IPM

School of Nano Science

IN THE NAME OF GOD

Iran University of Science and Technology

Effect of line and edge defects on β_{12}-borophene nanoribbons

By:

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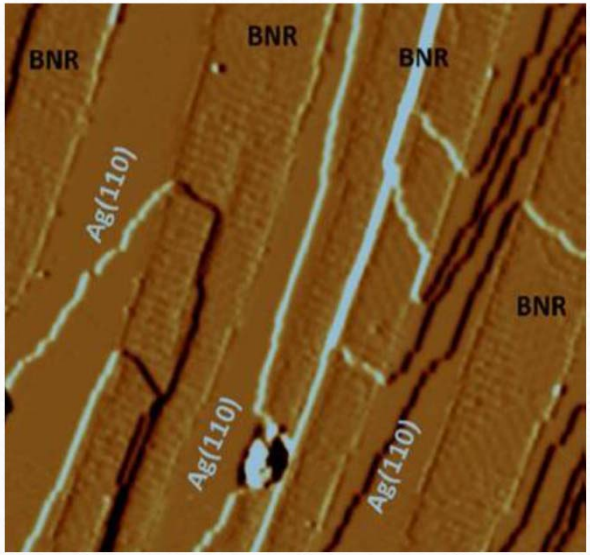
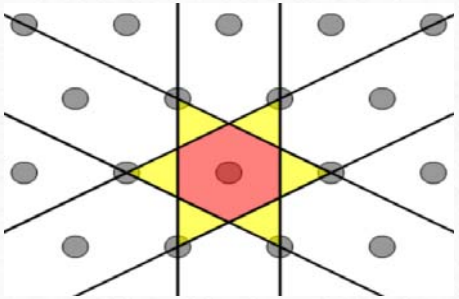
12 May 2022

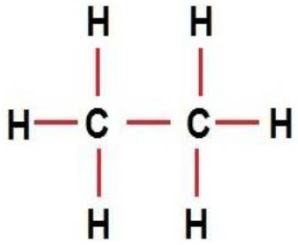
Introduction



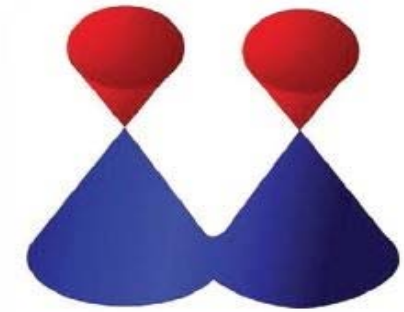
STM image of borophene nanoribbons on Ag (110) surface.



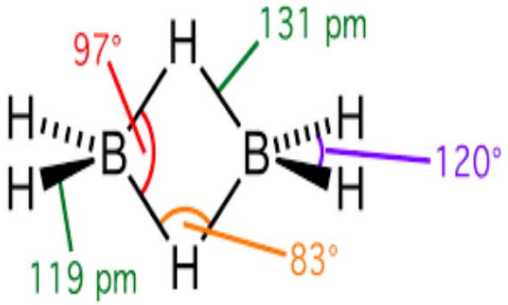
Dirac points in the Brillouin zone



Covalent band of C_2H_6



Dirac cones of borophene



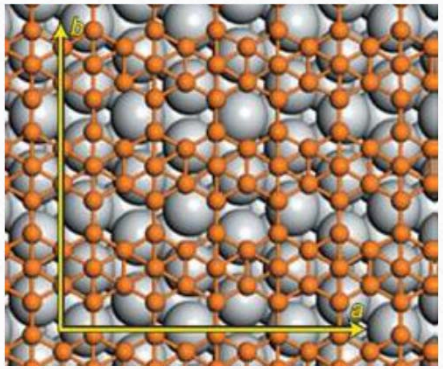
Banana band of B_2H_6

[1] B. Feng, J. Zhang, Q. Zhong, W. Li, S. Li, H. Li, P. Cheng, S. Meng, L. Chen, and K. Wu, Nat. Chem. **8**, 563.2016

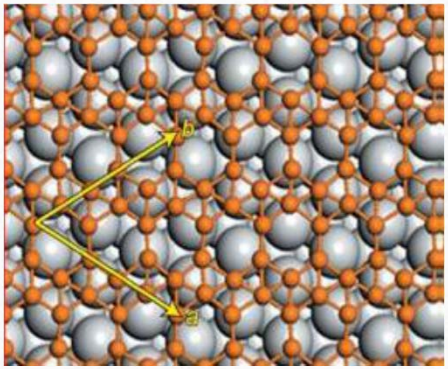
[2] Z.-Q.Wang, T.-Y. Lü, H.-Q.Wang, Y. P. Feng, and J.-C. Zheng, Front. Phys. **14**, 33403 (2019).

Different phases of borophene

Structures	Planar or buckling
δ_6	buckling
hr-sB	Planar
χ_3	Planar
β_{12}	Planar



β_{12}-borophene



χ_3- borophene

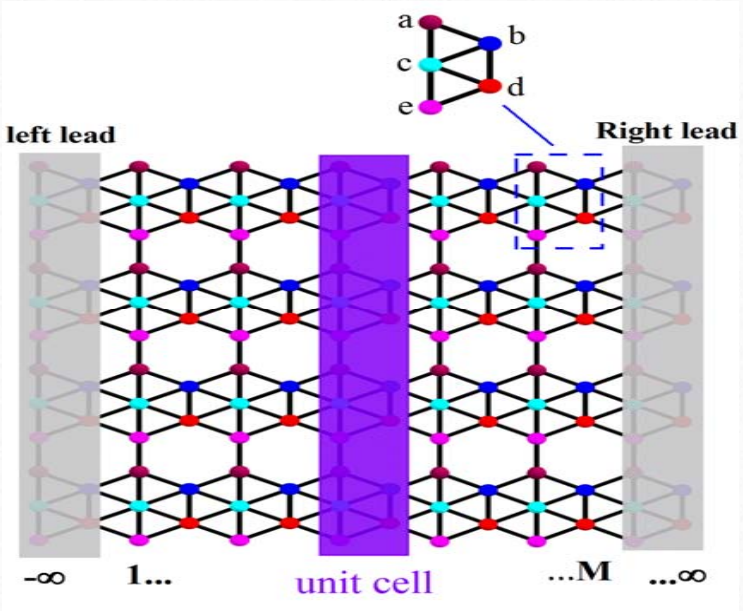
[3] H. Zhang *et al.*, "Dirac Nodal Lines and Tilted Semi-Dirac Cones Coexisting in a Striped Boron Sheet," *J. Phys. Chem. Lett.*, vol. 8, no. 8, pp. 1707–1713, 2017, doi: 10.1021/acs.jpclett.7b00452

Tight-binding Hamiltonian of β_{12}-borophene

پارامتر جهش	$t_{ab} = t_{de}$	$t_{ac} = t_{ce}$	$t_{bc} = t_{cd}$	t_{bd}	t_{ae}
مقدار	-2.04 eV	-1.79 eV	-1.84 eV	-1.91 eV	-2.12 eV
آنسایت انرژی	ε_a	ε_b	ε_c	ε_d	ε_e
مقدار	0.196 eV	-0.058 eV	-0.845 eV	0.196 eV	-0.058 eV
نحوه اعمال ولتاژ	+V	+V	0	-V	-V

Table of different parameters of β_{12}-borophene

$$H=-t\sum_{<i,j>\alpha} c^{\dagger}_{i\alpha}c_{j\alpha}+\sum_{i,\alpha} c^{\dagger}_{i\alpha}(\varepsilon_i+V_i)c_{i\alpha}+H.c.$$



Schematic illustration of a zigzag BNR. The primitive cell indicated by dashed blue rectangle contains five atoms with labels b, d, a, c and e which are colored by blue, red, wine, turquoise and magenta.

[4]C.-C. Liu, H. Jiang, and Y. Yao, Phys. Rev. B 84, 195430 (2011).

Non-equilibrium Green's function

$$G(E) = \frac{e^2}{h} Tr[\Gamma_L(E) g(E) \Gamma_R(E) (g(E))^{\dagger}]$$

$$\Gamma_{LR}(E) = i(\Sigma_{LR} - (\Sigma_{LR})^{\dagger}$$

$$\Sigma_{LR} = H_{01}^{\dagger} g_{00} H_{01}$$

$$(E^{+} - H_{00}) g_{00} = I + H_{-10}^{\dagger} g_{-10}$$

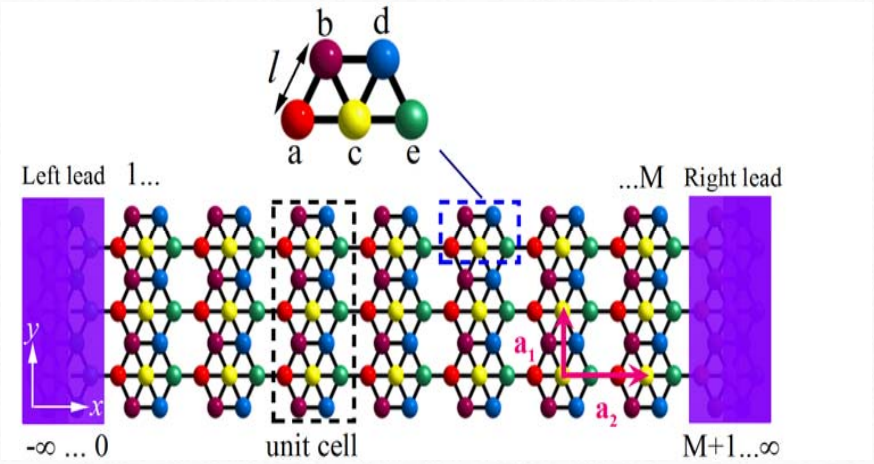
$$(E^{+} - H_{00}) g_{-l0} = H_{-10}^{\dagger} g_{-l-1,0} + H_{-10} g_{-l+1,0}$$

$$g_{00} = \Lambda g_{-10}$$

$$g_{00}(E) = \left[E^{\dagger}\mathbf{I} - H_{00} - H_{-10}^{\dagger}\ \Lambda\right]^{-1}$$

$$g_{l+1,0}(E) = \left[E^{\dagger}\mathbf{I} - H_{l,l} - H_{l,l+1}^{\dagger} g_{l,0} H_{l,l+1}\right]^{-1}$$

$$J_{m \to n}(E) = \frac{4e}{h} Im\,[H_{mn} G_{mn}]$$

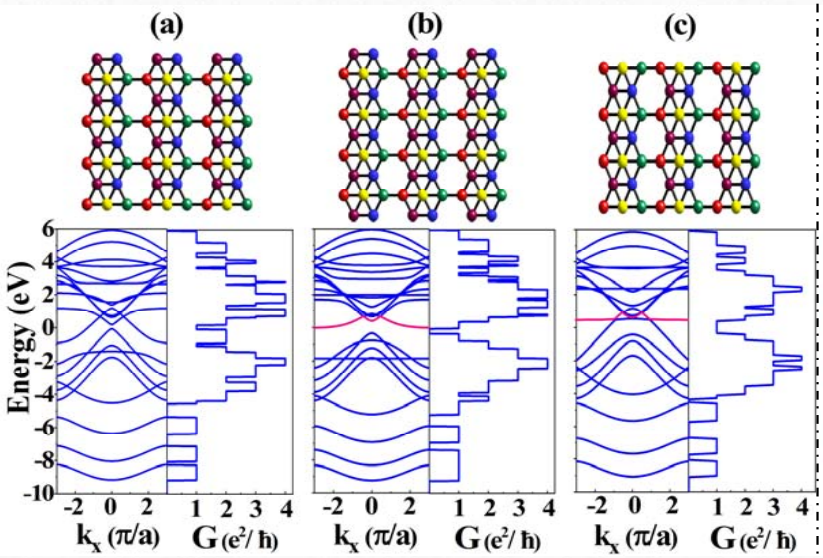


Schematic illustration of an armchair BNR. The primitive cell indicated by dashed blue rectangle contains five atoms with labels b, d, a, c and e which are colored by purple, blue, red, yellow and green, respectively.

[5] F. Norouzi *et al.*, "Controllable spin filtering and half-metallicity in β 12-borophene nanoribbons." *Phys. Rev. B.*, **104**(24) (2021), 245431.

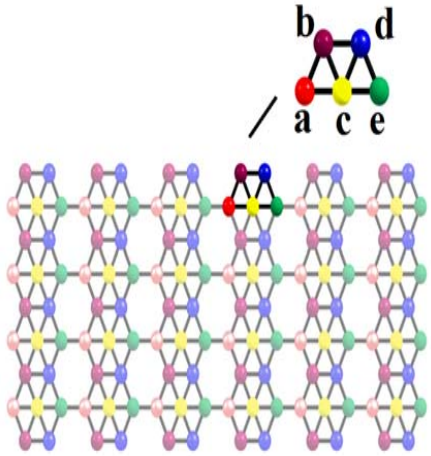
Results and Discussion

Effects of different edge shapes in ABNR

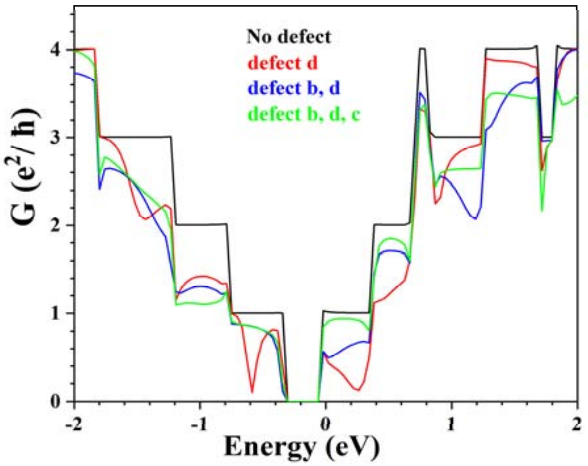


Top view of the atomic conjurations (upper) and the band structure and conductance for BNRs with different edge shapes (a) AF(b) AA and (c) FF edges. There are a at band near the Fermi (zero) energy for AA edges and a quasi at band for FF edges indicated by pink color.

Effects of edge defects in ABNR (armchair borophene nanoribbon)



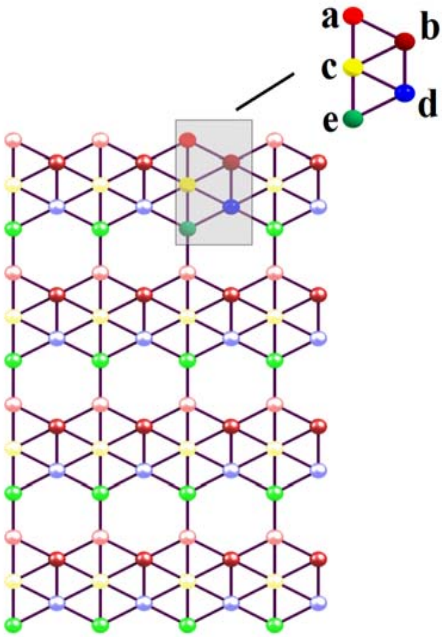
Schematic illustration of an armchair BNR.



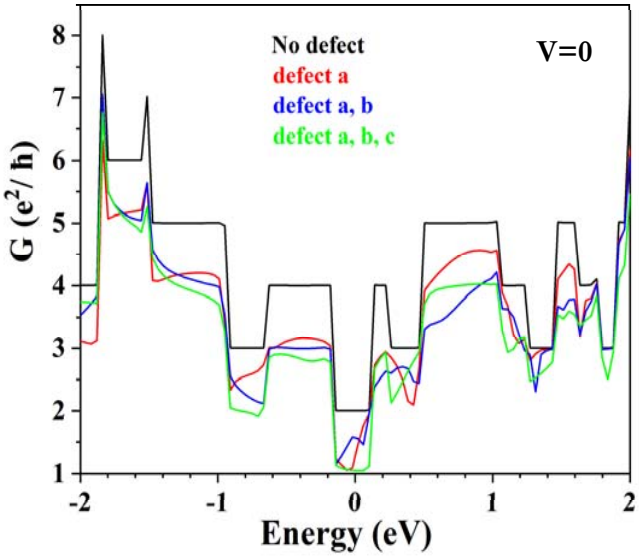
Charge conductance for a 22-ABNR in the Presence of different edge defects.

F. Norouzi *et al.*, "Controllable spin filtering and half-metallicity in β12-borophene nanoribbons." *Phys. Rev. B.*, **104**(24) (2021), 245431.

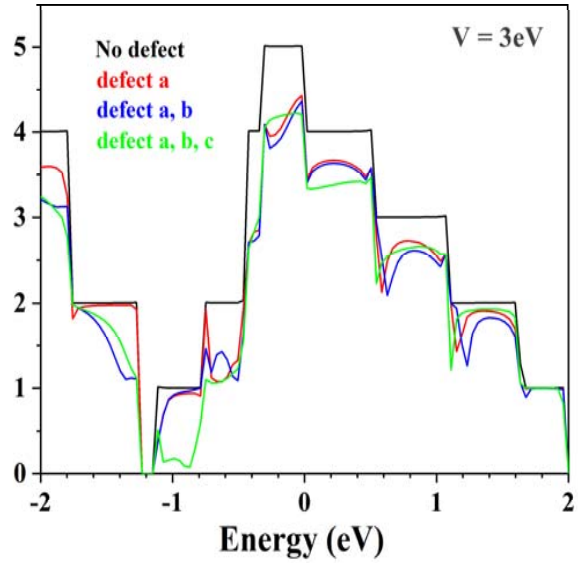
The edge defects in the presence of perpendicular electric field in ZBNR



Schematic illustration of a zigzag BNR.



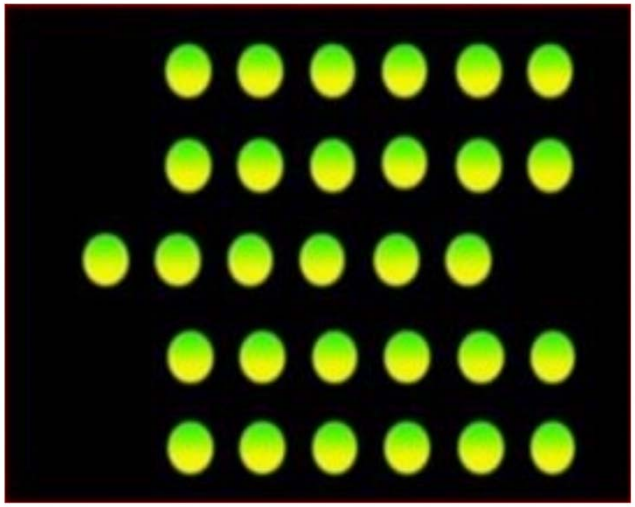
Charge conductance for a 20-ZBNR in the presence of different edge defects.



Charge conductance for a 20-ZBNR in the presence of different edge defects and perpendicular electric field.

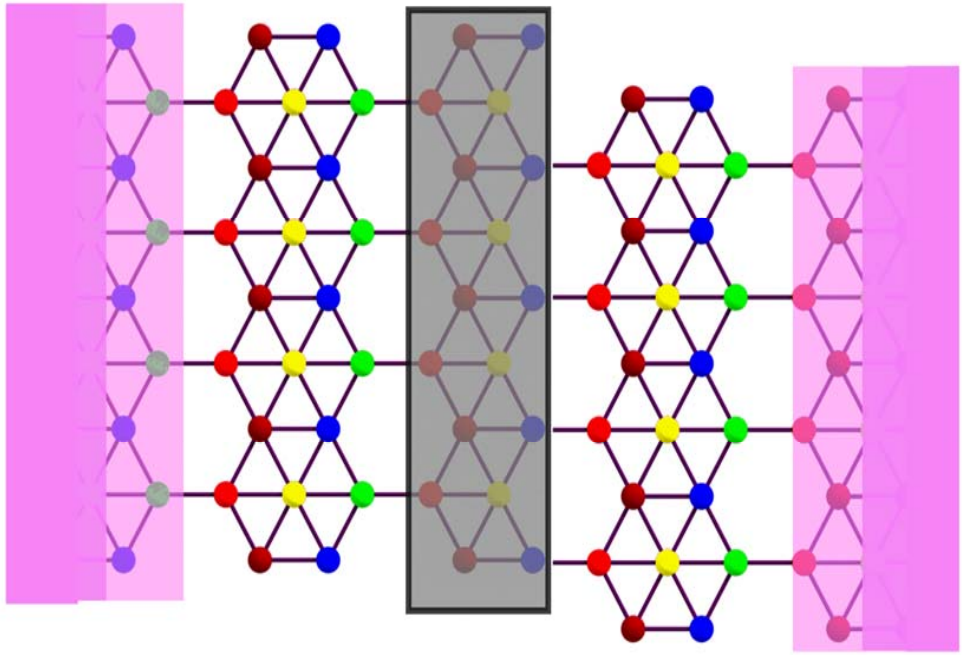
Line defects

When defects are formed in atomic arrangement along the line by displacement of group of atoms called line defects or dislocation.

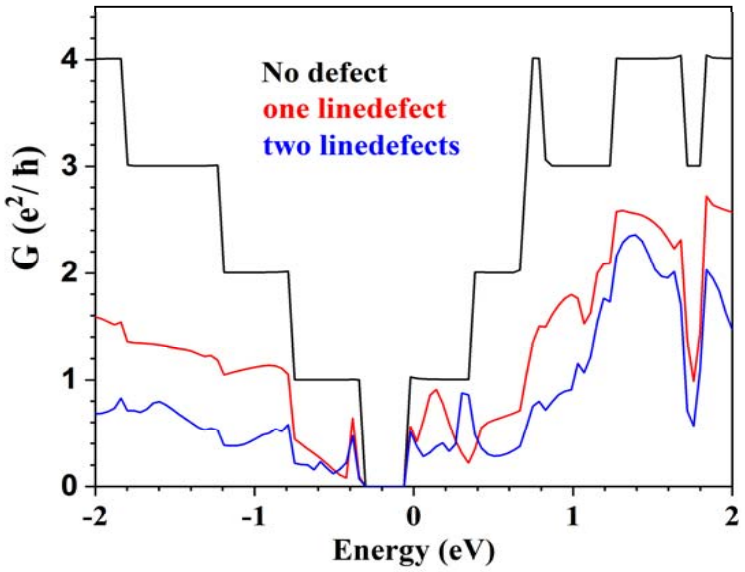


Line defects in solids

Effects of line defects in ABNRs

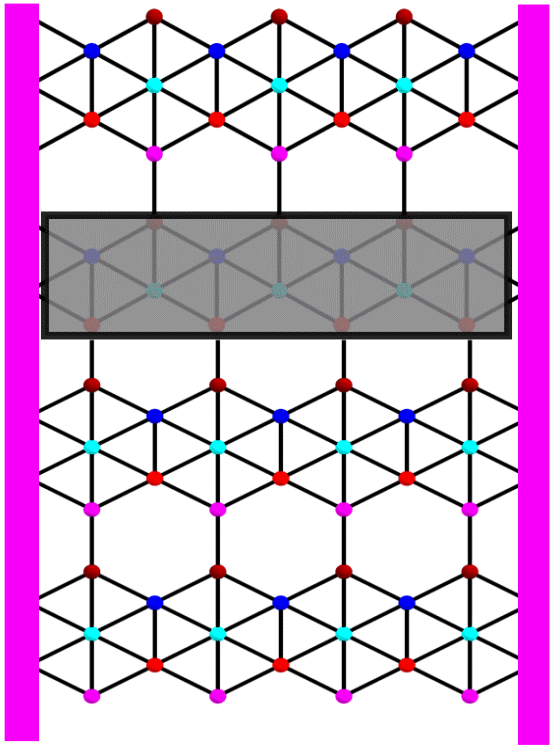


Schematic illustration of an ABNR in the presence of line defects.

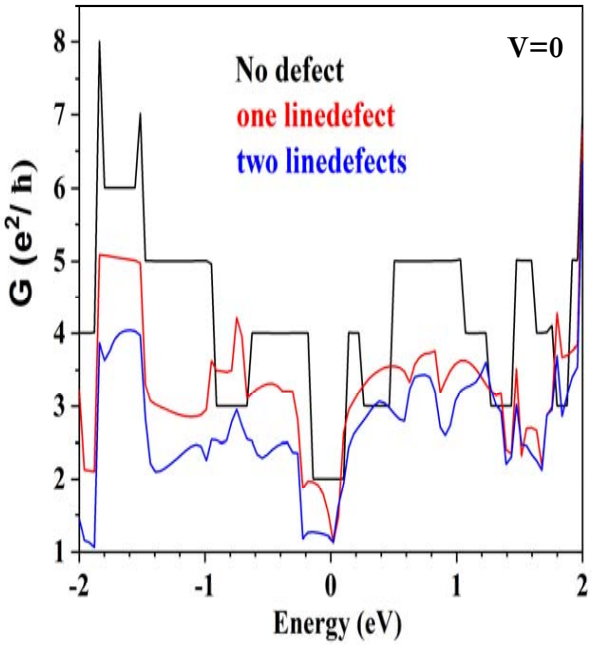


Charge conductance for an ABNR in the presence of different line defects.

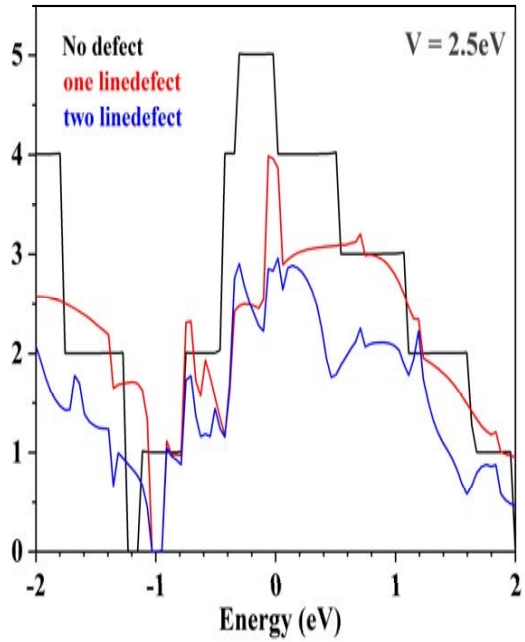
Effects of line defects in the presence of perpendicular electric field in ZBNR



Schematic illustration of a ZBNR in the presence of line defects.

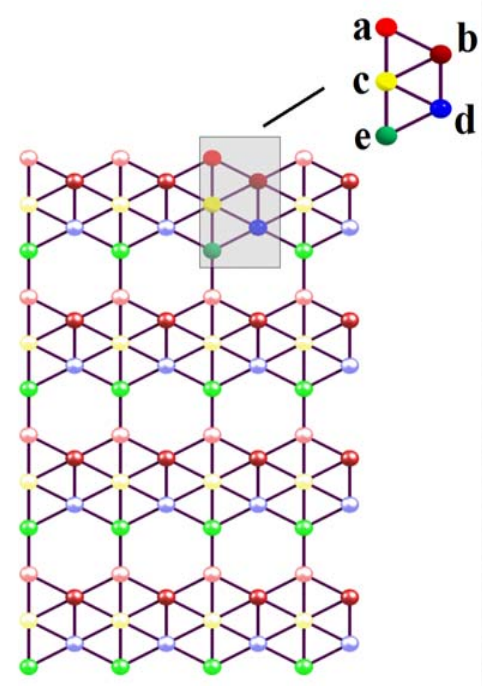


Charge conductance for a ZBNR in the presence of different line defects.

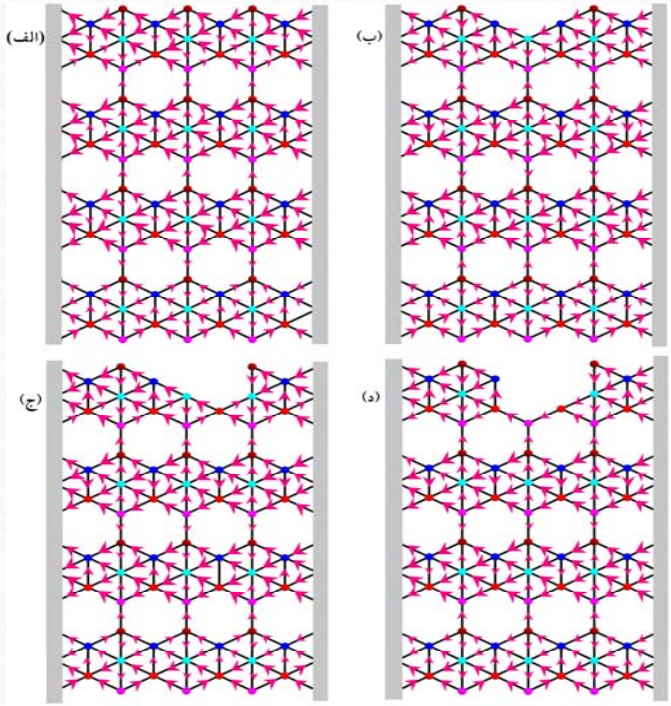


Charge conductance for a ZBNR in the presence of different line defects and perpendicular electric field.

Local currents density in ZBNR in the presence of different edge defects

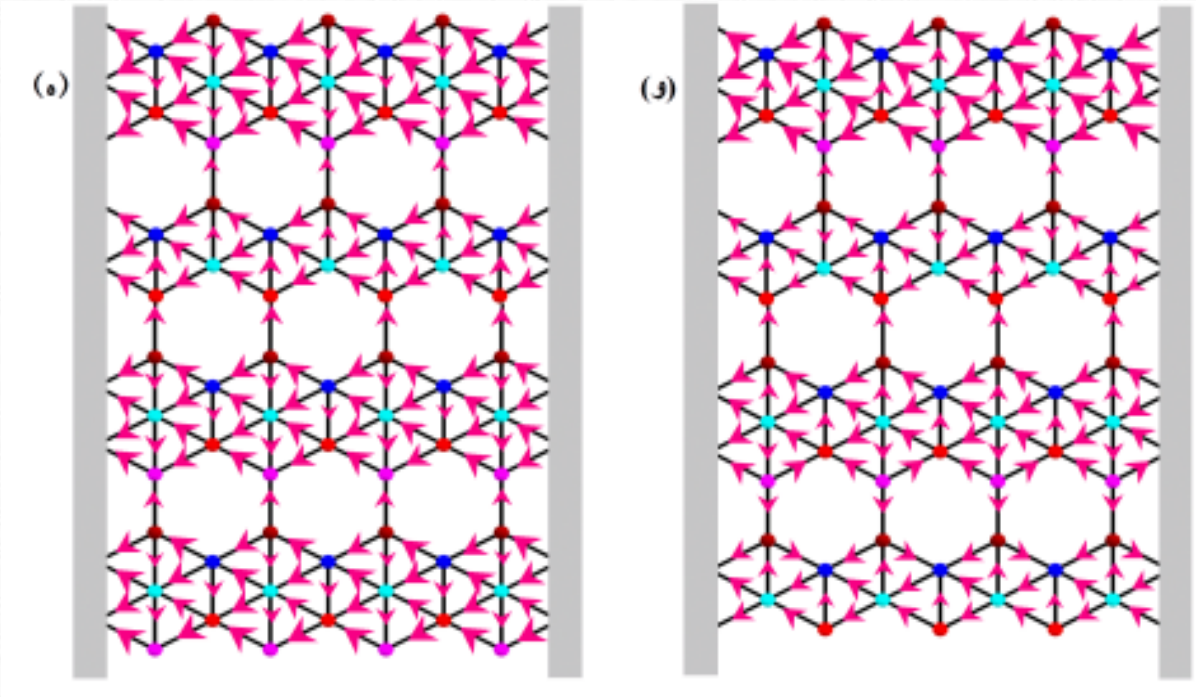


Schematic illustration of a ZBNR.



Local current distribution for a ZBNR in the presence of different edge defects.

Local currents density in the presences of one and two line defects in ZBNR



Local current distribution for a ZBNR in the presence of different line defects.

Conclusion

- ✓ The electronic properties of BNRs greatly depend on their edge structure. Here, ABNRs are semiconductor while BNRs with other edges are metal. For larger widths (i.e., N>27 atoms) all BNRs are metal.
- ✓ The band gap of ABNRs in the presence of line and edge defects remains unchanged and they do not lead to quasi-localized states.
- ✓ The conductance of ZBNRs in the presence of line and edge defects dramatically reduces so that applying a perpendicular electrical field can be lead to a transition from metal to semiconductor.
- ✓ The magnitude of the perpendicular electric field required for this transition in the presence of line defects for ZBNRs decreases.
- ✓ The local current density near the various edge defects decreases so that its amount for three-atom vacancy because of breaking the inversion symmetry of atoms in the honeycomb lattice is larger.
- ✓ The local current density passing through the line defects is smaller than other paths.

THANKS FOR YOUR ATTENTION