

Electronic Supporting Information

Sequential BN-doping Induced Tuning of Electronic Properties in Zigzag-edged Graphene Nanoribbons: A Computational Approach

Amrit Sarmah,^{a,*} Pavel Hobza^{a,b}

^aInstitute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo nam. 2, CZ-16610 Prague 6, Czech Republic

^bDepartment of Physical Chemistry, Palacky University, CZ-77146 Olomouc, Czech Republic

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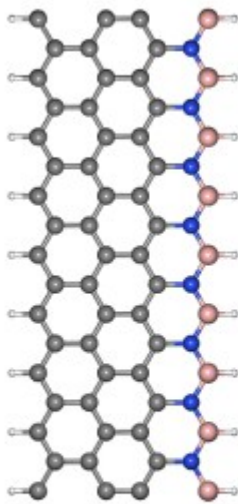
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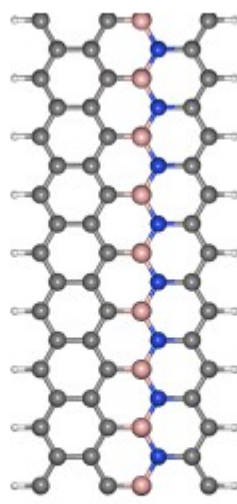
*Corresponding Author

E-mail Address: amrit.sarmah@marge.uochb.cas.cz (Amrit Sarmah)

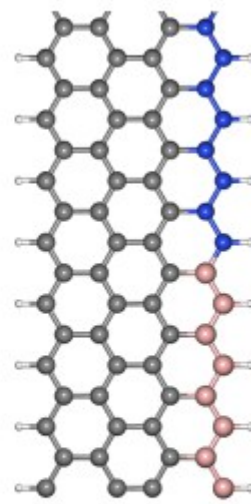
(a)



edge

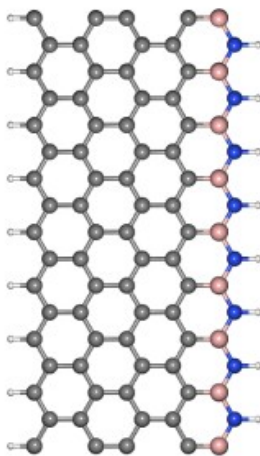


Off-edge

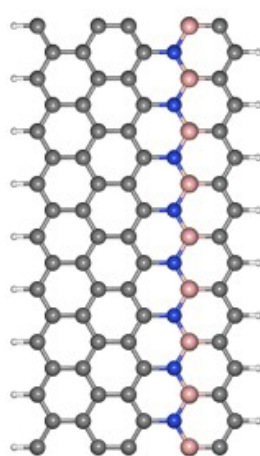


Half-half

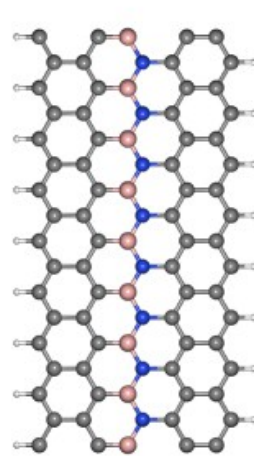
(b)



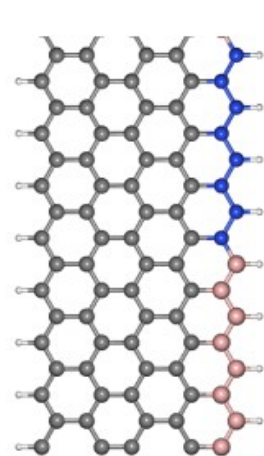
edge



Off-edge



center



Half-half

Fig. S1. The typical pictorial representation of the model 4 (a) and 5-ZGNR (b) systems and their corresponding doping pattern.

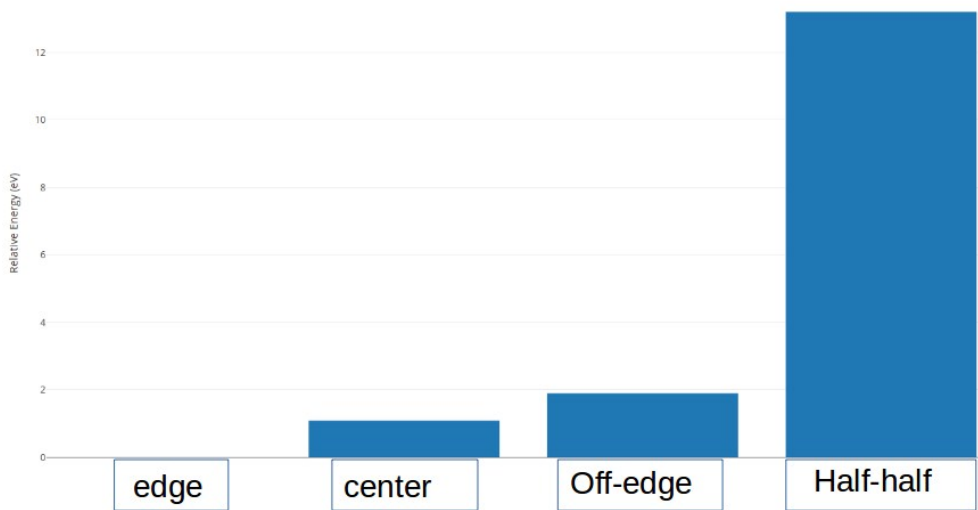


Fig. S2. A graphical representation of the relative energy values for four BN doped nanoribbon systems used in our present study. Here, the most stable system i.e., edge substituted ZGNR system is taken as the reference point and the other energies are plotted with respect to the reference system. Higher energy corresponds to lower stability.

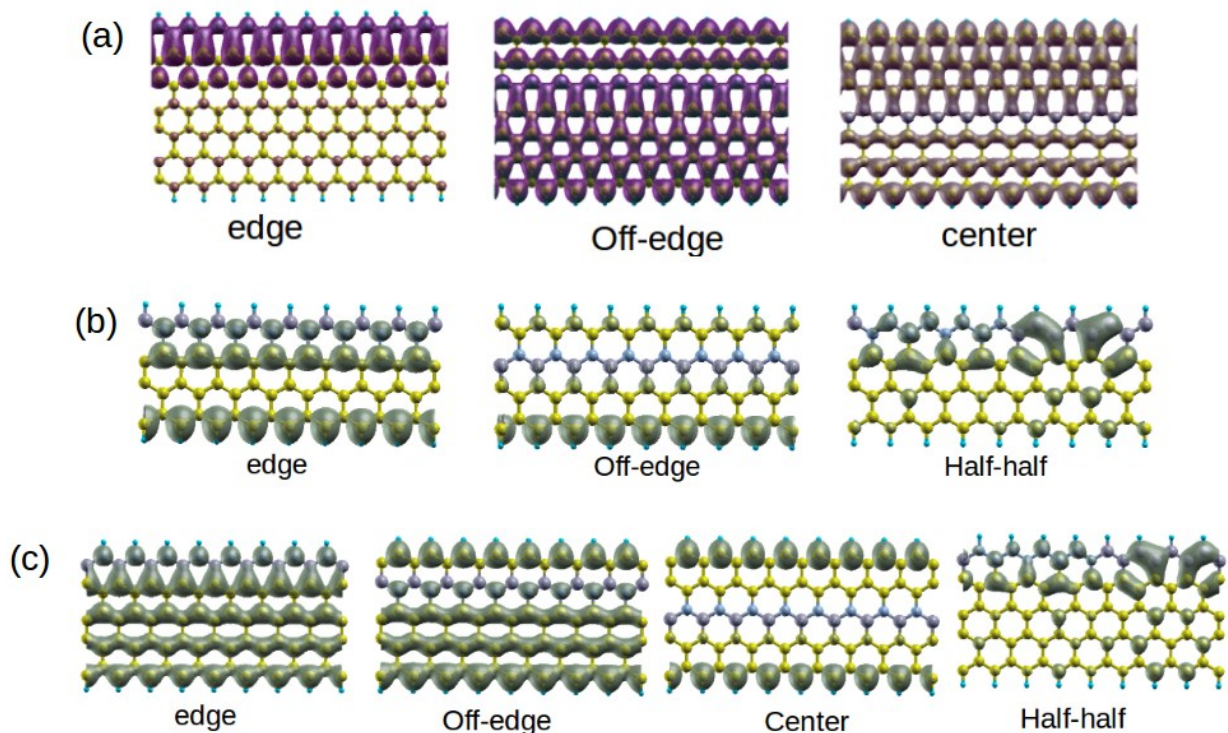
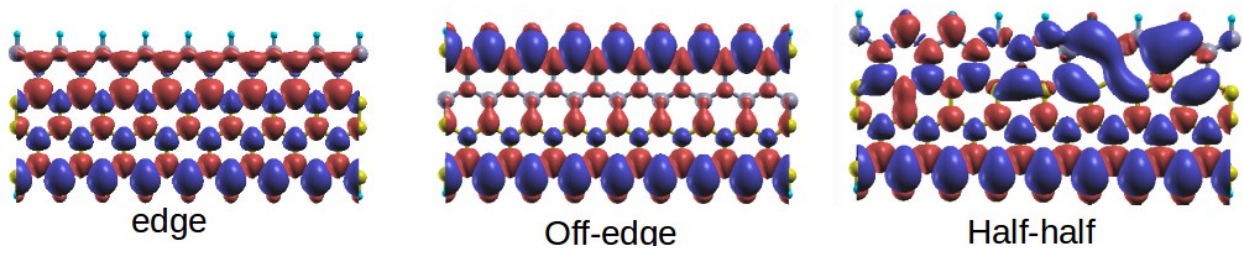


Fig. S3. The visual representation of the computed isosurface map for the distribution of local density of states (LDOS) for three BN-doped ZGNRs. (a) 4-ZGNR, (b) 5-ZGNR and (c) 7-ZGNR systems.

(a)



(b)

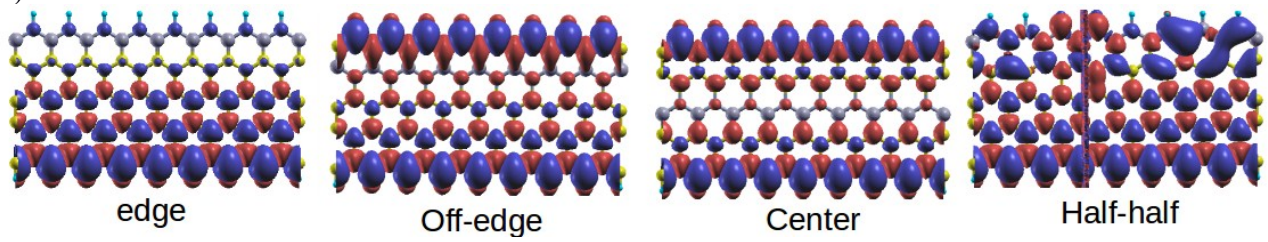


Fig. S4. The spin density distribution plots for the different BN-doped 4 (a) and 5-ZGNRs (b). The red and purple color regions in the plot represent the oppositely aligned excess spin densities.