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Study of the Effect of Mono Vacancy of Graphene Hexagonal-Boron Nitride Hybrid with Diamond Shaped h-BN Island

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The separation of single-atom-thick graphene from bulk graphite in 2004 [1] has led to the massive interest in other single layer materials with or without honeycomb structure by the scientific community. One of the stable one similar to graphene is the boron nitride in hexagonal form (h-BN). The ideal lattice match between graphene and h-BN make it possible to create graphene/h-BN in-plane hybrids (GBN) structure. The honeycomb lattice of carbon atoms makes it an attractive structure in fundamental physics and electronic devices, such as capacitors and field effect transistors (FETs)[2].
Avoiding defect during production of graphene or h-BN is almost impossible. In this study we determine the electronic properties of both the pristine and defective hybrid structure by performing electronic structure calculation within the density functional theory (DFT) framework, 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. The electronic band structure of the GBN hybrid with varied types of vacancies and sizes were analyzed thoroughly. The result obtained shows that the size of the island can alter the band gap of the system. Magnetism arises from vacancy defect was also analyzed. The higher the magnetization energy, the more stable magnetism the system has.

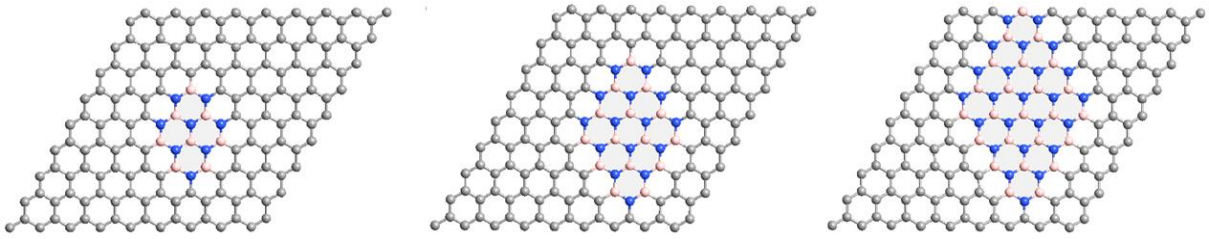

Figure 1. Optimized geometry of pristine in-plane hybrid of graphene/h-BN. The dark blue, grey and the light orange colors show N, C and B atoms respectively. It shows a graphene layout hosting an h-BN island at the middle.

References

[1] K. S. Novoselov *et al.*, "Electric field in atomically thin carbon films," *Science (80-.).*, 2004, doi: 10.1126/science.1102896.

[2] D. A. Areshkin and C. T. White, "Building blocks for integrated graphene circuits," *Nano Lett.*, 2007, doi: 10.1021/nl070708c.