 *Appl. Phys. Lett* 104: 143111