Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for manuscript

Line Defects and Induced Doping Effects in Graphene, Hexagonal Boron Nitride and Hybrid BNC

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Table 1S: Structures, composition and abbreviated names of O-I and its BN-doped structures in two ***A*** and ***Z*** directions.

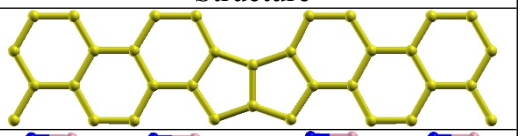
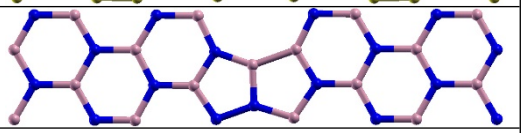
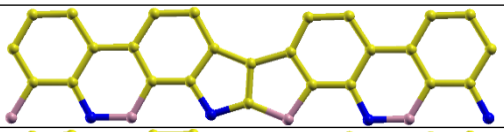
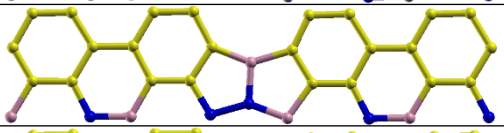
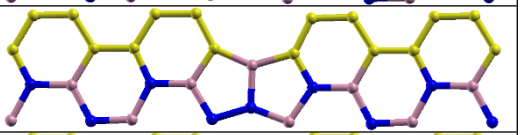
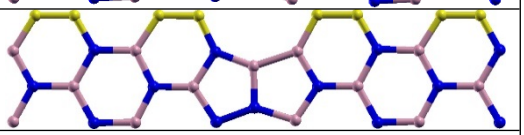
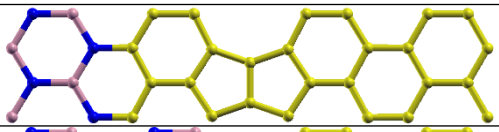
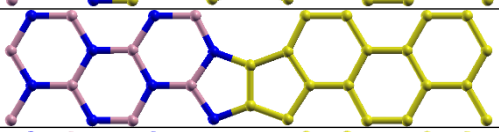
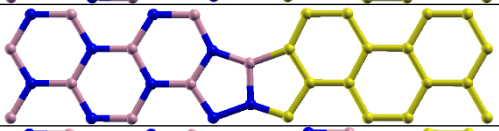
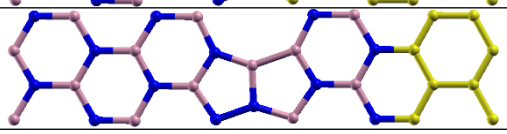
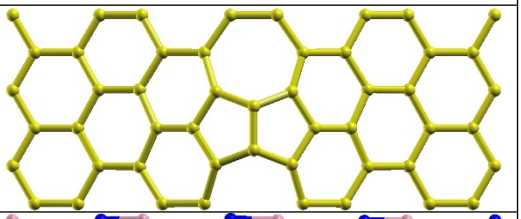
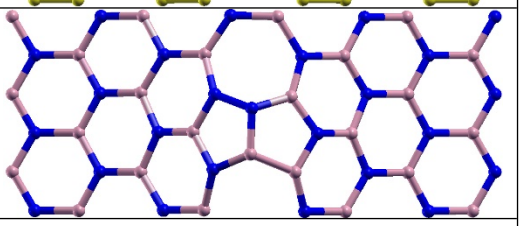
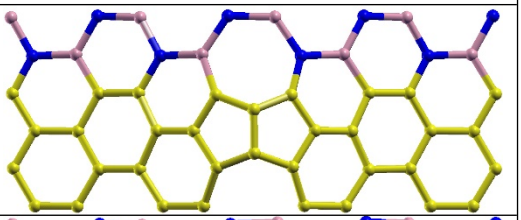
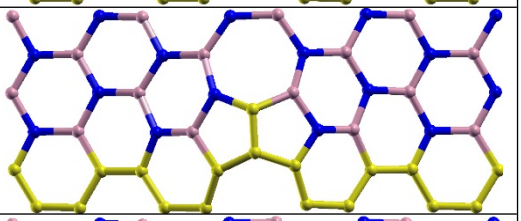
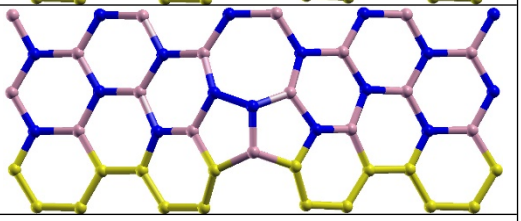
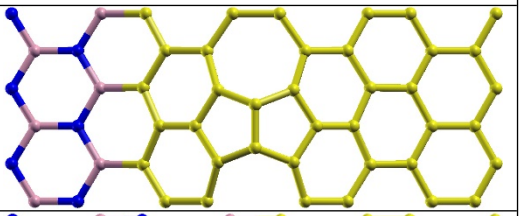
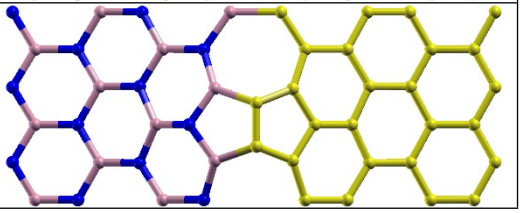
Name	Symbol for Names	Structure
G-585-ELD	O-I	
BN-585-ELD	O-II	
Doping of 585 ELD in ***A*** direction		
A-$B_4N_4C_{26}$-585-ELD	OA-I	
A-$B_5N_5C_{24}$-585-ELD	OA-II	
A-$B_9N_9C_{16}$-585-ELD	OA-III	
A-$B_{13}N_{13}C_8$-585-ELD	OA-IV	
Doping of 585 ELD in ***Z*** direction		
Z-$B_4N_4C_{26}$-585-ELD	OZ-I	
Z-$B_8N_8C_{18}$-585-ELD	OZ-II	
Z-$B_9N_9C_{16}$-585-ELD	OZ-III	
Z-$B_{13}N_{13}C_8$-585-ELD	OZ-IV	

Table 2S: Structures, composition and abbreviated names of H-I and its BN-doped structures in two ***A*** and ***Z*** directions.

Name	Symbol for Names	Structure
G-5775-ELD	H-I	
BN-5775-ELD	H-II	
Doping of 5775 ELD in ***A*** direction		
A-$B_8N_8C_{34}$-5775-ELD	HA-I	
A-$B_{16}N_{16}C_{18}$-5775-ELD	HA-II	
A-$B_{17}N_{17}C_{16}$-5775-ELD	HA-III	
Doping of 5775 ELD in ***Z*** direction		
Z-$B_6N_6C_{38}$-5775-ELD	HZ-I	
Z-$B_{12}N_{12}C_{26}$-5775-ELD	HZ-II	

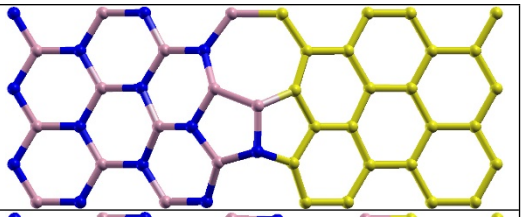
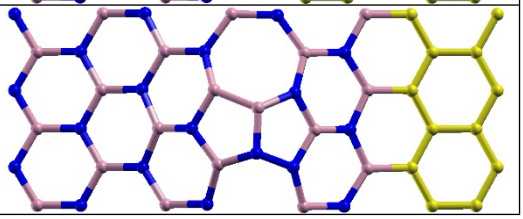
Z-$B_{13}N_{13}C_{24}$ -5775-ELD	HZ-III	
Z-$B_{19}N_{19}$ C_{12}-5775-ELD	HZ-IV	

Table 3S: Structures, composition and abbreviated names of G and its BN-doped structures in two ***A*** and ***Z*** directions (Counterpart of O-I and its BN-doped structures).

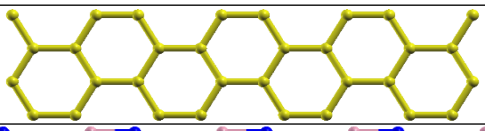
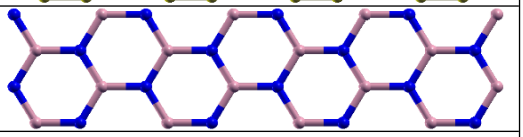
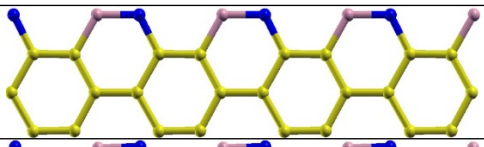
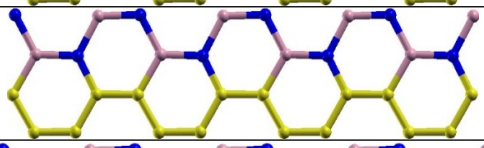
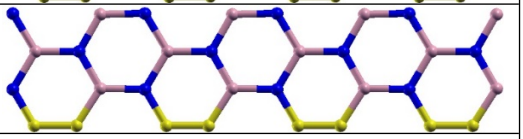
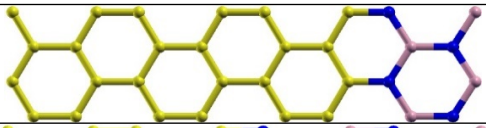
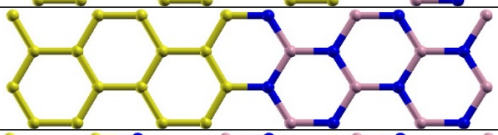
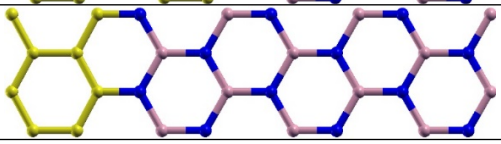
Name	Symbol for Names	Structure
G	PP0	
h-BN	PP1	
Doping of G in ***A*** direction		
A-$B_4N_4C_{24}$	PA-I	
A-$B_8N_8C_{16}$	PA-II	
A-$B_{12}N_{12}C_8$	PA-III	
Doping of G in ***Z*** direction		
Z-$B_4N_4C_{24}$	PZ-I	
Z-$B_8N_8C_{16}$	PZ-II	
Z-$B_{12}N_{12}C_8$	PZ-III	

Table 4S: Structures, composition and abbreviated names of G and its BN-doped structures in two ***A*** and ***Z*** directions (Counterpart of H-I and its BN-doped structures).

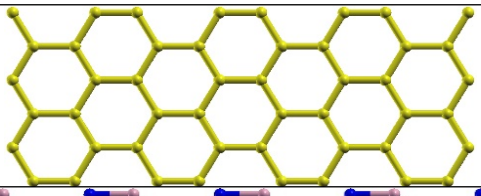
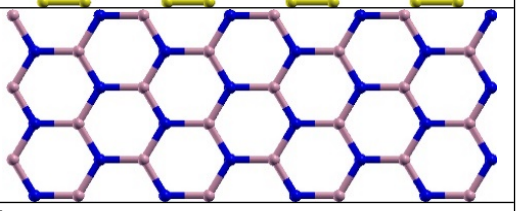
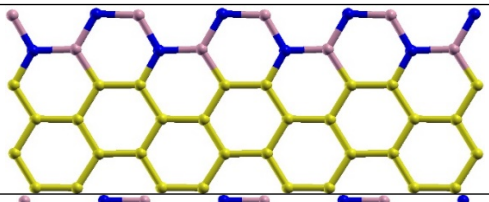
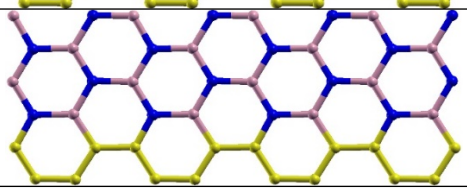
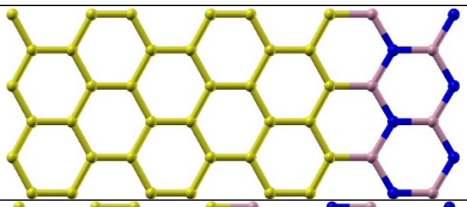
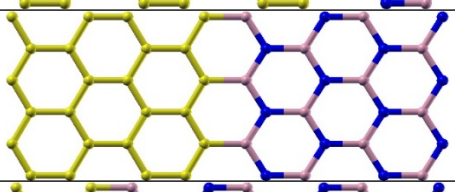
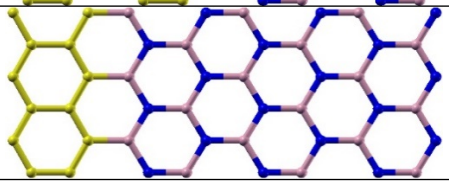
Name	Symbol for Names	Structure
G	PP0‘	
h-BN	PP1‘	
Doping of G in ***A*** direction		
A-$B_8N_8C_{32}$	PA-I‘	
A-$B_{16}N_{16}C_{16}$	PA-II‘	
Doping of G in ***Z*** direction		
Z-$B_6N_6C_{36}$	PZ-I‘	
Z-$B_{12}N_{12}C_{18}$	PZ-II‘	
Z-$B_{18}N_{18}C_{12}$	PZ-III‘	

Figure. 1S: Top and side views models of initial (a) and (d), relaxed (b) and (e) and full relaxed structures (c) and (f) of C_2 ad-dimmers linear adsorption on G sheet for embedded 585-ELD and 5775-ELD structures, respectively.

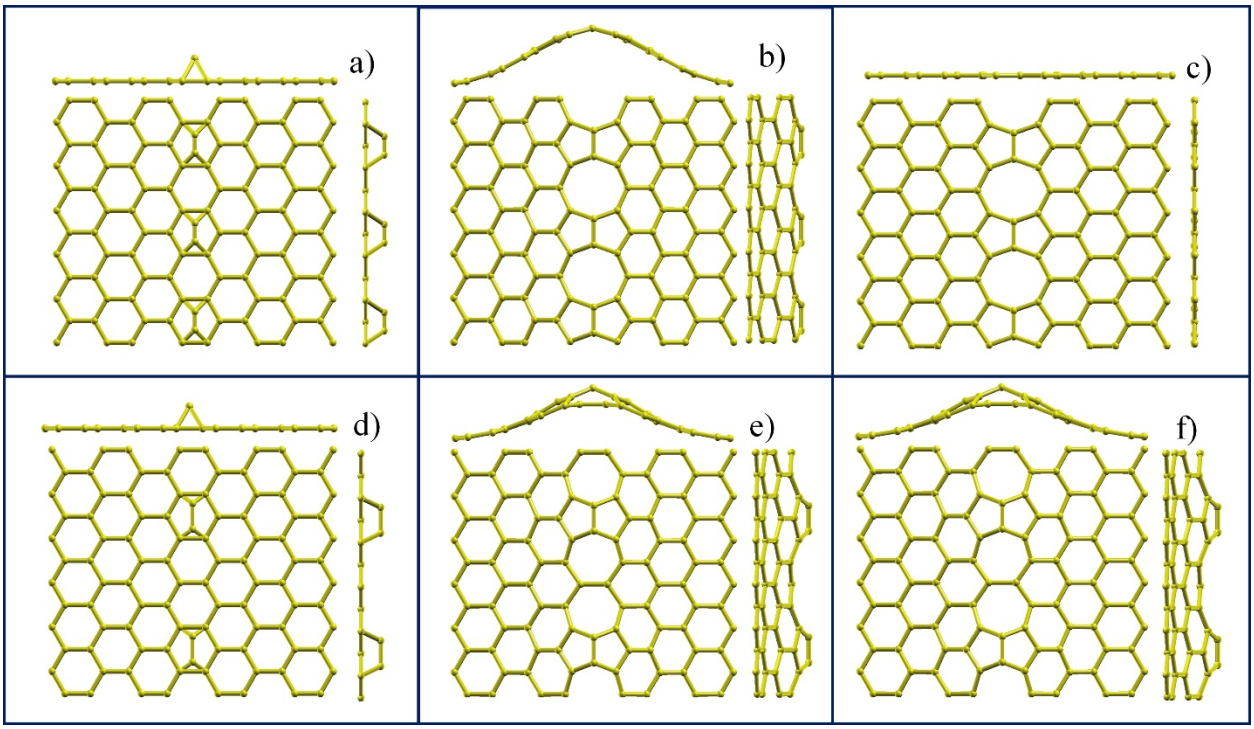


Figure. 2S: Unit cell of (a) 585 ELD along with rings label, ELD, ***A*** and ***Z*** directions, (b) 5775 ELD along with rings label, ELD, ***A*** and ***Z*** directions and (c) and (d) show zigzag N-edge and zigzag B-edge in both BN 585- and BN 5775-ELD structures (e) (L_c) . Length of the circumscribing ring 10.

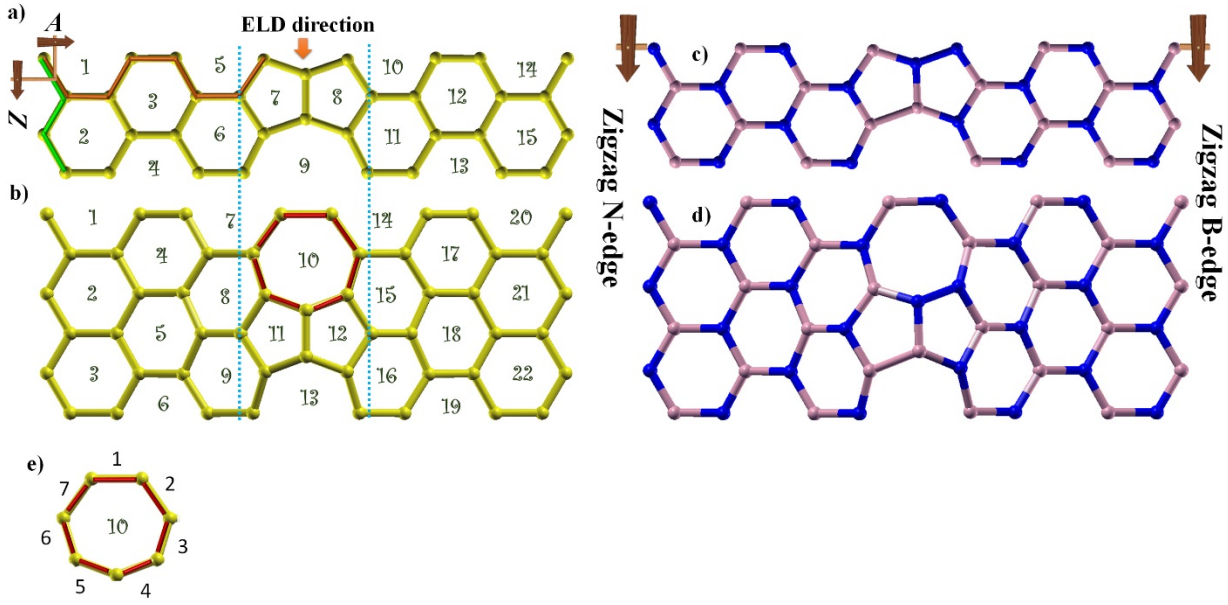


Figure. 3S: Electronic band structures of (a) G sheet along with VEBS and CEBS states and (b) *h*-BN sheet along with VEBS and CEBS states, total density of states for G sheet (projected density of state of 2p orbitals C atoms (inset)) (c) and (d) for *h*-BN sheet(projected density of state of 2p orbitals of B and N atoms (inset)), EPS plots mapped onto electron density values with isodensity values of 0.004 a.u. of (e) G sheet and (f) *h*-BN sheet.

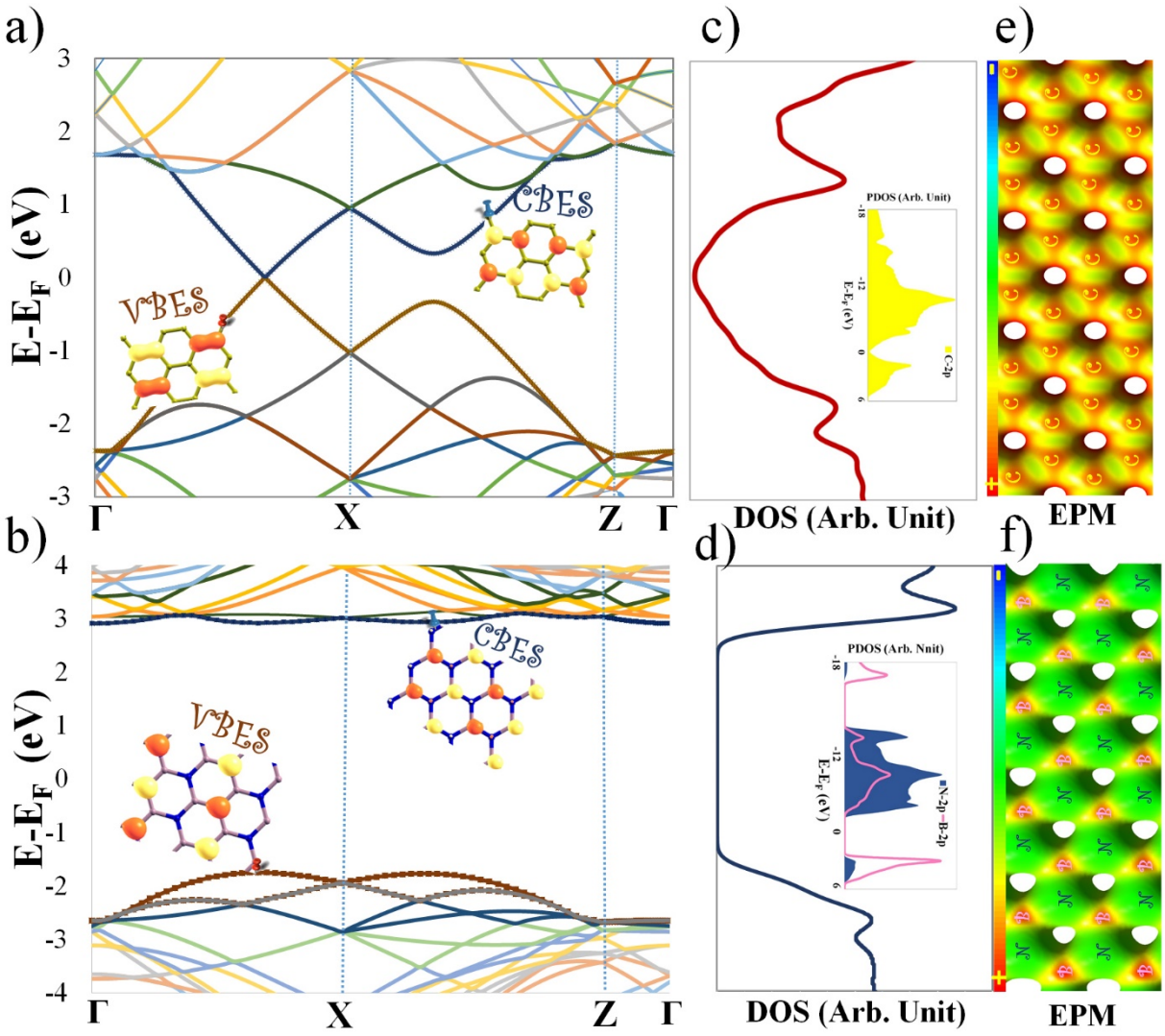


Figure. 4S: Conductance as a function of the energy (the Fermi energy E_F is set to zero) for the O-I and H-I structures.

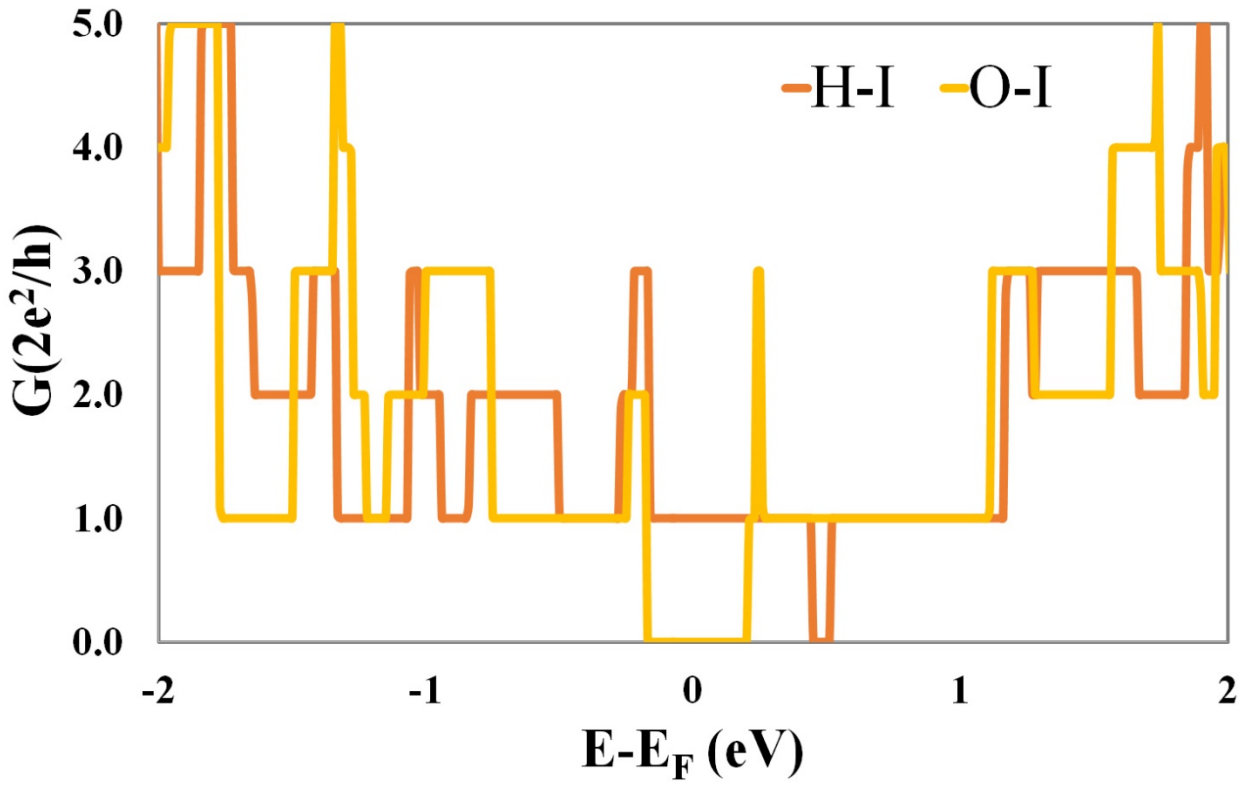


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Figure. 5S. Length of the circumscribing rings in (a) O-I and (b) H-I structures.

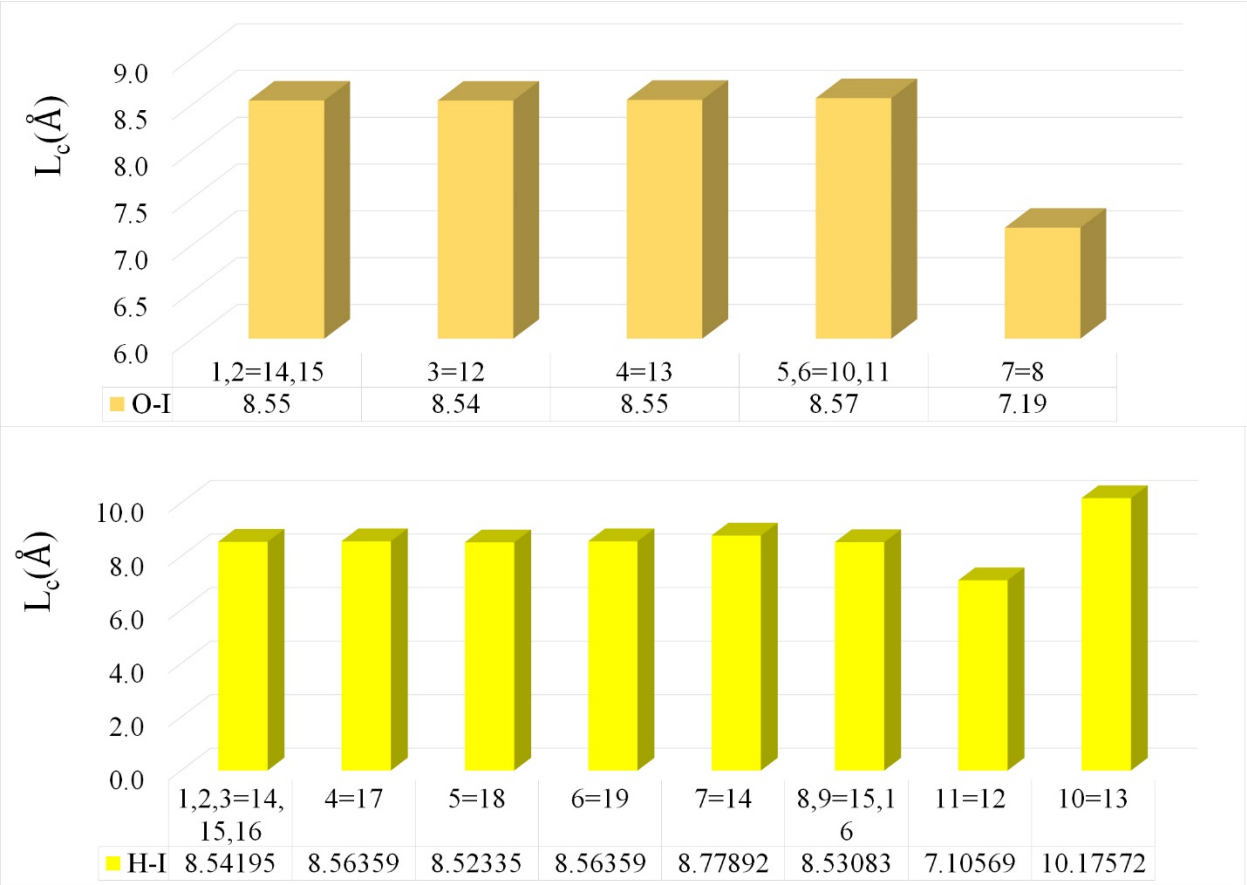

Figure 6S. Relative cohesive energy per atom with respect to pristine graphene sheet (Counterpart of O-I and its BN-doped structures), band gap and full relaxed unit cells of G sheet and its different BN-doped structures in two ***A*** and ***Z*** directions.

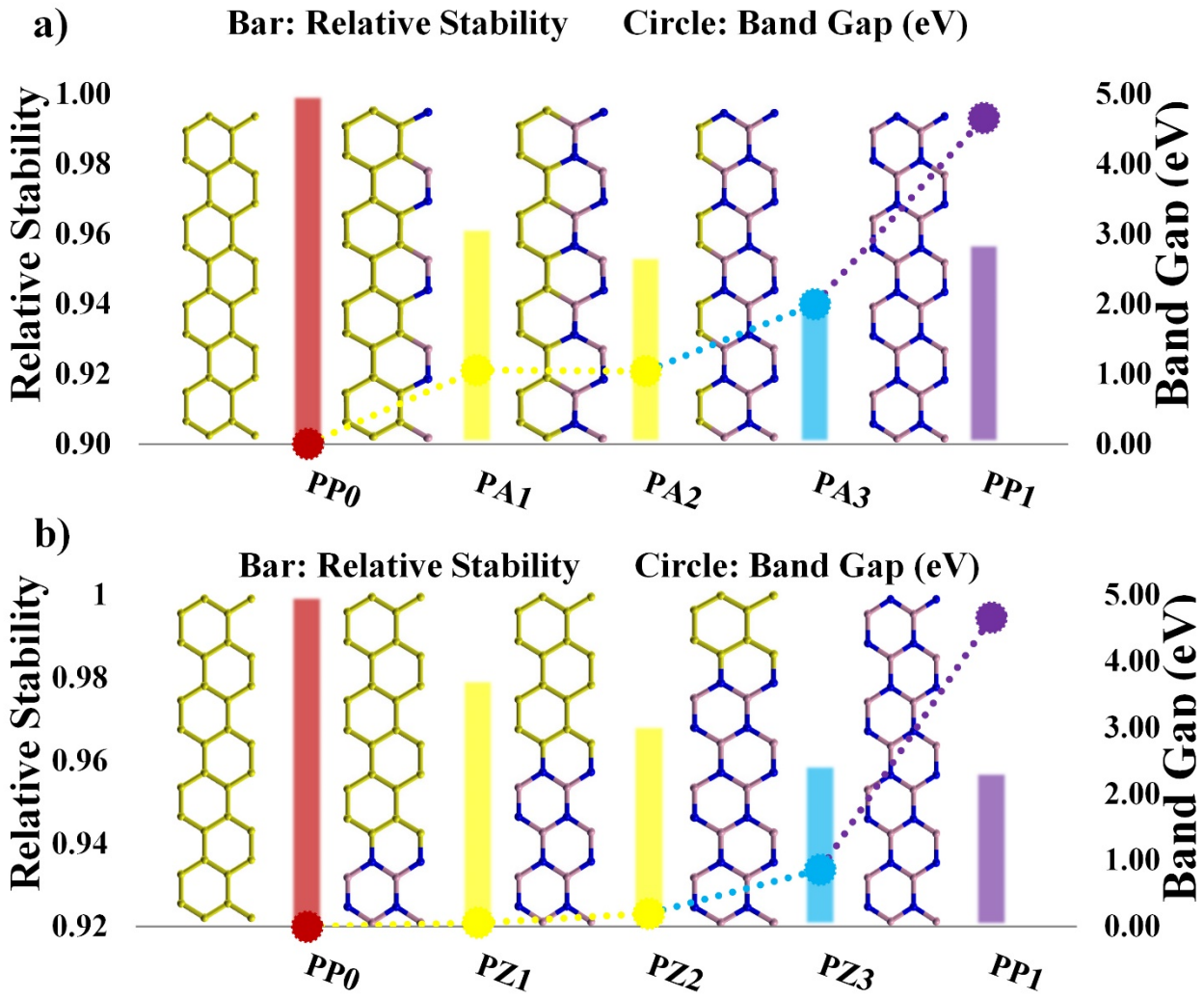

Figure 7S. Relative cohesive energy per atom with respect to pristine graphene sheet (Counterpart of H-I and its BN-doped structures), band gap and full relaxed unit cells of G sheet and its different BN-doped structures in two ***A*** and ***Z*** directions.