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Electronic Structure and Energetics of Corrugated Graphene Sheet

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1. Introduction

Ever since the synthesis of graphene[1], which is a carbon allotrope with a planar honeycomb molecular structure, there has been a wealth of theoretical and experimental studies of the physical properties of this exotic carbon allotrope[2,3]. Graphene is known to be a semimetal with zero density of states equal at the Fermi energy, which is due to the emergence of two linear dispersion bands at the Fermi level. These linear dispersion bands lead to massless electrons near the Fermi energy, which allows for a wealth of intriguing physics. For instance, graphene has an unusually low-energy electronic structure that gives it remarkable transport properties. Thus, graphene is now considered to possess great potential for advancing both low-dimensional sciences and the next generation of nanoscale electronic devices.

On the other hand, fundamental properties of graphene is strongly depends both on its network topology and the interlayer interactions with the underlying substrate composed of graphene layers or other materials, such as SiO_2. For instance, graphene sheet with defects is either semiconductor or metal depending on the mutual defect arrangements in graphene. Furthermore, for insulating substrates, such as SiO_2, HfO_2, and hexagonal-BN, because of the potential undulations, the hybridization, and the structural distortions induced by the atoms on substrates, graphene no longer has a linear dispersion band and instead has quadric bands with small but finite energy gaps. The multiplicity of electronic structures possible in graphene fascinates many in the field of low-dimensional surface and interface sciences, but it is difficult to exploit these properties in nanoscale electronic devices. In electronic devices, hybrid structures made in part from conventional materials are essential. Such hybrid structures are expected to have structural distortions in their graphene networks [4,5], which lead to electronic structure modulation. These properties hinder the graphene application in electronic devices. Thus, for device applications in future technologies, it is important to understand the electronic structure of these graphene hybrid structures. In particular, it is indispensable to explore the electronic structure of an isolated graphene sheet with long-range structural undulation by performing the first-principle total-energy calculations based on the density functional theory.

2. Methods

To study the electronic structure of graphene with the long-range structural undulation, we perform the first-principle total-energy calculations in the framework of the density functional theory (DFT) [6,7] on graphene sheet with structural corrugations introduced periodically along the armchair and zigzag directions. To express the exchange-correlation energy among the interacting electrons, we used the local density approximation (LDA) with a functional form fitted to a Monte-Carlo result for homogeneous electron gases [8,9]. Norm-conserving pseudopotentials generated using the Troullier-Martins scheme were adopted to describe the electron-ion interaction [10,11]. The valence wave functions were expanded in terms of the plane-wave basis set with a cutoff energy of 50 Ry. This cutoff provides sufficient convergence to investigate the relative stability of the various carbon phases.

Besides the DFT calculations, we also performed the tight-binding molecular-dynamics (TBMD) calculations on graphene with 18x18 lateral periodicity under several temperatures. The parameters of the TBMD method was developed for the research such as molecular dynamics studies of the liquid phase of carbon and also for the structures from small carbon clusters to a graphene sheet [12].

Fig. 1: Optimized geometry of the corrugated graphene with gradient angle of 40 degree. The corrugation is parallel to the armchair direction.

3. Results

Figure 1 shows an optimized geometry of the corrugated graphene sheet of which gradient angle is 30 degree, in which the corrugation is along the armchair direction. Our calculations show that the energy cost to induce such corrugations is 1 meV per C atom and 20 meV per C atom for the corrugation parallel to armchair and zigzag directions, respectively. For the corrugation along parallel to the armchair direction, the energy loss caused by the corrugation is negligible and independent of the width of the graphene

ribbon region and the curvature of the nanotube-like portion. On the other hand, along the zigzag direction, the total energy loss caused by the corrugation monotonically increases from zero to a few tens of meV as the gradient angle increases. Thus, the graphene favors corrugation along the armchair direction compared with that along the zigzag direction. Furthermore, the energetics confirms that the energy cost for corrugation is less than a few tens of meV so that the isolated graphene will generally have some structural undulation, such as the rippling and corrugation, on the nanometer scale. The fact also indicates that, in hybrid structures with substrates, graphene may exhibit variety in its morphology.

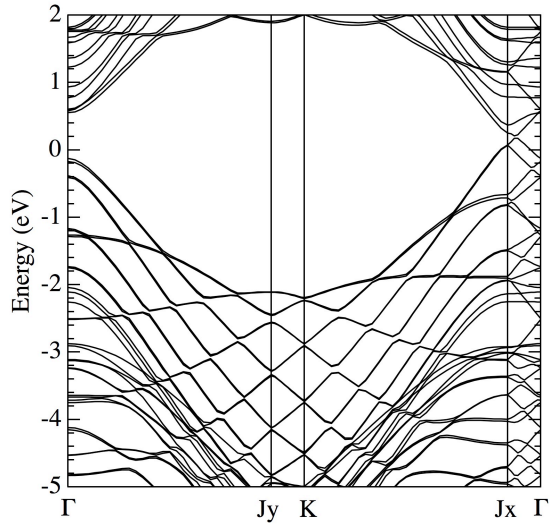

Fig. 2: Electronic structure of the corrugated graphene in which the corrugation is parallel to the armchair direction with gradient angle of 40 degree. The energy is measured from that of the Fermi level.

Figure 2 show the electronic energy band of the corrugated graphene sheet in which the corrugation is parallel to the armchair direction with the gradient angle of 40 degree. Here, the K point is folded in the vicinity of the J_y point on the J_y -Γ line. Near the Fermi level, the electronic structure maintains its features that correspond to an isolated graphene sheet without corrugation. However, by focusing on the vicinity of the K point, we found a tiny energy gap of about 5 meV (or less) that was independent of the curvature at the inflection region. The results indicate that the long-range structural undulations basically lead to the semiconducting electronic property on graphene sheet. Therefore, it is essential and important to design the graphene-based electronic devices by considering the hybrid structures taking account not only of substrate but also structural undulations.

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