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Combined effect of the perpendicular magnetic field and dilute charged impurity on the electronic phase of bilayer AA-stacked hydrogenated graphene

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ABSTRACT

We address the electronic phase engineering in the impurity-infected functionalized bilayer graphene with hydrogen atoms (H-BLG) subjected to a uniform Zeeman magnetic field, employing the tight-binding model, the Green's function technique, and the Born approximation. In particular, the key point of the present work is focused on the electronic density of states (DOS) in the vicinity of the Fermi energy. By exploiting the perturbative picture, we figure out that how the interaction and/or competition between host electrons, guest electrons, and the magnetic field potential can lead to the phase transition in H-BLG. Furthermore, different configurations of hydrogenation, namely reduced table-like and reduced chair-like, are also considered when impurities are the same and/or different. A comprehensive information on the various configurations provides the semimetallic and gapless semiconducting behaviors for unfunctionalized bilayer graphene and H-BLGs, respectively. Further numerical calculations propose a semimetal-to-metal and gapless semiconductor-to-semimetal phase transition, respectively, when only turning on the magnetic field. Interestingly, the results indicate that the impurity doping alone affects the systems as well, leading to semimetal-to-metal and no phase transition in the pristine system and hydrogenated ones, respectively. However, the combined effect of charged impurity and magnetic field shows that the pristine bilayer graphene is not influenced much as the functionalized ones and phase back transitions appear. Tuning of the electronic phase of H-BLG by using both types of electronic and magnetic perturbations play a decisive role in optical responses.

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1. Introduction

Graphene as a first two-dimensional (2D) carbon material is still a subject of extensive research in nanoscience in both scientific and engineering fields due to its remarkable electronic and physical properties such as the unconventional quantum Hall effect [1] and high carrier mobility [2–4]. However, the *pristine* graphene with inherent zero band gap is not applicable in logic circuits stemming from its fairly low on/off current ratio of about 4 [5]. To overcome this obstacle, one has to explore effective methods to open a band gap in its electronic spectrum, resulting in converting massless Dirac fermions to massive ones. In so doing, there are various approaches such as applying electric field [6,7], uniaxial strain [8,9], different substrates [10,11], cutting graphene [12,13], and chemical functionalization [14]. All of these ways break the electron–hole band symmetry and induce a finite (non-zero) band gap. To do the best way, one should be aware that the stability of the honeycomb lattice of graphene is conserved during the processes, i.e. during applying external perturbations. In addition on graphene, a new window in logic applications can be opened using the topological insulators with remarkable topological properties of edge states in dynamical superlattices [15]. Moreover, other applicable photonic Floquet topological insulators in honeycomb lattice of atomic ensembles give rise to fascinating features [16]. On the other hand, it is worthwhile to mention that for logic devices, the electro-optical properties of atomic systems alarm interesting outcomings [17,18].

Currently, hydrogenation of carbon materials has attracted considerable attention due to the widespread applications behind it. Hydrogenation of graphene induces different electronic and magnetic characterizations into the graphene, making it a proper candidate in logic devices with a non-zero band gap, which is estab-

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lished both theoretically and experimentally in Refs. [19–26]. It has been shown that the full adsorption of hydrogen (H) atoms on top of carbon (C) atoms in graphene opens a band gap of 3.43 eV [27] and a net magnetic moment of 1 μ_B (μ_B being the Bohr magneton constant) [28,29]. Furthermore, ferromagnetic and antiferromagnetic ordering for different couplings between H and C atoms are reported [23]. One of the important factors leading to different properties in the hydrogenation of graphene refers to the hydrogenation configuration. It implies that fully hydrogenated graphene, which is called graphane has different responses compared to the half-hydrogenated one [20,30]. In addition to hydrogen, other chemical functionalizations with F, OH, COOH, and O give rise to fascinating properties in graphene [13, 30–32]. The main goal of functionalization of graphene is destroying sp^2-hybridization indeed. It should be noted that the hydrogenation process is reversible in order to tune the electronic phase of the system [19,33].

Unlike monolayer graphene, tuning of the band gap and electronic properties in bilayer graphene is easier originating from the *interlayer* coupling between C atoms from the top and bottom layers [34]. The same ways used in monolayer graphene in order to induce a band gap can be used in bilayer graphene too [5–7, 34–38]. The arrangement of electronic bands in bilayer graphene shows that the system is a semimetal [39,40]. Furthermore, the chemical modification of few-layer graphene by H atoms has been investigated well experimentally [41]. They found that the properties of hydrogenated-few-layer graphene depend strongly on the number of layers. On the one hand, it has been shown that the hydrogenated bilayer graphene is a ferromagnetic semiconductor [35], which of course, like the monolayer case, the hydrogen site-dependent physical properties are expected [19,21,22,26, 42–45]. On the other hand, stacking of layers is important. Bilayer graphene has different types of stacking including the Bernal (AB-stacked), the simple (AA-stacked), twisted, and so on [46–49]. In AB (AA) staking case, A/B atom in the first layer corresponds to B/A (A/B) atom in the second layer. Bilayer graphene and its hydrogenated version inherently have large potentials in real applications [5,35,50]. Generally, the hydrogenation of single-layer graphene is much easier than the bilayer case [19,33]. Although most of the references above are on AB-stacked bilayer graphene, to the best of our knowledge, a few investigations of hydrogenated AA-stacked bilayer graphene have been done to date.

Recently, there have been several studies on the magnetic field effect on bilayer graphene [51,52]. As well known, the thickness of 2D materials tells us that only the coupling between the magnetic field and spin degrees of freedom is possible, not the orbit one. It is better to say that the coupling from spins is more dominant than the orbit ones in 2D systems. For this reason, applying a magnetic field leads to various physical properties. Also, investigation of hydrogenated bilayer graphene subjected to a magnetic field beam is interesting. In addition, as mentioned before, optimizing electronic properties of bilayer graphene requires to control the band gap which has been done by numerous methods [see the previous paragraph]. Interestingly, impurity doping effects is also one of the ways to tune the physical quantities of low-dimensional materials [53–59]. This is also appealing in condensed matter physics to see what the impurity effects on the electronic phase of hydrogenated bilayer graphene are.

Motivated by the provided insights on hydrogenated bilayer graphene and different effective factors, we raise this question: What are the electronic treatments of the impurity-infected hydrogenated bilayer graphene (H-BLG) subjected to a uniform magnetic field with different H configurations? To answer this question, we restrict ourselves to the basic quantity, electronic density of states (DOS). Although, as mentioned, there are numerous works on bilayer graphene theoretically, a few reports can be found on

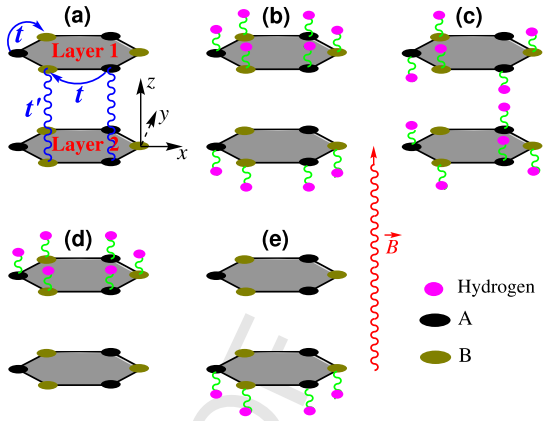

Fig. 1. (Color online.) Geometry of hydrogenated AA-stacked bilayer graphene for (a) pristine, (b) table-like, (c) chair-like, (d) r-table-like, and (e) r-chair-like case. The *intralayer* and *interlayer* hopping energies are labeled by t and t', respectively. The perpendicular magnetic field is also applied in the z-direction as $\vec{B}$.

the combined effects of magnetic field and impurity on H-BLG. In this paper, theoretical calculations are performed using the tight-binding Hamiltonian model and the Green's function approach. Also, the electron–impurity interaction effect between the host electrons of H-BLG and the external impurities is considered by means of the Born approximation and T-matrix method. The details will be shown later. We report the electronic phase transition and mid states stemming from various interactions. In other words, here we show that how one can control the electronic properties of H-BLG for future logic applications.

The paper is organized as follows. In Sec. 2, we describe the effective Hamiltonian model for H-BLG in the presence of the magnetic field in detail in which the special attention is paid to the way of hydrogenating. In Sec. 3, we introduce the Born approximation and T-matrix in order to find the interacting Green's functions. Then, we calculate DOS using the Green's function elements derived from the perturbed Hamiltonian. The results will be presented in Sec. 4 and to conclude, we summarize our remarkable findings in Sec. 5.

2. Model description

The intent of this section is to introduce the model addressing H-BLG lattice to allow for a systematic and routine assessment of electronic phase transition. To describe the dynamics of Dirac fermions in presence of magnetic field, the following tight-binding model Hamiltonian has been used [60]:

$$\hat{\mathcal{H}} = \sum_{i,j}\sum_{\sigma,\sigma'}\sum_{\alpha,\beta}\left[t_{ij\sigma'}^{\alpha\beta\sigma} + \epsilon_i^{\alpha\sigma}\delta_{\alpha\beta}\delta_{ij}\delta_{\sigma\sigma'}\right]\hat{c}_i^{\dagger\alpha\sigma}\hat{c}_j^{\beta\sigma'} + g\mu_B B/2\sum_{i,l}\left[\hat{a}_{li,\uparrow}^{\dagger}\hat{a}_{li,\downarrow} + \hat{b}_{li,\uparrow}^{\dagger}\hat{b}_{li,\downarrow} + \text{H.c.}\right], \quad (1)$$

wherein $t_{ij\sigma'}^{\alpha\beta\sigma}$ defines the hopping integral between an electron with spin σ from subsite α in the unit cell i to another electron with spin σ' from subsite β in the unit cell j. $\epsilon_i^{\alpha\sigma}$ is the on-site energy for an electron with spin σ from subsite α in the unit cell i. The hydrogen contribution with spin up is included in the on-site energy. Also, l is used for the layer index. In this work, five forms of hydrogenation are considered, namely pristine, table-like, chair-like, reduced table-like (r-table-like), and reduced chair-like (r-chair-like). Since our structure is considered as bilayer including four atoms per unit cell [A_1, B_1, A_2, and B_2] without hydrogenation, as illustrated in Fig. 1(a), by considering one H atom

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