Physica E 65 (2015) 36–43

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Quasi-particle spectrum in trilayer graphene: Role of onsite coulomb interaction and interlayer coupling

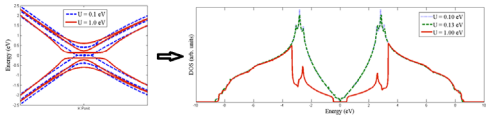
Sanjay Kumar *, Ajay

Department of Applied Science and Engineering, Indian Institute of Technology Roorkee, Saharanpur Campus-Saharanpur, 247001, India

HIGHLIGHTS

- Analysis of the quasi-particle spectrum in trilayer graphene.
- The expressions are obtained using Green's function equations of motion approach.
- Enhancement in Coulomb interaction energy generates a gap at Fermi level.
- Enhancement in $t_\perp$, Introduce a finite DOS at Fermi point in ABC-stacking.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 6 May 2014
Received in revised form
21 July 2014
Accepted 14 August 2014
Available online 23 August 2014

Keywords:
Trilayer graphene
Electronic spectrum
Tight binding hamiltonian
Stacking order

ABSTRACT

Stacking dependent quasi-particle spectrum and density of states (DOS) in trilayer (ABC-, ABA- and AAA-stacked) graphene are analyzed using mean-field Green's function equations of motion method. Interlayer coupling (t_1) is found to be responsible for the splitting of quasi-particle peaks in each stacking order. Coulomb interaction suppresses the trilayer splitting and generates a finite gap at Fermi level in ABC- while a tiny gap in ABA-stacked trilayer graphene. Influence of $t_\perp$ is prominent for AAA-stacking as compared to ABC- and ABA-stacking orders. The theoretically obtained quasi-particle energies and DOS has been viewed in terms of recent angle resolved photoemission spectroscopic (ARPES) and scanning tunneling microscopic (STM) data available on these systems.

1. Introduction

Graphene is single layer of sp^2 bonded carbon atoms arranged in a hexagonal lattice {(interpenetrating two tringular sub-lattices (say A and B)}. The electronic spectra of graphene (monolayer) depicts a gapless band structure leading to highly conducting states close to Dirac points [1–11] (specified by $K=2\pi/a$ $(1/3,1/3\sqrt{3})$ and $K'=2\pi/a$ $(1/3,-1/3\sqrt{3})$). Since the experimental isolation of Graphene [2] and later development of multilayer graphene structures, these materials have shown an exponential growth in the experimental and theoretical researches focused to understand electronic properties for potential applications in electronic devices. Bilayer graphene exhibits two possible stacking orders i.e. AB- and AA-stacking, AB-stacked bilayer graphene consists of two coupled graphene layers placed in such a way so that the B sublattice atoms of upper layer are situated directly above the A sublattice atoms of the lower layer [4,12–16]. While, crystal structure of AA-stacked bilayer is such that all A (B) sub-lattice atoms of top layer lie exactly above the A (B) sub-lattice atoms of respective bottom layer [12,15,16]. The inter-planar spacing for AB stacking and AA stacking are of the order of 3.35 Å and 3.55 Å respectively [8,15–17]. Also, AB-stacked bilayer graphene has parabolic band dispersion with tunable band gap of the order of 0.25 eV under the influence of perpendicular electric field [5,18–22] and no such gap was found in monolayer graphene.

In trilayer graphene, there exist two stable stacking orders which are ABC-stacking (rhombohedral) order and ABA-stacking (Bernal) order, while AAA-stacking has been found in intercalated graphite [23–25]. The crystal structure of ABC-stacked trilayer graphene is such that, one sublattice of top layer lies exectly above the center of hexagons of bottom layer as shown in Fig. 1(a). Whereas, in ABA-stacking, all atoms of topmost layer lie exactly on

* Corresponding author. Tel.: +91 9557282112.
E-mail address: sanjaybharatiyiitr@gmail.com (S. Kumar).

http://dx.doi.org/10.1016/j.physe.2014.08.010
1386-9477/

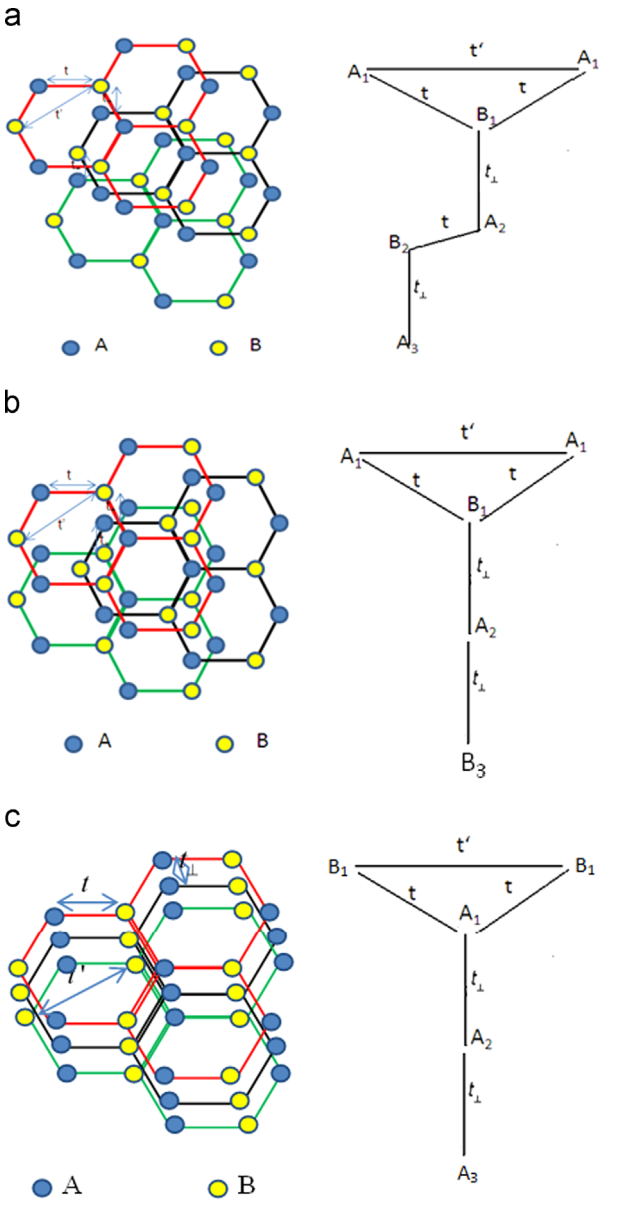


Fig. 1. Crystal structure of (a) ABC-stacked, (b). ABA-stacked and (c). AAA-stacked trilayer graphene.

top of bottommost layer [26] as shown in Fig. 1(b). Among all the three stacking orders, AAA-stacked trilayer graphene has the simplest cystal structure, where all atoms of adjacent upper layer lie exactly on top of neighbor lower layer as in Fig. 1(c). The electronic band structure of trilayer graphene depends on nature of stacking sequence [27,28]. ABA-stacked trilayer graphene has a combination of linear and parabolic band dispersion with a zero band gap while ABC-stacked trilayer graphene has cubic band dispersion with a tunable band gap of the order of 0.12 eV under the application of perpendicular electric field [26,28–36]. Also near the Dirac points, electrons in ABA-stacked trilayer graphene behave as both massive and massless Dirac fermions whereas in ABC-stacked trilayer graphene their behavior is like massive fermions [31,37–40]. Simple hexagonal or AAA-stacked trilayer graphene exhibits an energy dispersion relation that looks like a combination of three monolayer linear (massless) bands with a zero band gap with three Dirac points near its Fermi level [41]. The first principle investigation of the electronic band structure of AAA-stacked trilayer graphene showed that perpendicular electric field does not open up a band gap in the band structure of hexagonal trilayer graphene close to Dirac points [42].

To study the electronic structure of graphene, ARPES and STM measurements are the reliable and powerful probes. Ohta et al. [24] experimentally (by using ARPES) studied band structure of multilayer graphene and found that the splitting of π-bands depend upon onsite Coulomb interaction, number of layers and their interaction. Yankowitz et al. [43] have found, by using STM measurements, that stacking order plays an important role in determining the existence of gate tunable band gap in trilayer graphene as ABC-stacked graphene shows an electric field tunable band gap whereas ABA-stacked show a metallic behavior. Recently, Menezes et al. [44] have studied the quasi-particle band structure of ABA- and ABC-stacked trilayer graphene through ab initio density-functional theory (DFT) and many-body calculations within GW approximation. They have also reproduced the values of various hopping parameters. However, it will be a subject of interest to study the influence of hopping parameters and onsite Coulomb interaction energy on DOS in these systems.

Therefore, in light of above facts, stacking order, hopping parameters and onsite electron-electron interaction [24,27,28] play important role in determining the electronic structure and transport behavior of trilayer graphene. It is important to attempt tight binding studies related to electronic spectra [45–48] of trilayer graphene in different stacking arrangement by including contribution of next-nearest-neighbor hopping (t') and interlayer coupling ($t_\perp$) parameters along with onsite Coulomb interaction energy (U). For this purpose we have used tight binding model Hamiltonian and employed Green's function technique within mean-field approximation to compare the theoretically obtained quasi-particle energies and DOS results with the recent available experimental (ARPES & STM) data [5,24,43,48].

2. Theoretical formulation

Crystal structure of ABC-stacked trilayer graphene is such that one triangular sublattice of top layer lies exactly above the center of hexagon in bottom layer and there are six carbon atoms per unit cell as schematically shown in Fig. 1(a). Therefore, only half of the atoms of three mono-layers are strongly coupled by interlayer hopping, while rest half atoms are weakly coupled [30]. Tight binding model Hamiltonian of ABC-stacked trilayer graphene within two triangular sub-lattice approaches in momentum space is given by:

$$H_{ABC-Trilayer} = H_{Intralayer} + H_{Interlayer} \tag{1}$$

$$H_{Intralayer} = -\sum_{k,\sigma,r=1,2,3} t_k\{a^+_{rk\sigma}b_{rk\sigma} + h.c.\} - \sum_{k,\sigma,r=1,2,3} t'_k\{a^+_{rk\sigma}a_{rk\sigma} + b^+_{rk\sigma}b_{rk\sigma} + h.c.\} + \frac{U}{2}\sum_{k,k',\sigma,r=1,2,3}\{a^+_{rk\sigma}a^+_{rk'-\sigma}a_{rk'-\sigma}a_{rk\sigma}\} + \frac{U}{2}\sum_{k,k',\sigma,r=1,2,3}\{b^+_{rk\sigma}b^+_{rk'-\sigma}b_{rk'-\sigma}b_{rk\sigma}\} \tag{1a}$$

$$H_{Interlayer} = -t_\perp\sum_{k,\sigma}\{b^+_{1k\sigma}a_{2k\sigma} + b^+_{2k\sigma}a_{3k\sigma} + h.c.\} \tag{1b}$$

where, t and t' are nearest-neighbor and next-nearest-neighbor hopping parameters on triangular sub-lattices, respectively. Also $t_\perp$ is interlayer coupling parameter and U is onsite Coulomb interaction energy in each triangular sub-lattice. The $a^+_{rk\sigma}(b_{rk\sigma})$ creates (annihilates) an electron on sub-lattice A (B) with momentum k and spin σ. Also [4,7,8,10,11], $t_k = t\{3+f(k)\}^{1/2}$ and $t'_k = -t'\{3+f(k)\}^{1/2}$, where