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Band-Gap tuning of graphene by dual $AuCl_3$-Acceptor and N-Donor doping: A first principle study

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ABSTRACT

Graphenes dual-doped by $AuCl_3$-acceptor and N-donor have been investigated using the first principle calculations. The band gaps of the dual-doped graphenes are opened. Three supercell models of dual-doped graphenes were calculated for comparison. With the increasing of N-$AuCl_3$ distance, the band-gap width of graphene decreases, but the work function and the formation energy (E_{form}) of graphene increases. We suggest the changes of band-gap width and Fermi level are attributed to the charge redistribution between N, $AuCl_3$ and graphene. The change of E_{form} is originated from the variations of L_{C-N}(Å) and L_{C-C}(Å) caused by the interaction between $AuCl_3$ and graphene layer.

1. Introduction

Graphene, a two-dimensional (2D) monolayer structure of carbon, has attracted intense attention since its first successful preparation in 2004 [1]. Graphene has been widely used in many applications such as solar cells [2], composites [3–5], field emission sources and vacuum electronic devices [6,7]. In these areas, graphene shows interesting optical and electrical properties such as high transmittance, high surface area, strong electrical conductivity, easy to modify and mass production [8–11].

Through exploring the band structure of graphene, it is possible to get a deeper understanding and more rational use of the special optical and electrical properties of graphene. Thus, the band gap opening of graphene becomes an interesting work. Researchers have studied the methods to open the band gap of graphene, such as single-doping [12] or dual-doping with donors and acceptors [13,14], molecule absorbing [15,16], and B-N embedding [17–19].

Dual-doping with donors and acceptors is a good way to open the band gap of graphene. Especially, B-N dual doping has been investigated by many researchers, because the radii of B and N atom are similar with that of C atom. However, B acceptors and N donors are both substitutional defects. Dual doping with high concentration may strongly degrade the lattice integrity of graphene and decrease the electrical properties such as carrier mobility [13,14]. $AuCl_3$ is an acceptor-like molecule for graphene and does not substitute the C atoms, because the Au^{3+} ions can be reduced to Au clusters through a charge transfer from the graphene surface [20–22]. Thus, the N-$AuCl_3$ dual doping may provide a way to open the band gap of graphene with less substitutional defects. However, to our best knowledge, so far there has few calculation studies on the band-gap tuning of graphene by N-$AuCl_3$ dual doping.

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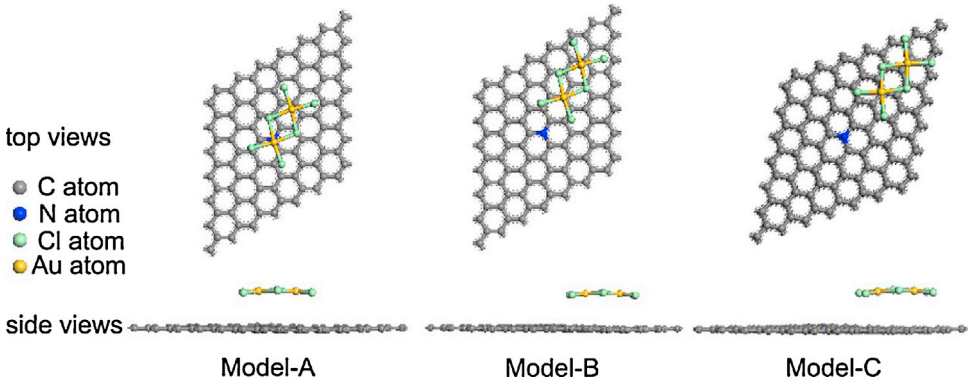

Fig. 1. The top and side views of three supercell models for dual-doped graphenes.

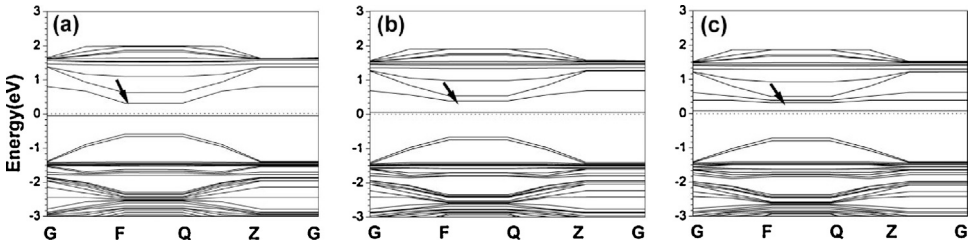

Fig. 2. The band structures of (a)-(c) dual-doped graphenes for model A, B and C, respectively. The arrows denote the positions of band-gaps. The Fermi levels are located at 0 eV and signified by horizontal red lines.

In this paper, the band-gap tuning of graphene by $AuCl_3$-acceptor and N-donor dual doping were studied using the first-principle calculations. Results show that the band-gaps of graphenes are successfully opened. Three supercell models of dual-doped graphenes were calculated for comparison. The band structures, the density of states (DOS), the partial density of states (PDOS), the formation energies (E_{form}) and the charge densities difference of the three supercell models were comprehensively investigated.

2. Models and methods

All the calculations were performed by CASTEP package based on density functional theory and all the models have been optimized successfully. We chose the projector augmented wave method (PAW) [23] to signify electron-ionic core interaction. Using Perdew Burke Ernzerhof (PBE) [24] of the generalized gradient approximation (GGA) to treat the electron exchange and correlation.

We build $7 \times 7 \times 1$ supercells of pristine and dual-doped graphenes. Each supercell has 98 carbon atoms. In the dual-doped graphene system, a carbon atom was substituted by a nitrogen atom and then an $AuCl_3$ molecule was adsorbed on the surface of graphene. A vacuum layer with a thickness of 20 Å was set to keep the adjacent graphene layers without interaction. In Fig. 1, in order to study the effect of Au-N distances on the graphene electronic properties, we constructed three supercell models with different Au-N distances for comparison. The Au-N distances for model A, B and C were 3.757, 5.561 and 6.731 Å, respectively. The cutoff energy of the plane wave was set to be 350 eV, and k-point meshes with a reciprocal space resolution of $2\pi \times 0.03$ Å^{-1} were used for Brillouin zone sampling to ensure the error bars of the total energies were less than 1 meV/atom.

3. Results and discussion

Fig. 2 shows the calculated band structures of doped graphenes. The band-gap width of pristine graphene is zero [25,26]. As for the doped graphenes, the conduction band minimums are higher in energy than the corresponding valence band maximums, which indicates the band-gaps successfully opened by the N-$AuCl_3$ dual doping. The Fermi level of model A is in the band-gap, which is similar with previous study for graphene by B and N doping [27]. However, the Fermi levels of model B and C are in the valence band, which suggests the effective charge transfer for $AuCl_3$ is larger than that for N atoms.

The calculated band-gap values for model A, B and C are listed in Table 1. The $d_{Au\text{-}N}$ values are the distances between N and Au atoms. Clearly, the band-gap width of graphene decreases with the increasing of N-$AuCl_3$ distance. Model A has the largest band-gap width (0.398 eV) with the smallest N-$AuCl_3$ distance of 3.757 Å.