Tuning the band gap of graphene by implanting a diamond shaped h-BN island

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Keywords: graphene, h-BN, band gap
Discipline: Physics

Introduction

The discovery of graphene in 2004 has led to the massive interest in other single layer materials by the scientific community. One of the most stable single layer material similar to graphene is hexagonal boron nitride (h-BN) [1]. The high conductivity of graphene makes it hard to simply turn its band gap on and up. Tuning the band gap will increase its application in optoelectronic and nanoelectronics devices. Several techniques have been suggested to open an energy gap between the valence and conduction band of graphene [2,]. In our study we proposed a hybrid structure to tune the band gap of graphene by implanting a diamond shaped h-BN island on graphene nanosheet.

Methodology

We determine the electronic properties of the hybrid structure by performing electronic structure calculation within the density functional theory (DFT) frame work, with the generalized gradient approximation (GGA) PW91 functional. For geometry optimizations, electronic and density of states (DOS) computations we used the Vienna Ab Initio Simulation Package (VASP, version 5.3) employing the projected augmented wave (PAW) method.

Result

The result obtained from our calculations shows a direct proportional relationship between the size of h-BN island and the band gap of the hybrid structure, as depicted in Table 1. Some carbon atoms were removed and replaced with boron and nitrogen atom to create the h-BN island. The energy needed to create the island is called island formation energy, and it's given by the formula in Eq. 1. The optimized geometry of the three hybrid structures are depicted in Figure 1.

$$E_{\text{if}} = (E_{G@h-BN} + Y\mu[B_{bulk}] + Z \times \mu[N_{bulk}] - (E_{h-BN_{162}} + (Y+Z) \times \mu[C_{atom}]) \quad (1)$$

Table 1. Island formation energy and the band gap of pristine h-BN(D)@G

Name	Island form energy (eV)	Band gap (meV)
4h-BN(D)@G	113.3	170.6
9h-BN(D)@G	210.2	355.3
16h-BN(D)@G	334.0	492.5

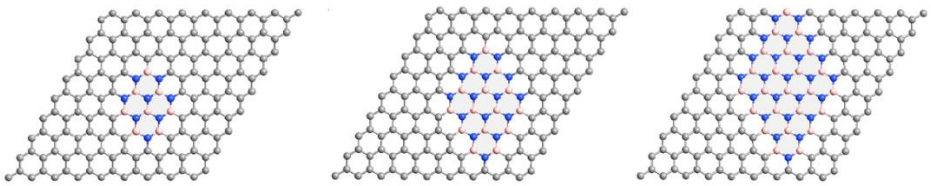

Figure 1. Optimized geometry of in-plane hybrid of graphene and h-BN GBN heterostructure. The dark blue, grey and the light orange colors show N, C and B atoms respectively.

References

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