Bulletin of Pure and Applied Science
Physics, Vol.41D No.2,
July-December 2022 P.81-85
Original Research Article

Print version ISSN 0970 6569
Online version ISSN 2320 3218
DOI: 10.5958/2320-3218.2022.00015.X
Available online at www.bpasjournals.com

Band Structure and Spatial Localization of Electrons in Twisted Bilayer Graphene Nanoribbons

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Received on 28.07.2022
Revised on 30.09.2022
Accepted on 30.10.2022
Published on 15.12.2022

ABSTRACT We have studied the band structure, density of states and spatial localization of electron in twisted bilayer nanoribbons by means of tight binding calculation. In Chiral geometries, edge states are also related to the presence of zig-zag edge atoms, although they presented remarkable size effects. Physical properties of chiral graphene nanoribbons and general edges can have a stong dependence on chirality. We have analysed the properties of edge states in twisted bilayaer ribbons, explaining their energy dispersion and spatial localization. The different splittings were found in edge bands due to the inhomogeneous interplay coupling. For stacked zig-zag atoms the coupling was larger than corresponding edge states splitted apart, but edge states stemming from regions with stacking, where the interlayer coupling was smaller and gave rise to zero energy bands. We have also been found that in the edge regions where top and bottom zig-zag terminations were stacked, inter-ribbon tunneling between the dispersions less zero energy states created bonding and antibonding combination with energies away from the energy of the Dirac point. The obtained results were found in good agreement with previously obtained results.

KEYWORDS Band Structure, Saptial localization, twisted bilayer, nanoribbon, chiral graphene, energy dispersion, splitting edge band, Dirac Point.

How to cite this article: Mishra A., Yadav J.P., Kumar A. (2022). Band Structure and Spatial Localization of Electrons in Twisted Bilayer Graphene Nanoribbons. *Bulletin of Pure and Applied Sciences- Physics,* 41D (2), 81-85.

INTRODUCTION

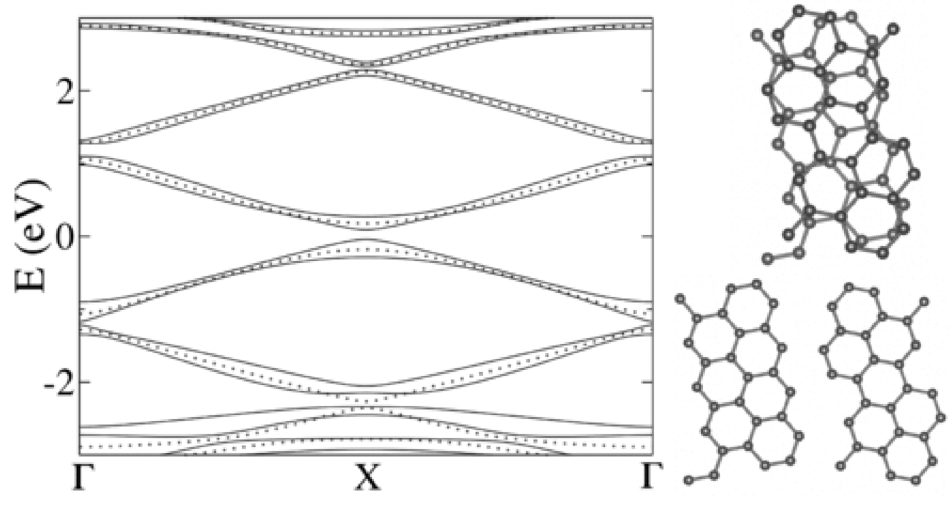
Trambly et al. (2010) [1] and Morell et al. (20202) [2] presented that for low rotation angles states near the Fermi level are mostly localized, with a strong localization, giving rise to the bright areas of the Moire pattern. The flattering of the bands with diminishing angle has been experimentally observed in angle-dependent Van-Hove singularities revealed in density of states measured by scanning tunneling spectroscopy [3-5] and by an increase of the intensity of Raman modes measured in twisted bilayer graphene samples [6-7]. There is not a controllable way to produce twisted bilayer graphene with a given angle, although some growth methods are more prone to yield twisted bilayers [8]. It was shown that graphene nanoribbons can be obtained by unzipping carbon nanotubes [9-10]. In this way twisted bilayer nanoribbons have been obtained by unzipping chiral multiwalled nanotubes [11]. Chiral graphene nanoribbons have edges with a mixture of armchair and zig-zag components. It has been theoretically established that all edges, with the exception of the pure armchair, presented zero energy localization state with a predominant weight at the edge atoms [12-13]. In pure zig-zag nanoribbons zero energy states were strongly localized at these atoms [14-15]. The dependence of the electronic properties of twisted bilayer graphene on the relative rotation angle between layers has attracted many theoretical [16-24] and experimental works [25-27]. If the rotation angle between the two graphene layers is large the system behaves as if it were composed of two uncoupled layers [28] with a linear dispersion relation and the same Fermi velocity as monolayer graphene. Singh et al. [29] developed a model for the miniband gap and related non parabolic dispersions at the limiting of bismuth-antimony. They have studied band edges and electronic phases as function of grow the orientation. They have found that layer width has large variation of phases and orientationless. Mishra and Kumar (2021) [30] studied electronic properties of graphene. The graphene nanoribbon sensitivity was dependent on matching condition and it was also found that conductivity was reduced.

METHOD

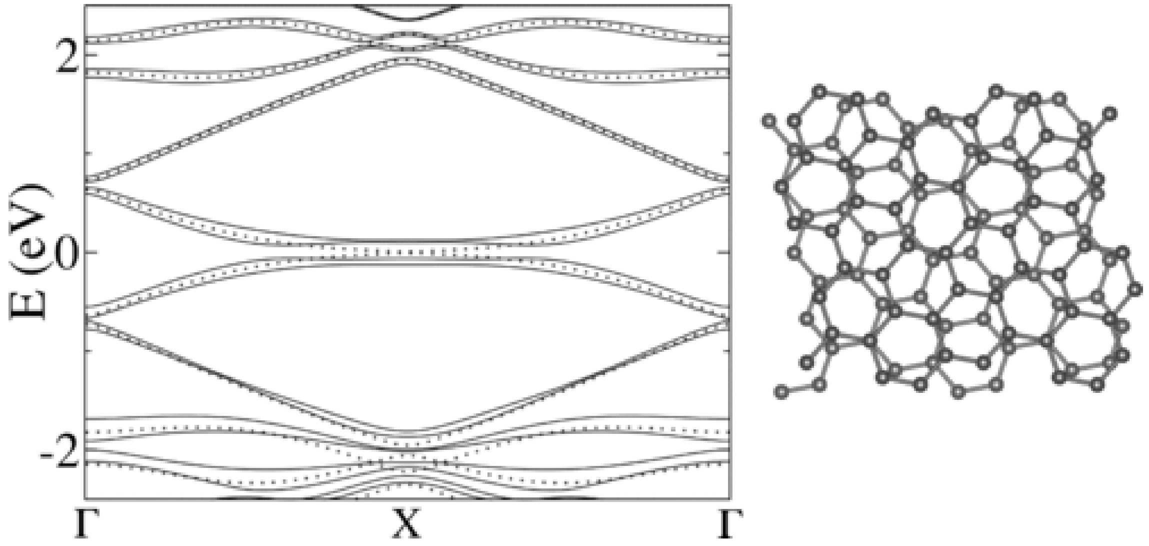
Unit cell of a commensurate twisted bilayer graphene was obtained by rotating a Bernal-Stacked bilayer. The rotation axis passes through a site which has an atom in a layer situated at the center of a hexagon of the other layer. In order to choose commensurate unit cell, a point of the crystal with co-ordinates $r = ma_1 + na_2$, where *m* and *n* are integers, was rotated to an equivalent site $t_1 = na_1 + ma_2$. The graphene lattice vectors are given by $a_1 = \frac{a}{2}\left(\sqrt{3} - 1\right)$ and $a_2 = \frac{a}{2}\left(\sqrt{3}, 1\right)$ and $a = 2.46\text{Å}$ is the graphene lattice constant. The unit cell vectors of the bilayer twisted cell can be chosen as $t_1 = na_1 + ma_2$ and $t_2 = -ma_1 + \left(n + m\right)a_2$. Bilayer unit cells built in this way are usually labeled by the indices $\left(n, m\right)$. The corresponding relative rotation angle between layers is given by $\cos\theta = \left(n^2 + 4mn + m^2\right)/2\left(n^2 + mn + m^2\right)$. The repetition of twisted bilayer graphene cell with $n = \left(m + 1\right)$ along either t_1 or t_2, yielded a chirial ribbon with edges having a predominantly armchair component. We have considered ribbons with minimal edges i.e. those with a minimum number of edge nodes with co-ordination number 2. The width of the ribbon was given by an integer multiple N of its width vector t_1. We have labeled the ribbons as $N\left(2m + n, n - m\right)\left[\left(n, m\right)\right]$, where $\left(2m + n, n - m\right)$ are the edge, *N* the width and $\left(n, m\right)$ identities the Moire geometry. For sufficiently small relative rotation angle, below 10°, distinct regions were found in twisted bilayer graphenes. There are areas with stacking, others with stacking and there are also regions which were seemed to be obtained by a relative translation, called slip. The obtained results were compared with previously obtained results.

RESULTS AND DISCUSSION

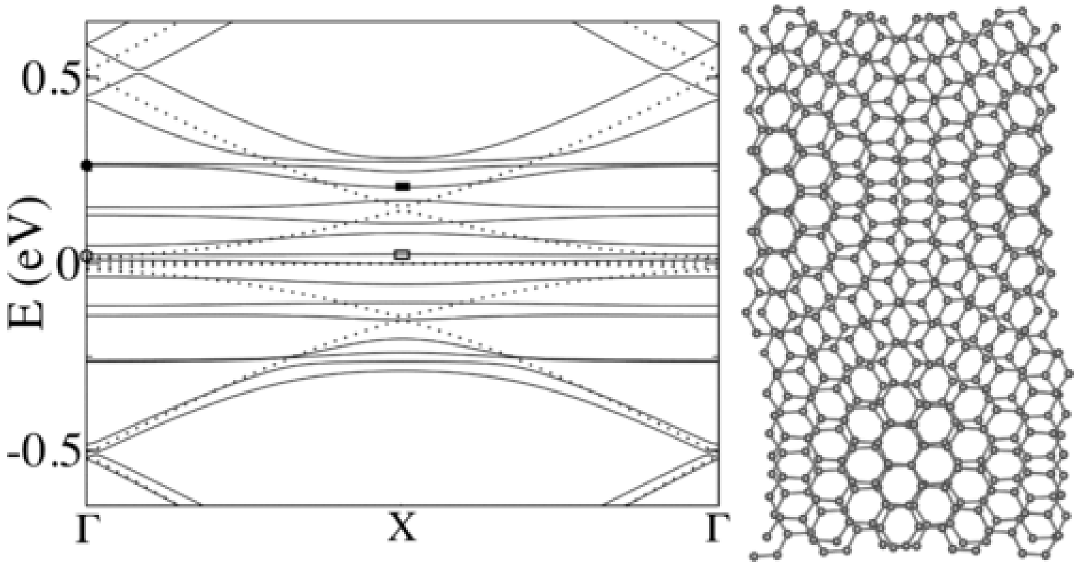
Graph (1) shows the bilayer geometry and the two components monolayer ribbons separately, which also shows their corresponding band structures. The (4,1) edge was decomposed as (3,0) + (1,1) in the right panels of graph (1), it is seen that the edge has only one armchair (1,1) step. This step is located at different parts of the suspended edges, so that they do not lie on top of each other. The orientation of the (1,1) steps is different in the two nanoribbons, in order to super impose them with a perfect stacking, a mirror reflection on a plane perpendicular to that of the ribbon is needed, in addition to a translation. Being related by a mirror reflection, the band structure of the two monolayer ribbons are equal. Having a (3,0) zigzag component, the (4,1) edge has the zero energy band. The monolayer ribbon should have two edge bands and therefore the bilayer ribbon has four. These edge bands are split apart and is seen in the left panels as shown in graph (1). The behavior is different from that of zigzag ribbons, due to the boundary condition for chiral edges mixes both sublattices. Such mixing leaded to the coupling of edge states at opposite sides of each monolayer ribbon, so that size effects produced the opening of a gap. The gap between the two edge bands in the monolayer ribbon is wider than for the bilayer ribbon. Coupling between the two ribbons splits the bands but the ribbon is so narrow. The 2(4,1)[(2,1)] twisted bilayer nanoribbons shown in graph (2). In the monolayer ribbon, the two edge bands are coupled, they touch at the edge of the Brillounin zone as $m=1$, M is at the Brillounin zone boundary × and their splitting at T is also smaller. With a (13,1)[(5,4)] twisted bilayer nanoribbons is splited from a (5,4) twisted bilayer graphene which has relative rotation angle $\theta = 7.34^o$ and 244 atoms in the unit cell. The corresponding ribbon have a (13,1) edge, which decomposed as a (12,0)+(1,1). This bilayer ribbon has 16 edge states. For smaller relative rotation angles as in the case in the unit cell for the ribbon m=4 so the M point is folded at T is shown in graph (3). The obtained results were compared with previously obtained results of theoretical and experimental research works and were found in good agreement.



Graph 1: Band structures of the 1(4,1)[(2,1)] twisted bilayer nanoribbon (solid lines) and of the corresponding monolayer ribbon (dotted lines). The geometry of the unit cell and its constituent monolayers are shown on the right.



Graph 2: Left Panel: Band structures of the 2(4,1)[(2,1)] twisted bilayer nanoribbon (solid lines) and of the corresponding monolayer ribbon (dotted lines). Right panel: Unit cell of the 2(4,1)[(2,1)] twisted bilayer nanoribbon.



Graph 3: Left panel: Band structure of the 1(13,1) [(5,4)] twisted bilayer nanoribbon (solid lines) and of the corresponding monolayer ribbon (dotted lines). Small circles and boxes indicate the *k* point of the bands selected to show the local density of states.

CONCLUSION

We have studied band structure and spatial localization of electrons in twisted bilayer graphene nanoribbons. We have found that due to the spatially inhomogeneous interlayer coupling, edge states streaming from regions with stacking are closer to the energy of the Dirac point, where as those arising from stacked edge states are splitted in energy due to the stronger interlayer coupling. We have found that the bands with energies less than 0.2 eV are mainly localized in the regions of the edges while edge bands farther from Fermilevel energy corresponding to the edge sites following the moire pattern of the bulk. As opposed to bulk bilayer graphene for which states near the Dirac point are localized in stacked regions. The obtained results were found in good agreement with previously obtained results.

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