International Students Science Congress

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

BY

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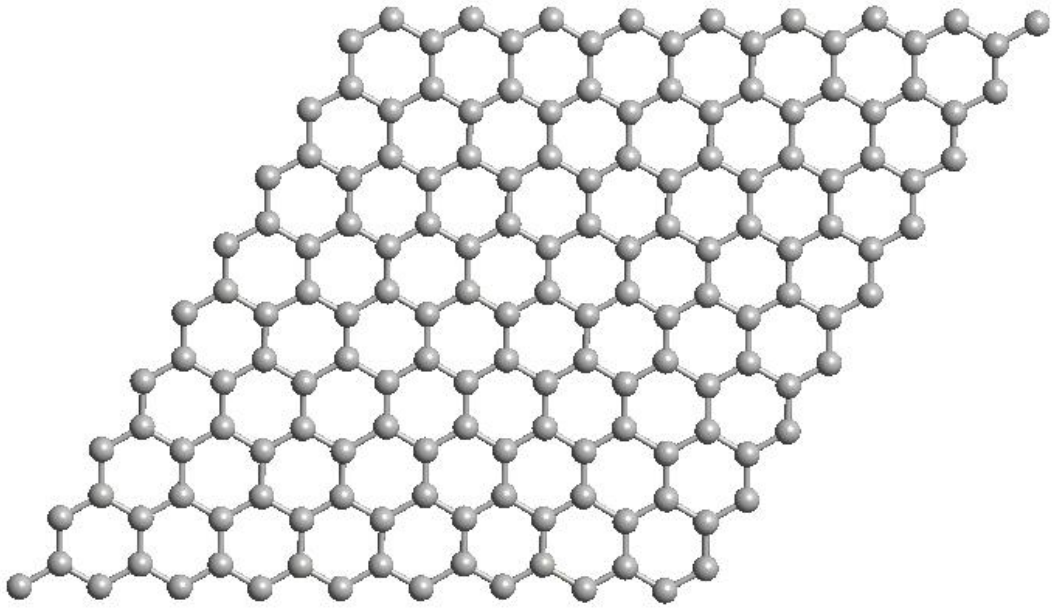
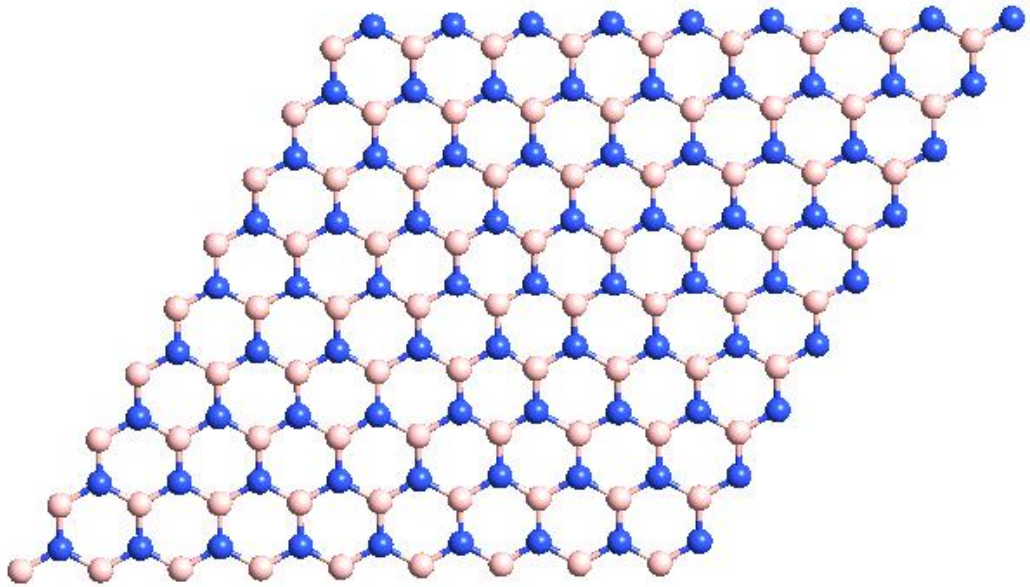
KEY RESEARCH QUESTION

Study of in-plane graphene/hexagonal boron nitride heterostructure by employing first principle calculations within the Density Functional Theory frame-work.



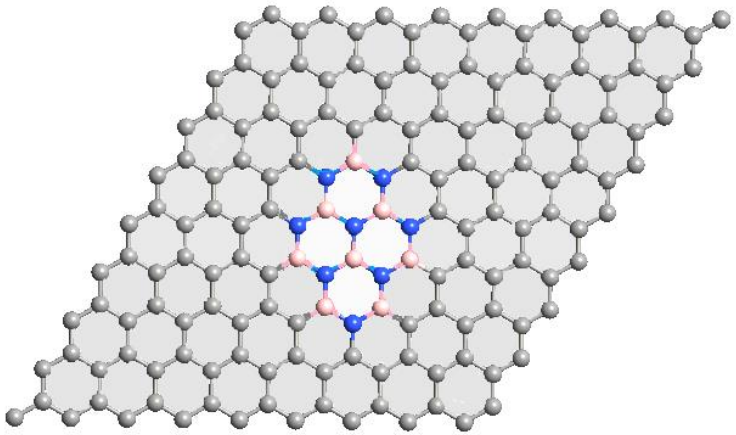
Graphene



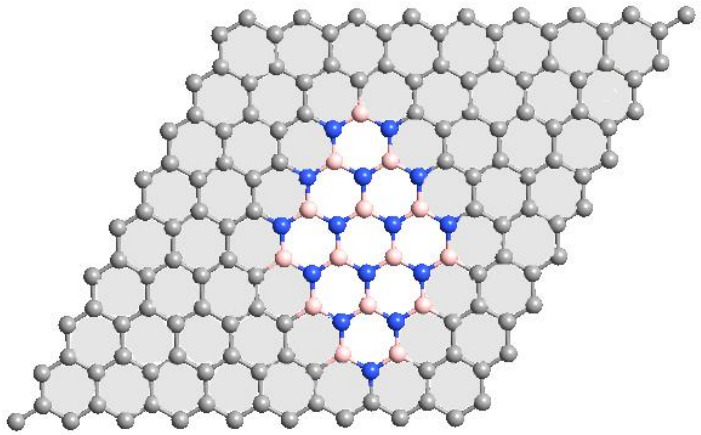
h-BN

KEY RESEARCH QUESTION

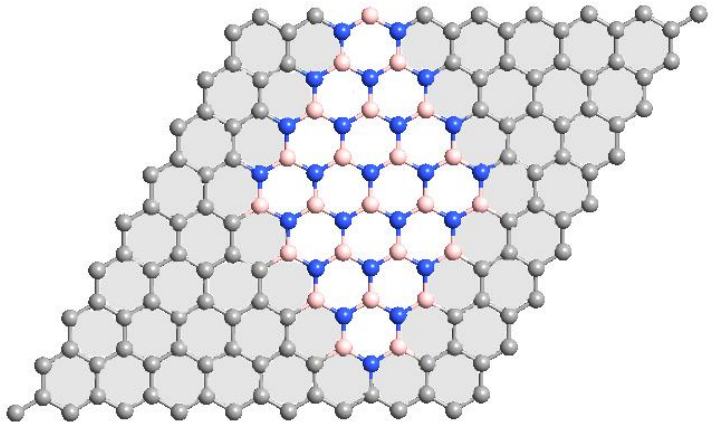
The hybrid structure showing Graphene layout with h-BN island for different island sizes



G-Diamond1

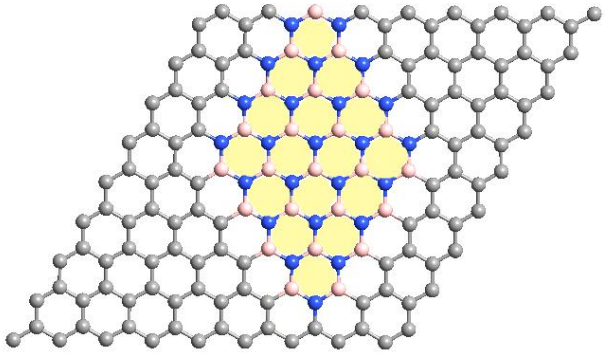


G-Diamond2

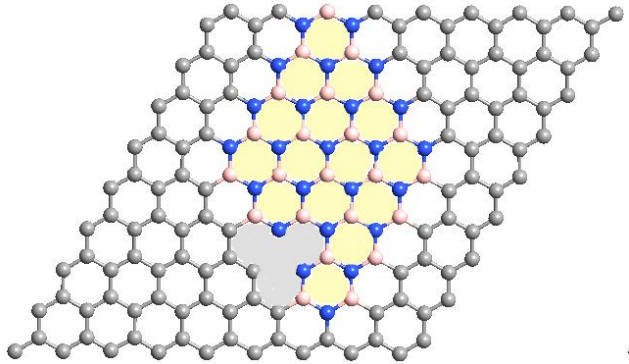


G-Diamond3

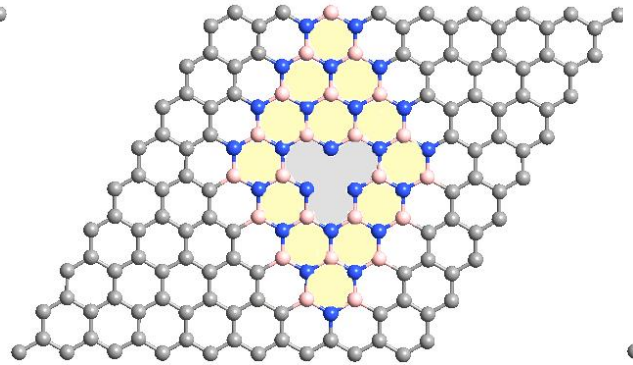
Vacancies of hybrid structure showing graphene layout with h-BN island



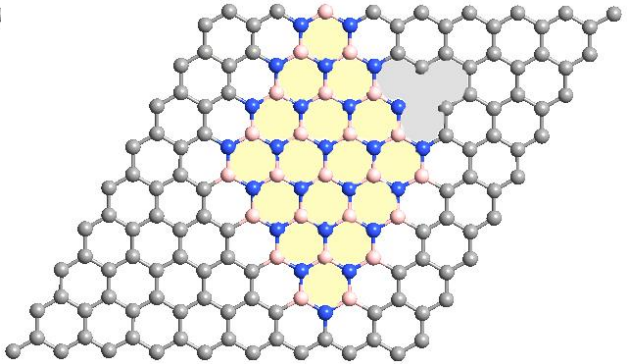
Pristine



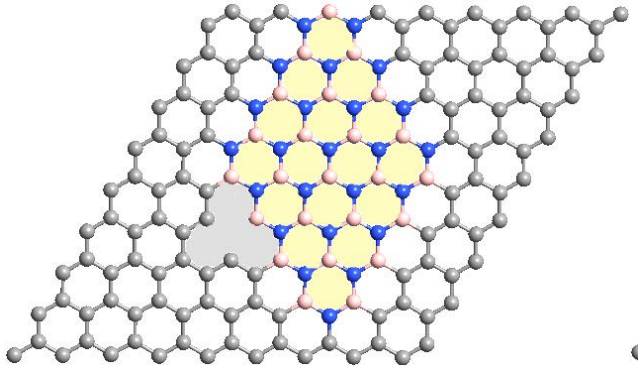
VB



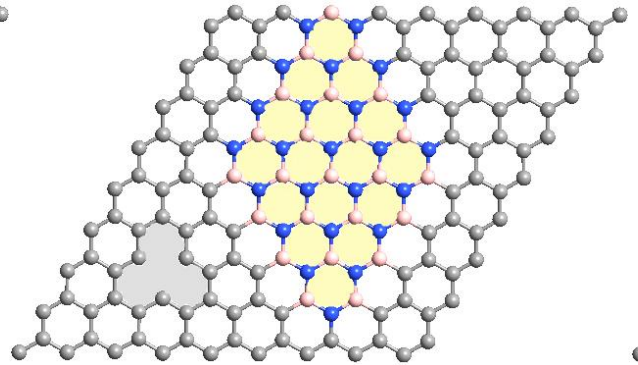
VBM



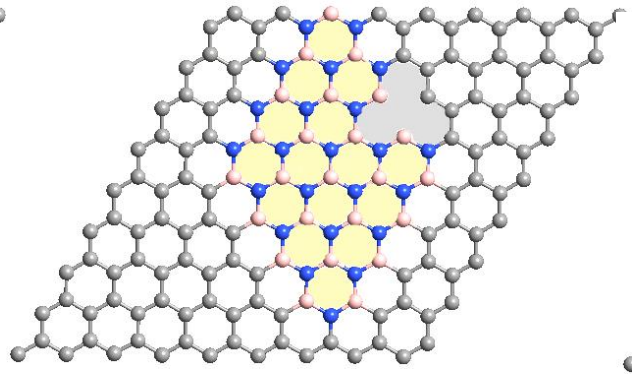
VC1



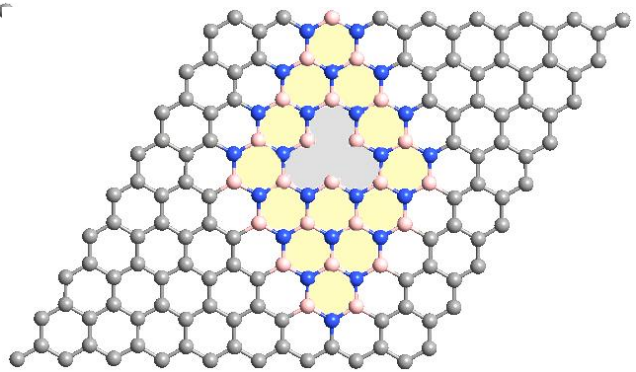
VC2



VCM



VN



VNM

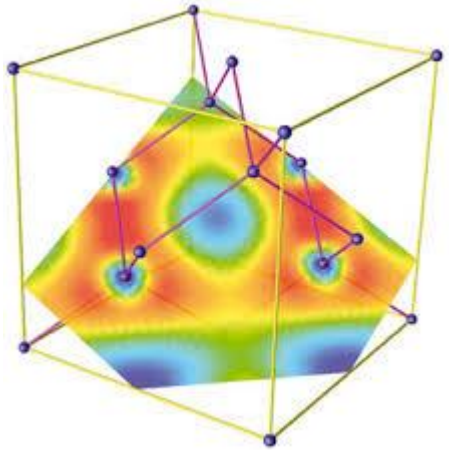
METHODOLOGY

- Virtual NanoLab

- Is a commercial point-and-click software for simulation and analysis of physical and chemical properties of nanoscale devices

METHODOLOGY

- The Vienna Ab initio Simulation Package, better known as VASP, is a package for performing ab initio quantum mechanical calculations using either Vanderbilt pseudopotentials, or the projector augmented wave method, and a plane wave basis set.

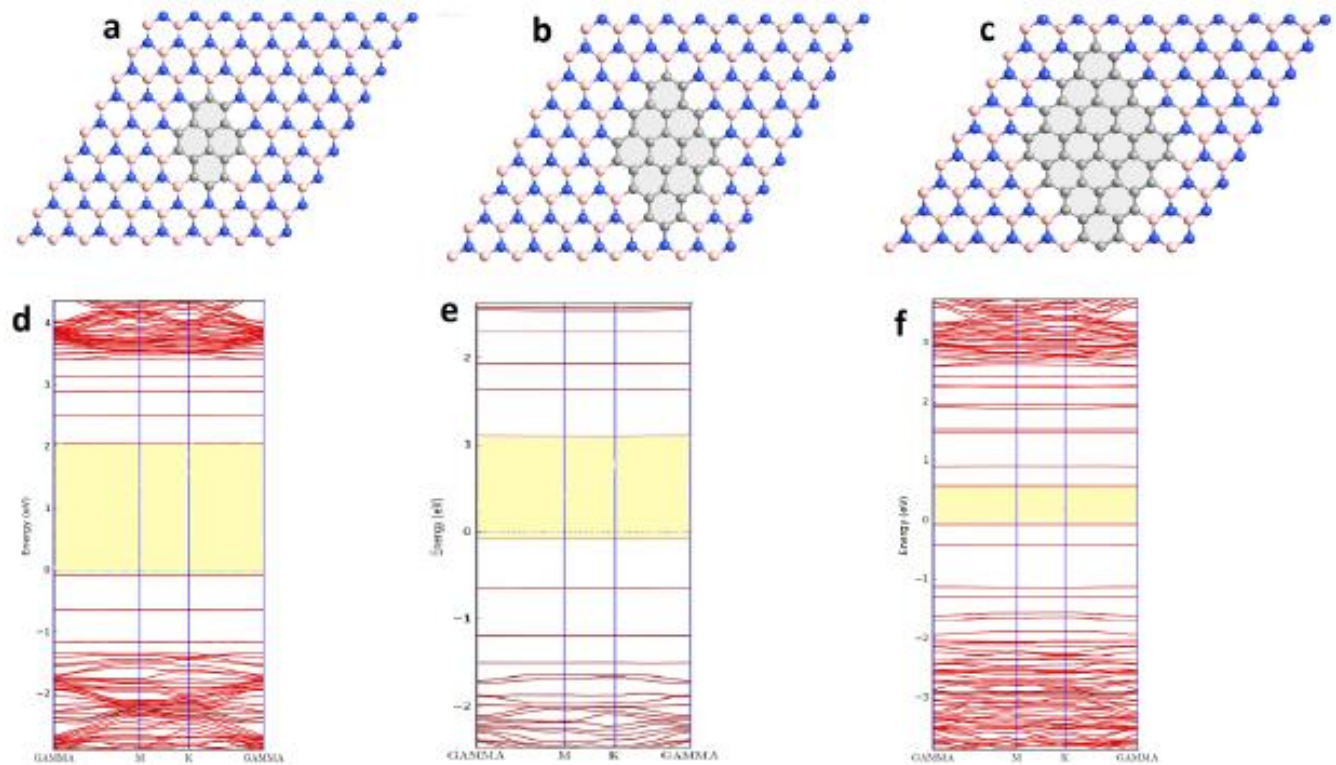


Island formation energy E_{if} of the pristine hybrid, Energy per atom and the band gap. All the hybrids are h-BN layout with diamond shaped graphene island.

System	Name	Energy (meV/atom)	Formation Energy E_{if} (eV)	Band gap (meV)
$C_{16}B_{73}N_{73}$	4h-BN(H)@G	-8.843	120.7	2131
$C_{30}B_{66}N_{66}$	9h-BN(H)@G	-8.861	224.4	1185
$C_{48}B_{57}N_{57}$	16h-BN(H)@G	-8.887	357.2	653

Magnetization energy ΔE_m, E_a Energy per atom, μ magnetic moment, formation energy E_f and E_g the band gap at the last column. NM means the hybrid is nonmagnetic. Hybrids of $C_{16}B_{72}N_{73}$ shows zero band gap therefore its metallic in nature.

System	Name	E_a (eV)	ΔE_m (eV)	μ (μ_B)	E_f (eV)	E_g (eV)
$C_{16}B_{72}N_{73}$	4h-BN(H-VB_L)@G	-8.784	-74.8	1.0	21.78	metallic
$C_{16}B_{72}N_{73}$	4h-BN(H-VB_I)@G	-8.804	-294.9	-1.0	25.02	0.35
$C_{15}B_{73}N_{73}$	4h-BN(H-VC_{I2})@G	-8.803	-0.20	NM	25.10	1.32
$C_{15}B_{73}N_{73}$	4h-BN(H-VC_{I1})@G	-8.800	-99.80	NM	24.61	0.32
$C_{15}B_{73}N_{73}$	4h-BN(H-VC_i)@G	-8.796	-249.10	NM	25.65	0.95
$C_{16}B_{73}N_{72}$	4h-BN(H-VN_L)@G	-8.798	-103.20	1.0	24.42	0.41
$C_{16}B_{73}N_{72}$	4h-BN(H-VN_I)@G	-8.802	-260.80	1.0	23.79	1.05
$C_{30}B_{65}N_{66}$	9h-BN(H-VB_L)@G	-8.816	-615.70	3.0	21.97	0.02
$C_{30}B_{65}N_{66}$	9h-BN(H-VB_I)@G	-8.821	-82.40	-0.4	9.44	0.43
$C_{29}B_{66}N_{66}$	9h-BN(H-VC_{I2})@G	-8.818	-45.90	NM	24.62	0.20
$C_{29}B_{66}N_{66}$	9h-BN(H-VC_{I1})@G	-8.820	-0.40	NM	25.04	1.21
$C_{29}B_{66}N_{66}$	9h-BN(H-VC_i)@G	-8.810	194.30	2.0	26.24	0.51
$C_{30}B_{66}N_{65}$	9h-BN(H-VN_L)@G	-8.816	-99.80	1.0	24.49	0.21
$C_{30}B_{66}N_{65}$	9h-BN(H-VN_I)@G	-8.819	-38.10	1.0	23.92	0.15
$C_{48}B_{56}N_{57}$	16h-BN(H-VB_L)@G	-8.845	-549.80	3.0	8.49	0.24
$C_{48}B_{56}N_{57}$	16h-BN(H-VB_I)@G	-8.848	-16.10	1.0	8.99	0.02
$C_{47}B_{57}N_{57}$	16h-BN(H-VC_{I2})@G	-8.847	-0.70	NM	24.73	0.68
$C_{47}B_{57}N_{57}$	16h-BN(H-VC_{I1})@G	-8.847	-114.80	2.0	24.62	0.15
$C_{47}B_{57}N_{57}$	16h-BN(H-VC_i)@G	-8.838	-9.30	NM	25.98	0.52
$C_{48}B_{57}N_{56}$	16h-BN(H-VN_L)@G	-8.845	-43.90	1.0	24.06	0.03
$C_{48}B_{57}N_{56}$	16h-BN(H-VN_I)@G	-8.847	-210.60	1.0	23.69	0.56



The hybrid structure indicating the comparative sizes of each graphene island (a) 4h-BN(H)@G (b) 9h-BN(H)@G(c) 16h-BN(H)@G. Also the electronic band structure of the corresponding hybrids is shown (d) Band structure of 4h-BN(H)@G (e) band structure of 9h-BN(H)@G (f) band structure of 16h-BN(H)@G. The yellow portion indicate the band gap area

conclusion

- We create the in-plane GBN heterostructure by implanting graphene island on hexagonal boron nitride substrate and vice-versa. And create some vacancies at different location on the system. We realized that the vacancy defect we created does not necessarily lead to structural instability; although surface distortion and reconstruction were observed.
- Hybrids that contain smaller island sizes shows metallic properties and exhibit a substantial amount of magnetic moment for possible localized spin utilization. We can also report that the band gap of graphene or h-BN can be tuned by implanting appropriate size of graphene sheet on an h-BN substrate, and vice- versa.

Thank you