OCTAGONAL DEFECT LINES IN GRAPHENE STRUCTURES

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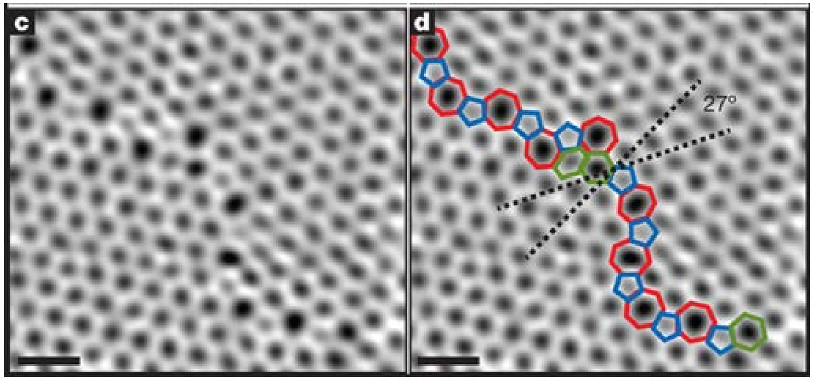
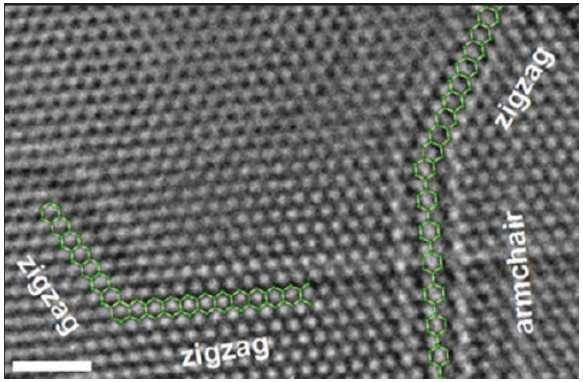
topological **pentagon/heptagon** defects

- junctions between zigzag/armchair ribbons and grain boundaries

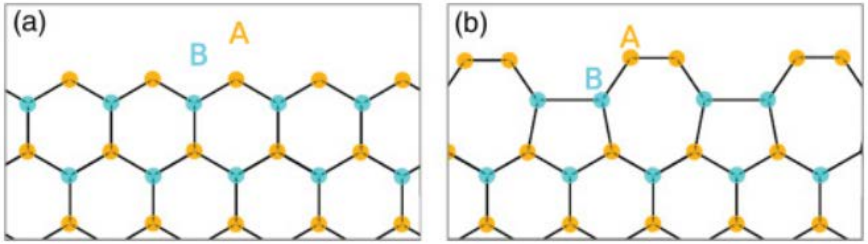


X.T. Xia,, et. al.,
Science 323, 1701, 2009

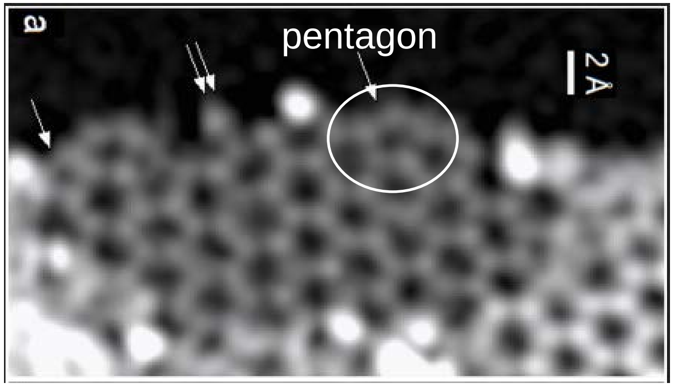


P.Y. Huang, at. al..,
Nature 469, 389, 2011)

- edge reconstructions in graphene nanoribbons



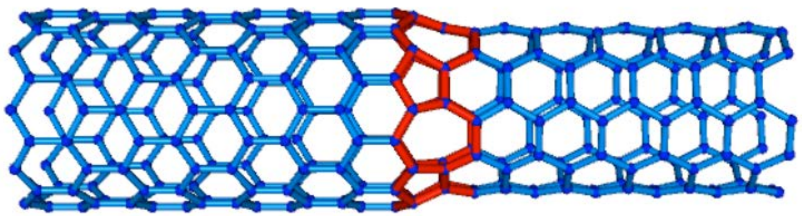
J. Rodriguezs, et. al.,
Phys. Rev. B 84, 155435, 2011



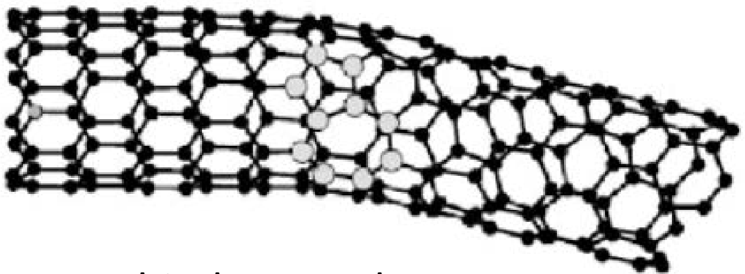
O.L. krivanek et.al.
Ultramicroscopy, 110, 935, 2010

topological **pentagon/heptagon** defects

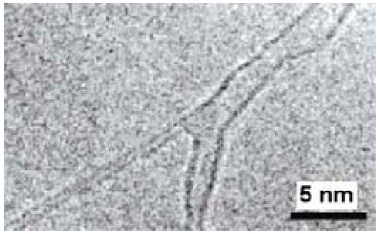
- junctions between carbon nanotubes

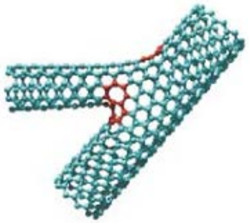


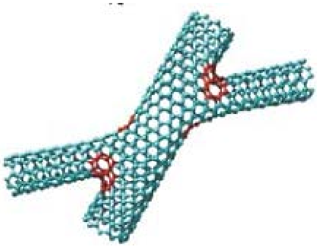
zigzag (2n,0) – armchair (n,n); **n** pairs 5/7



chiral nanotubes





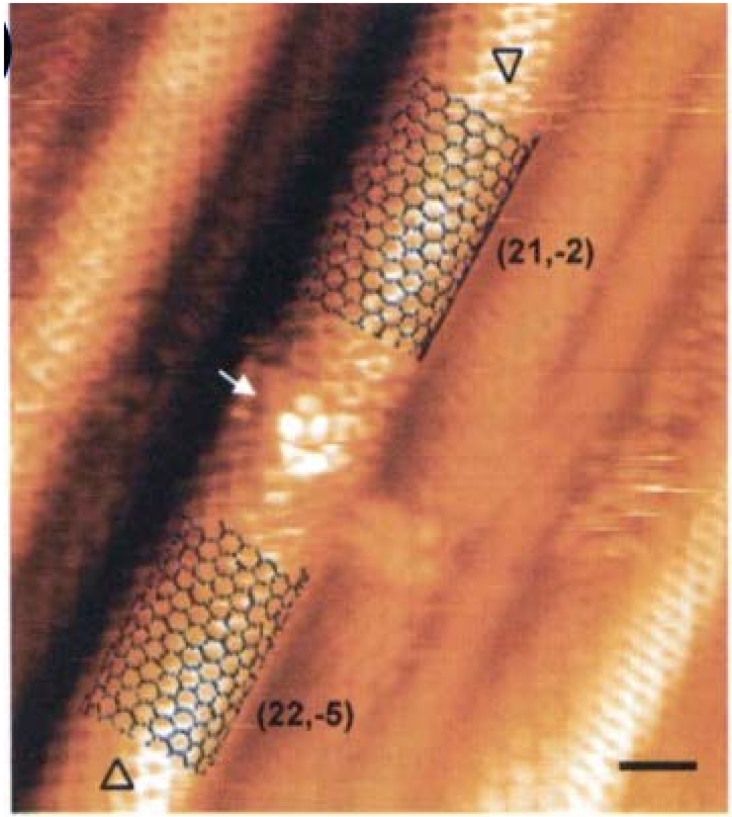


M. Terrones et al.
Phys. Rev. Lett. 2002

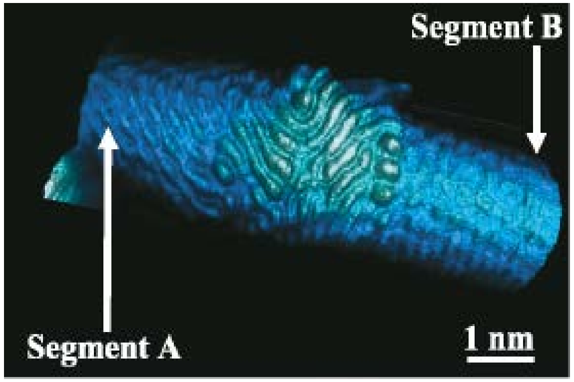
branchings

Interface localized states

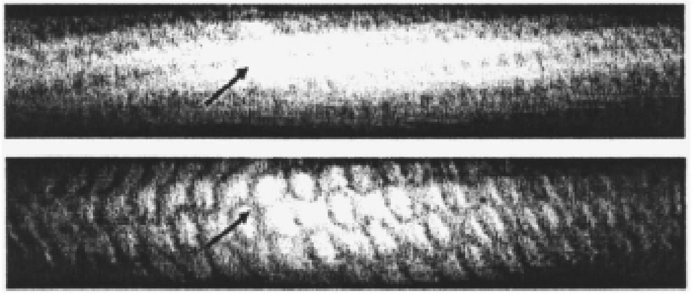
rolled up gtaphene junctions



M. Ouyang, et. al.,
Science 291, 97, 2001



Ishigami et. al.
Phys Rev Lett 93, 196803, 2004c



Kim et .al
Phys Rev B 71, 235402, 2005

For a long time it has been commonly assumed that
interface localized states (ILS) are due to topological defects …

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interface localized states (ILS) are due to topological defects …

2009

H. Santos, A. Ayuela, WJ, L. Chico, and M. Pelc
Phys. Rev. B 80, 035436

we have shown that ILS are due to zigzag parts of the edges of the joined tubes (structures)

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2011

WJ, A. Ayuela, M. Pelc, H. Santos, and L. Chico
Phys. Rev. B 83, 235424

we have introduced simple rules and diagrams allowing to determine (foresee) the existence, localization and degeneracy of edge-localized states at Fermi level for any shape of the graphene edge

PHYSICAL REVIEW B 83, 235424 (2011)

Edge states and flat bands in graphene nanoribbons with arbitrary geometries

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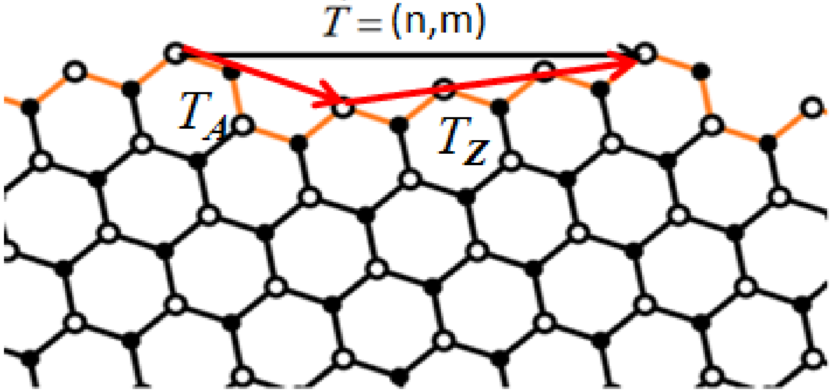
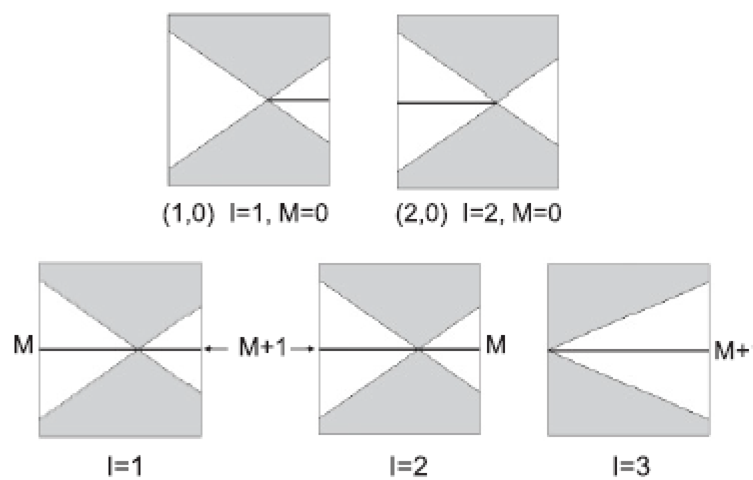
[1]Instytut Fizyki UMK, Grudziądzka 5, PL-87-100 Toruń, Poland
[2]Centro de Física de Materiales CFM-CPM CSIC-UPV/EHU, Departamento de Física de Materiales (Facultad de Química, UPV) and Donostia International Physics Center, ES-20080 San Sebastián/Donostia, Spain
[3]Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, ES-28049 Madrid, Spain
(Received 19 January 2011; published 29 June 2011)



$T_A=(m,m)$, $T_Z=(n-m,0)$

PHYSICAL REVIEW B 83, 235424 (2011)



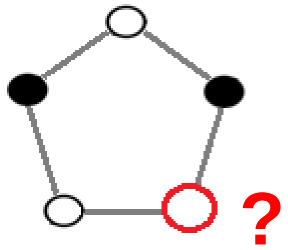
$$n-m = l + 3M$$

The fundamental condition for the existence of localized states (flat bands) at Fermi energy

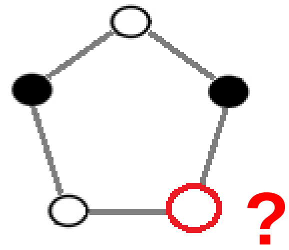
(at least in tight-binding approach)

is

localization of the wavefunction at one sublattice only

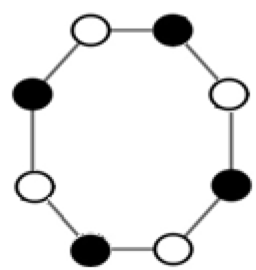


Pentagon, heptagon defects mix strongly graphene sublattices
-usually they cannot localize states exactly at Fermi level



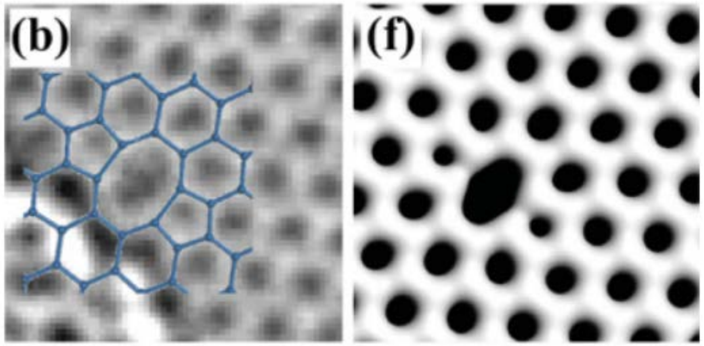
Pentagon, heptagon defects mix strongly graphene sublattices
-usually they cannot localize states exactly at Fermi level

in contrast, octagonal defects need not to mix sublattices
-they can yield localized states at E_F

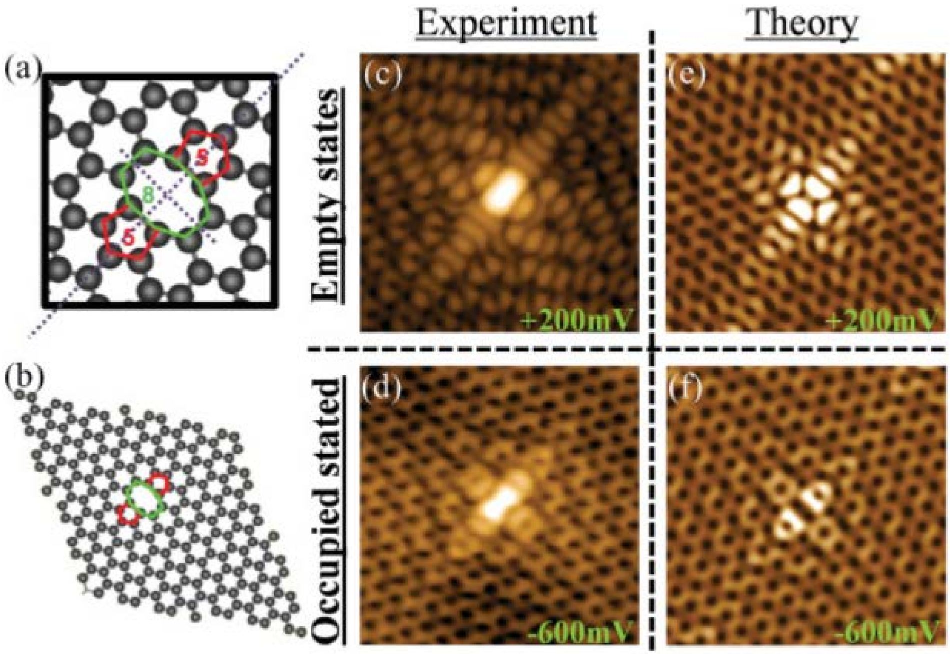


Octagonal defects

divacancies



Y. Kim, et. al.,
Phys. Rev. B 84, 2011

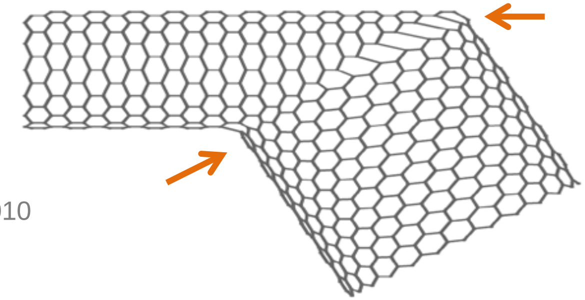


M.M. Ugeda, et. al., Phys. Rev. B 85, 2012

Octagonal defects

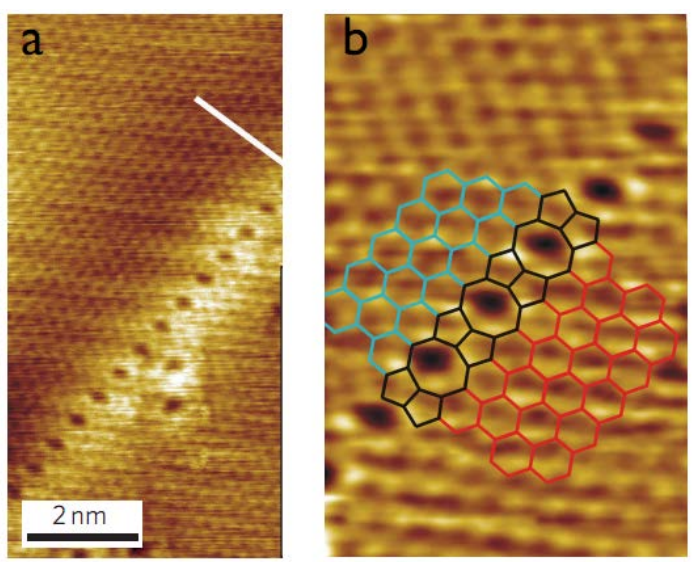
(strongly) curved systems

diagonal junctions between CNs



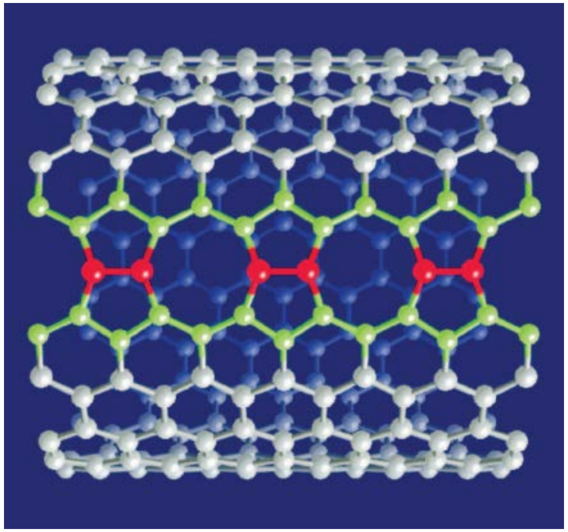
W. Jaskolski, et. al.,
phys. stat. sol. C7, 2010

line defects in graphene



J. Lahiri et. al., Nature nanotech. 5, 2010

line defects in carbon tubes



S. Okada, et. al., Phys. Rev. B 74, 2006

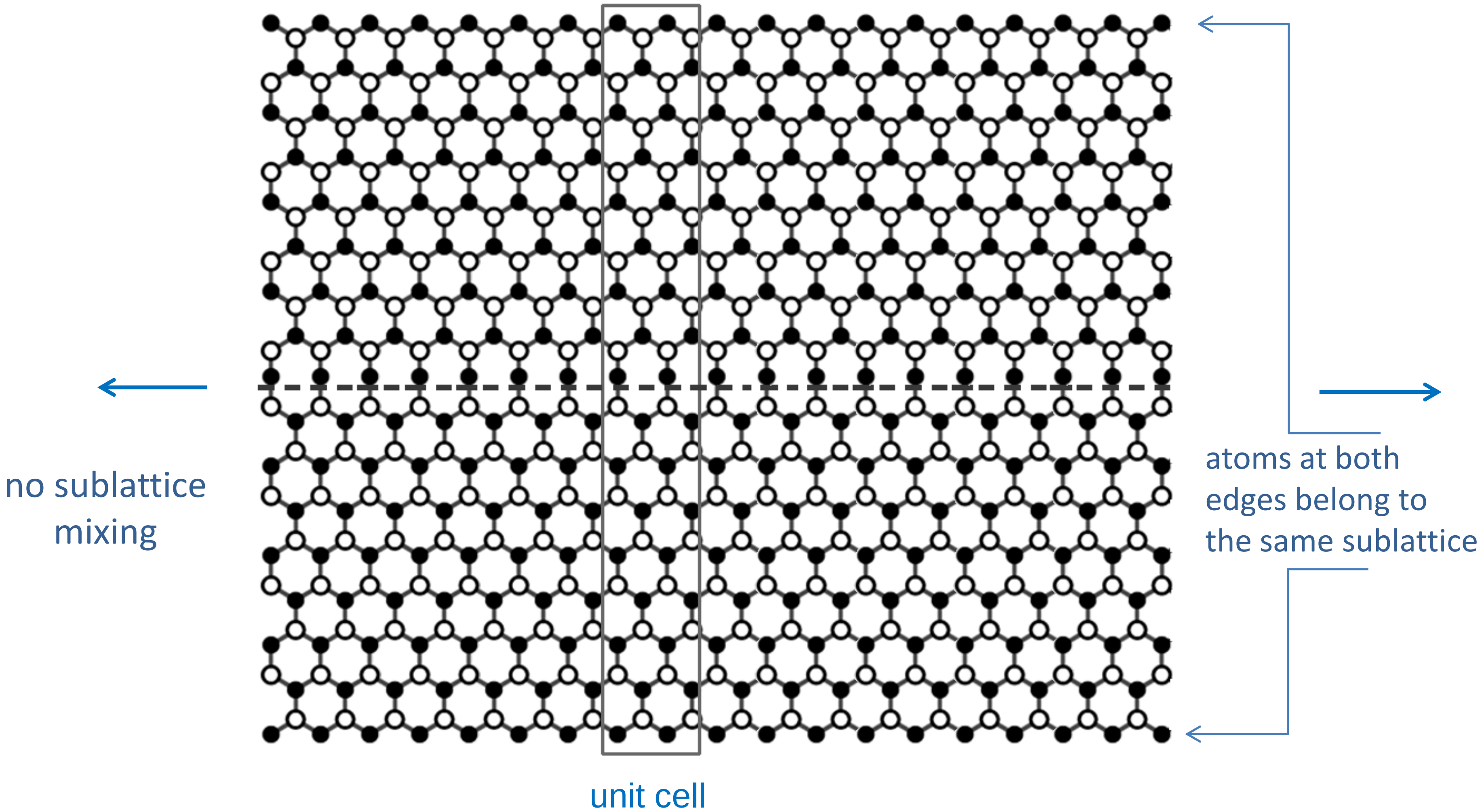
We study graphene nanoribbons and carbon nanotubes containing defect lines built of octagonal rings.

We show that octagonal defects localize states at Fermi energy even if their appearence mixes both graphene sublattices.

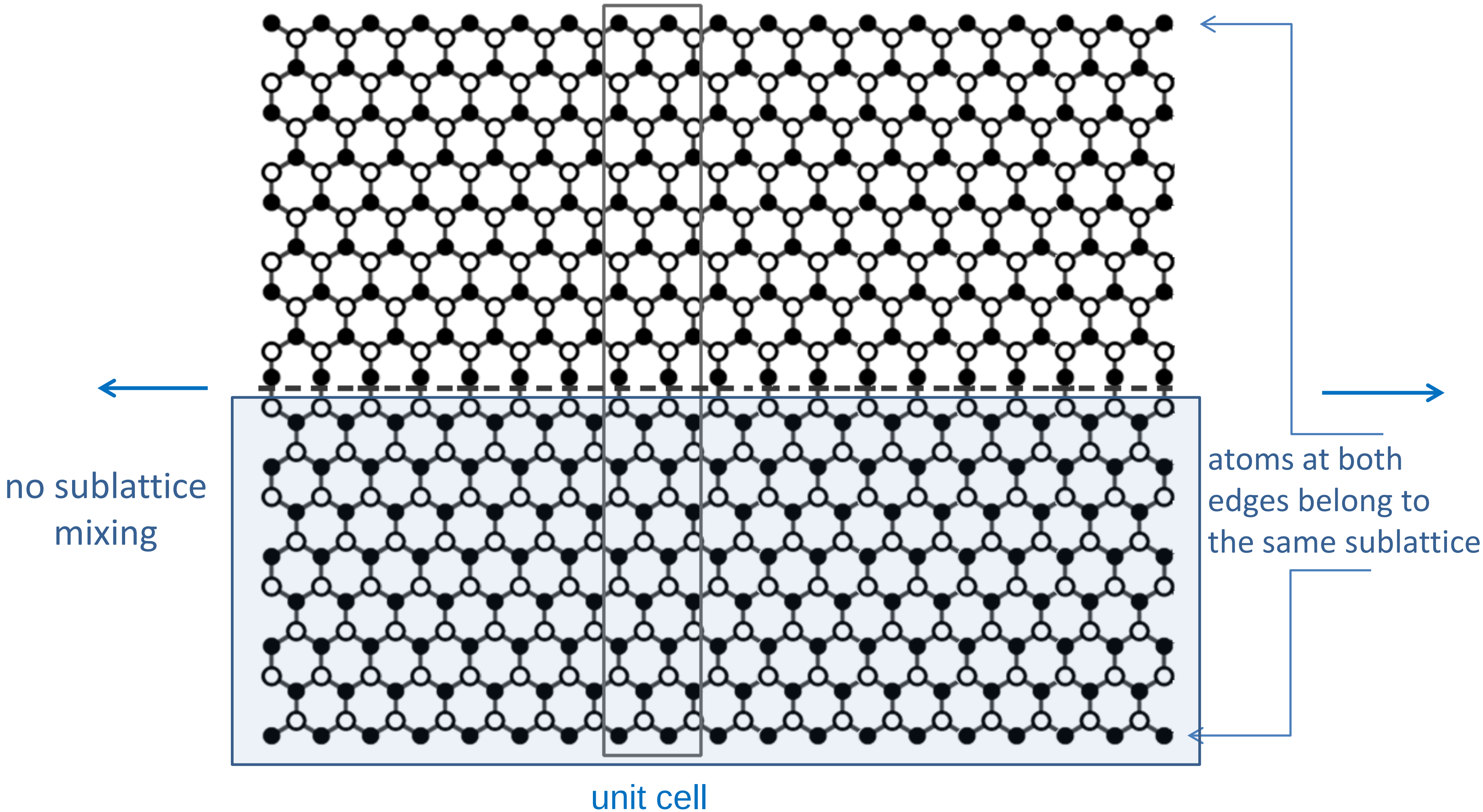
In some cases they may lead to spontaneous magnetization.

Calculation method: π-electron tight-binding approximation.
Electron interaction effects are taken into account by means of the Hubbard model.

Localization at octagons is explained using simple rules presented in our previous paper on graphene ribbons with arbitrary edges(2011), but it is the presence of octagons, which focuse localization at E_F



zigzag GNR with defect line built of octagonal rings
equals to
two connected ZGNR, one of them having one edge of the Klein type



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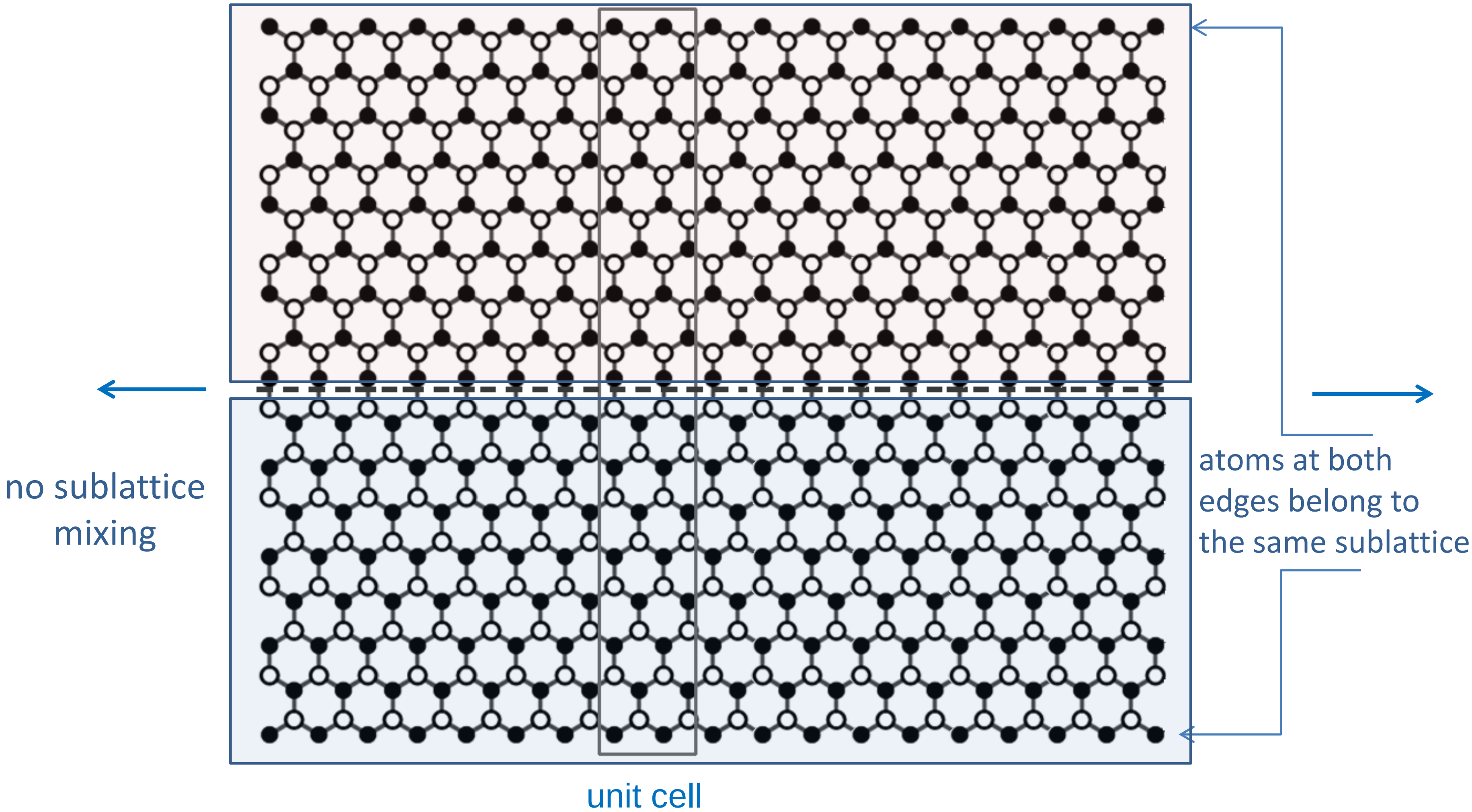

zigzag GNR with defect line built of octagonal rings
equals to
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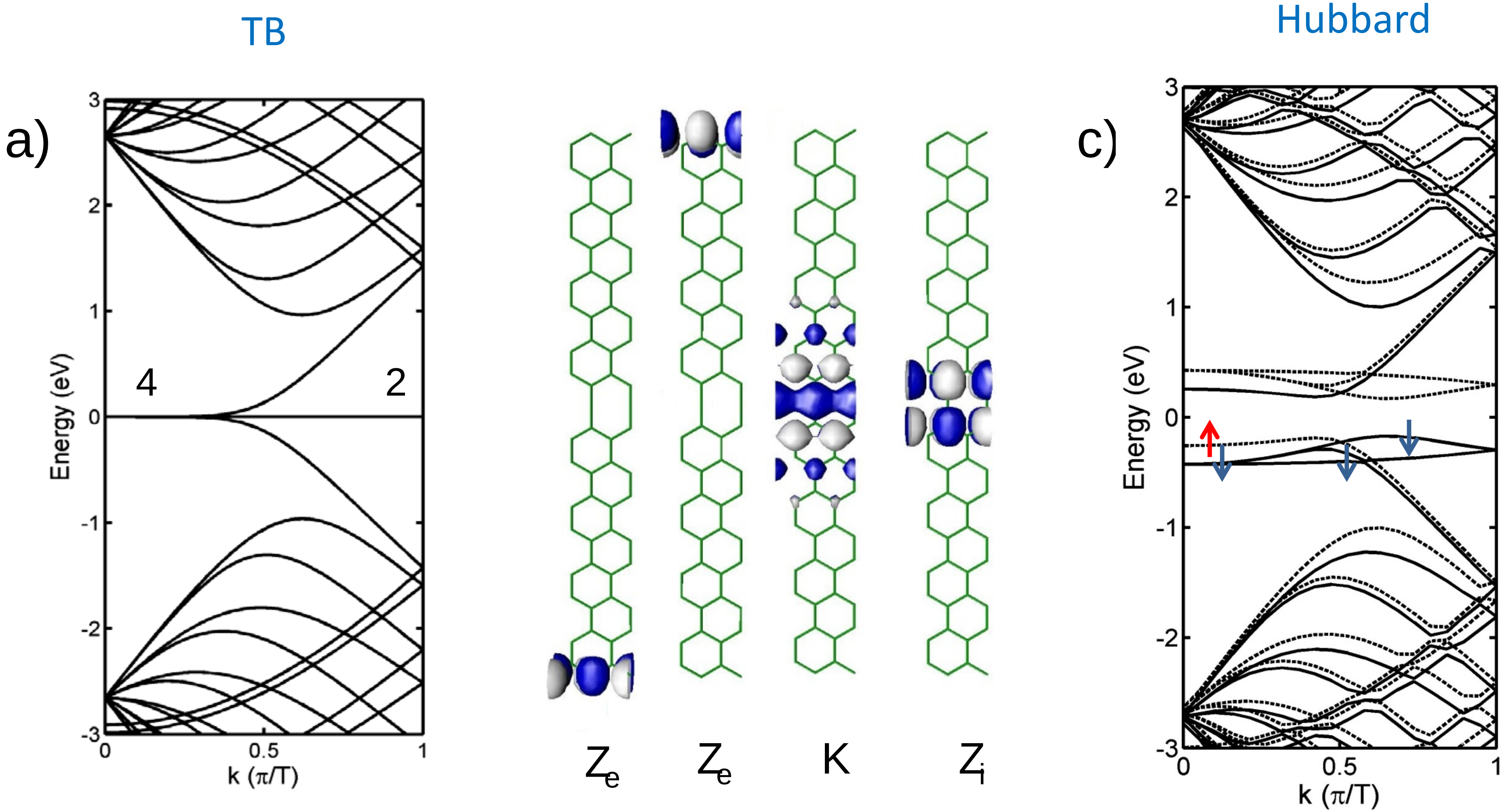
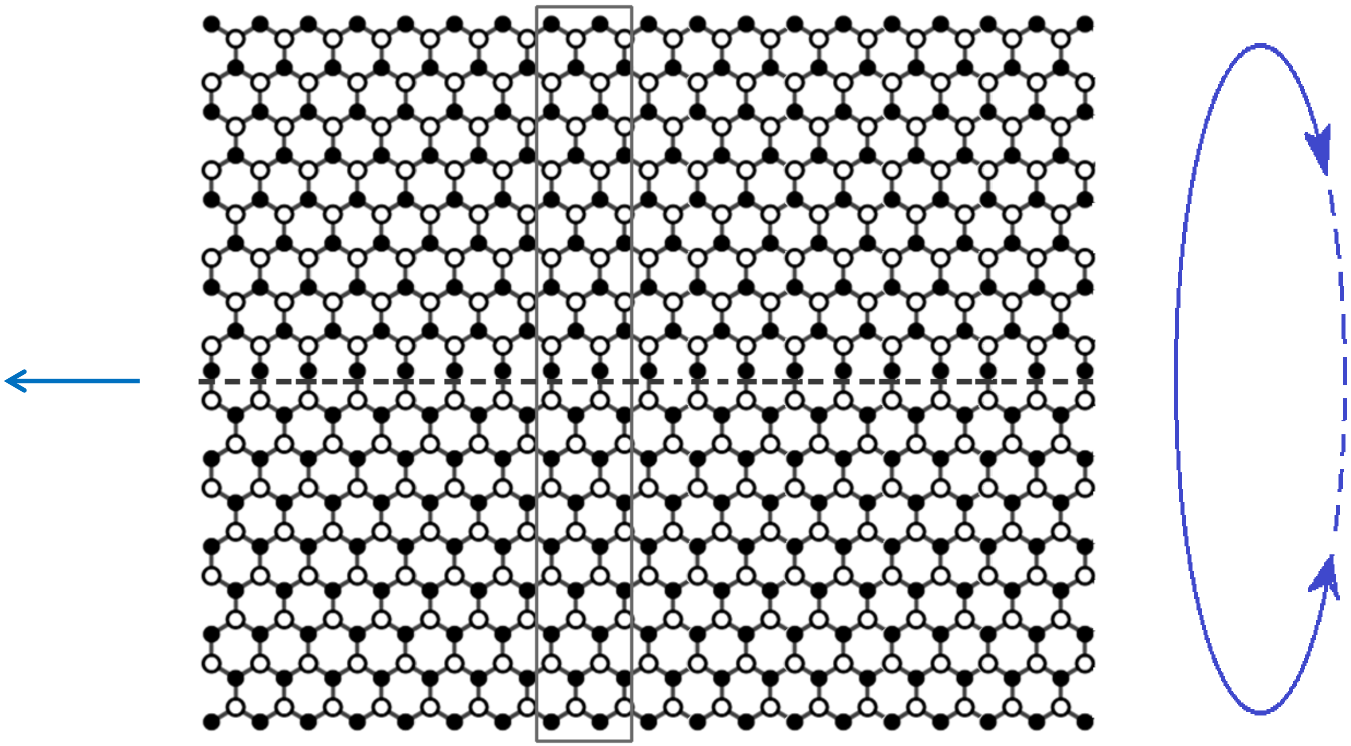
results

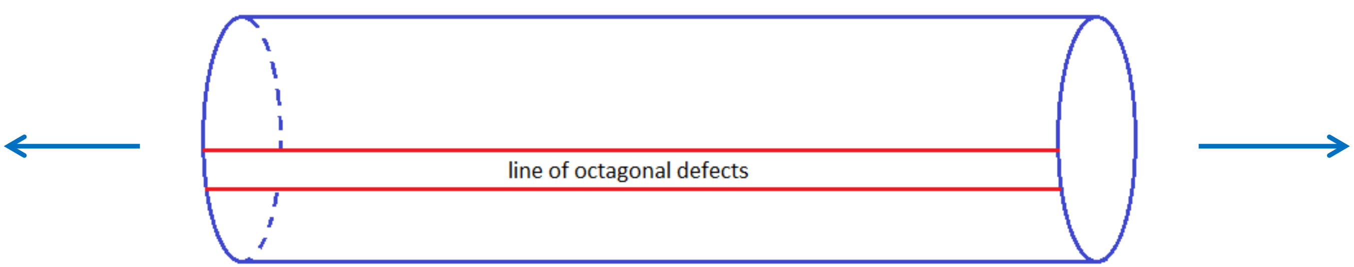


calculated magnetization equals $2\mu_B$
consistent with Lieb theorem -
two sublattice atoms imbalance in the unit cell

Rolled up zigzag GNR with defect line built of octagonal rings
i.e.,
armchair carbon nanotube with octagonal defect line alnog the axis



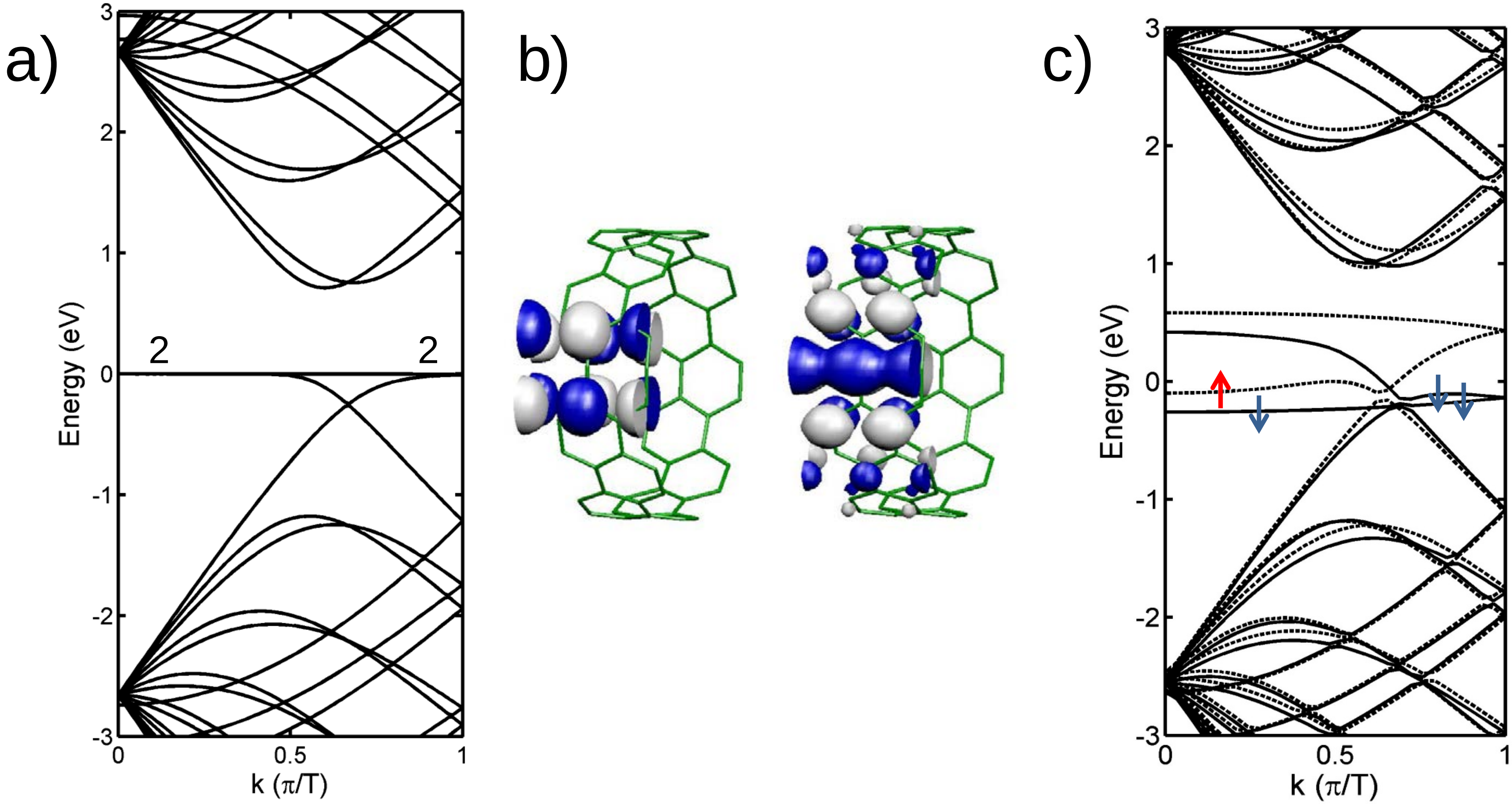
global sublattice mixing!



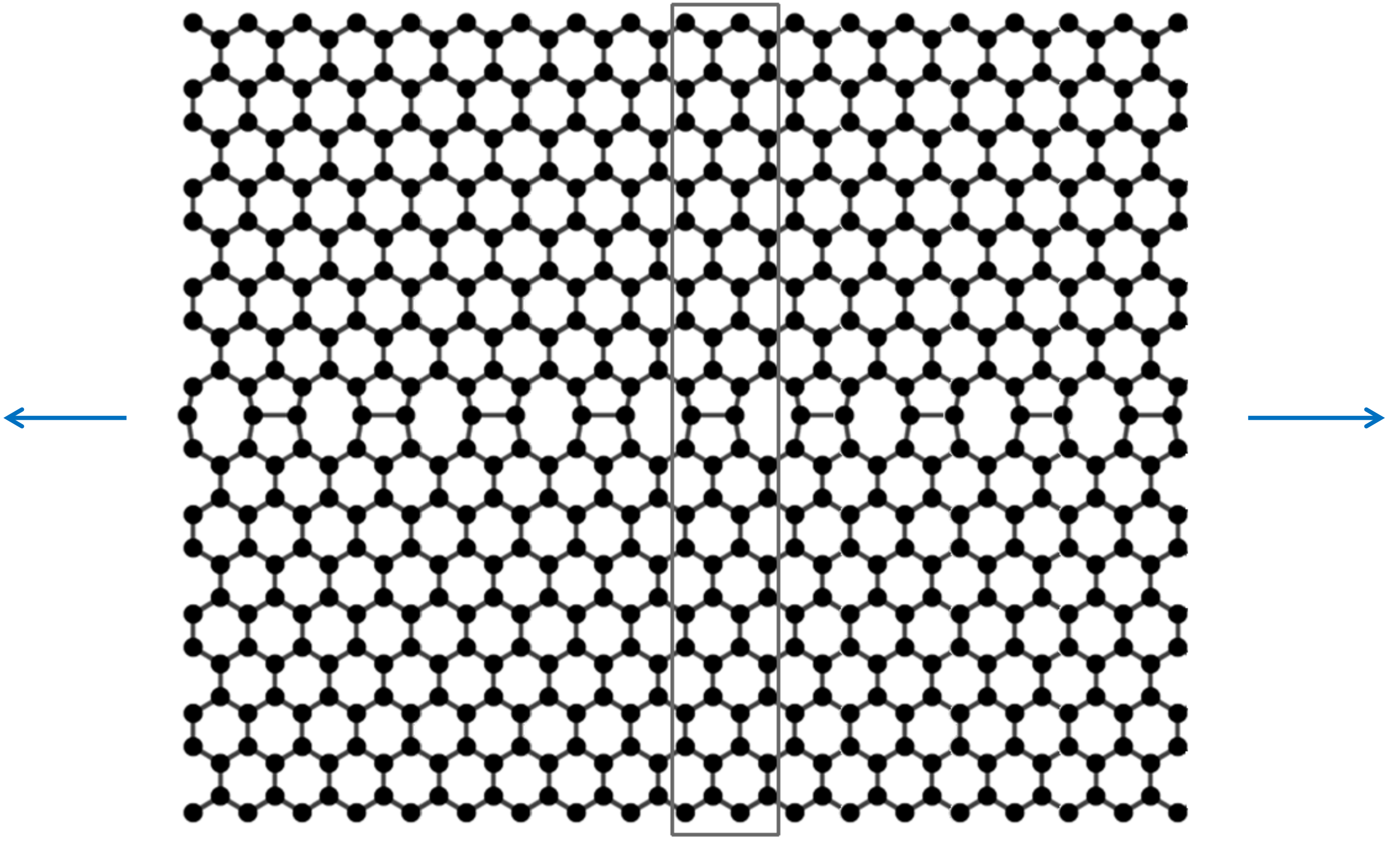
results

TB

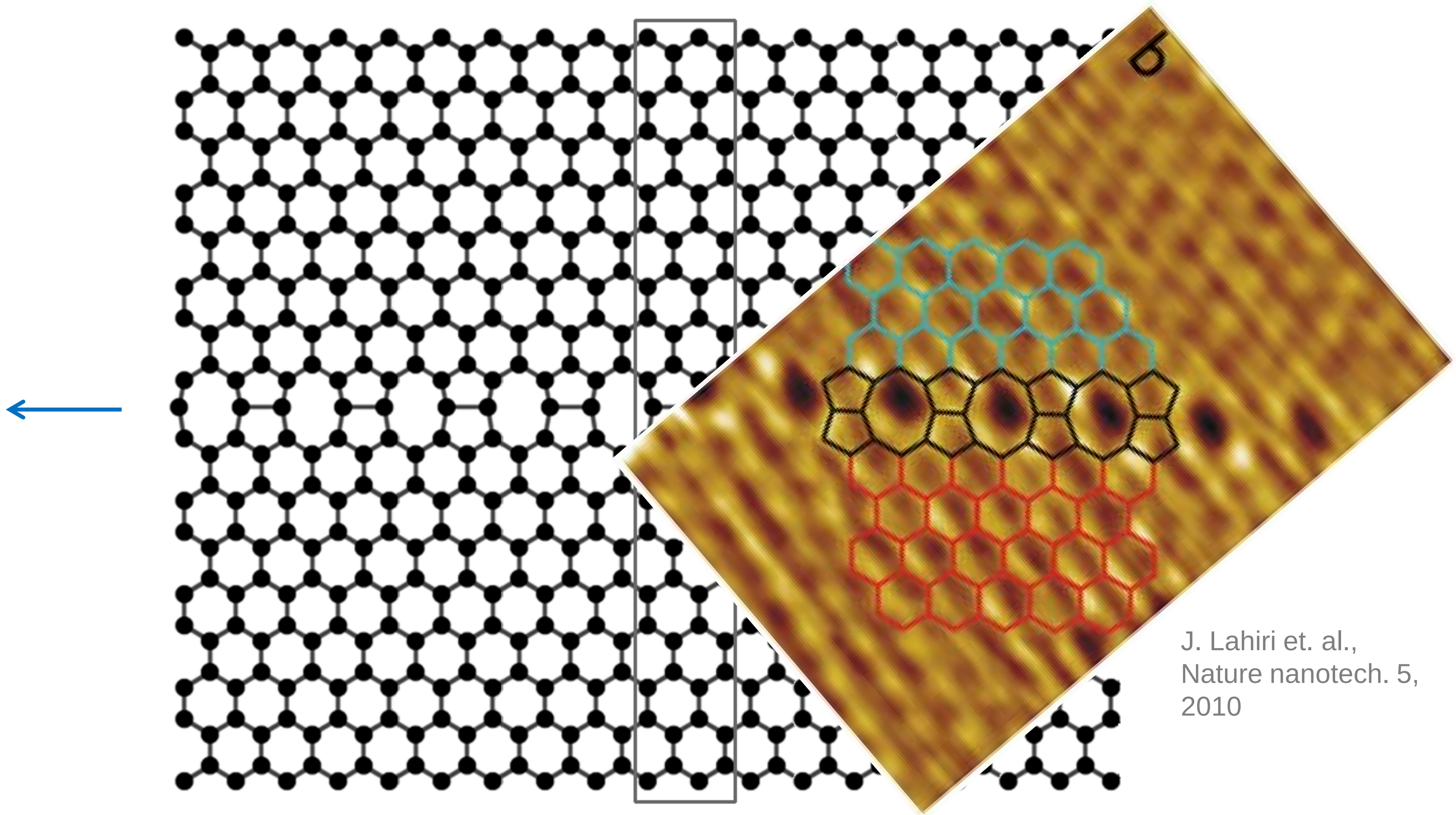
Hubbard



magnetization ~ $0.6\mu_B$



zigzag GNR with defect line built of octagonal and pentagonal rings



J. Lahiri et. al.,
Nature nanotech. 5,
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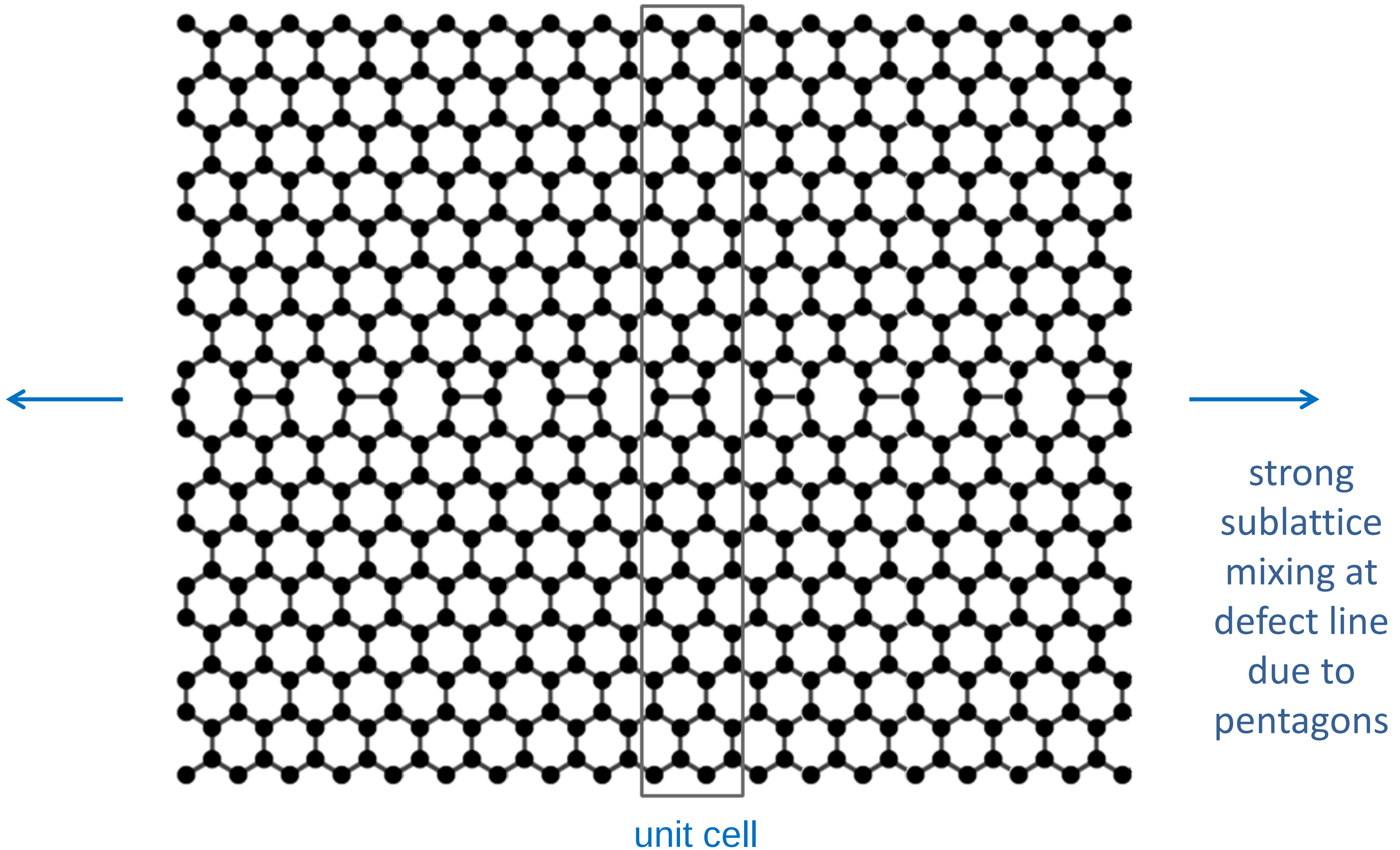

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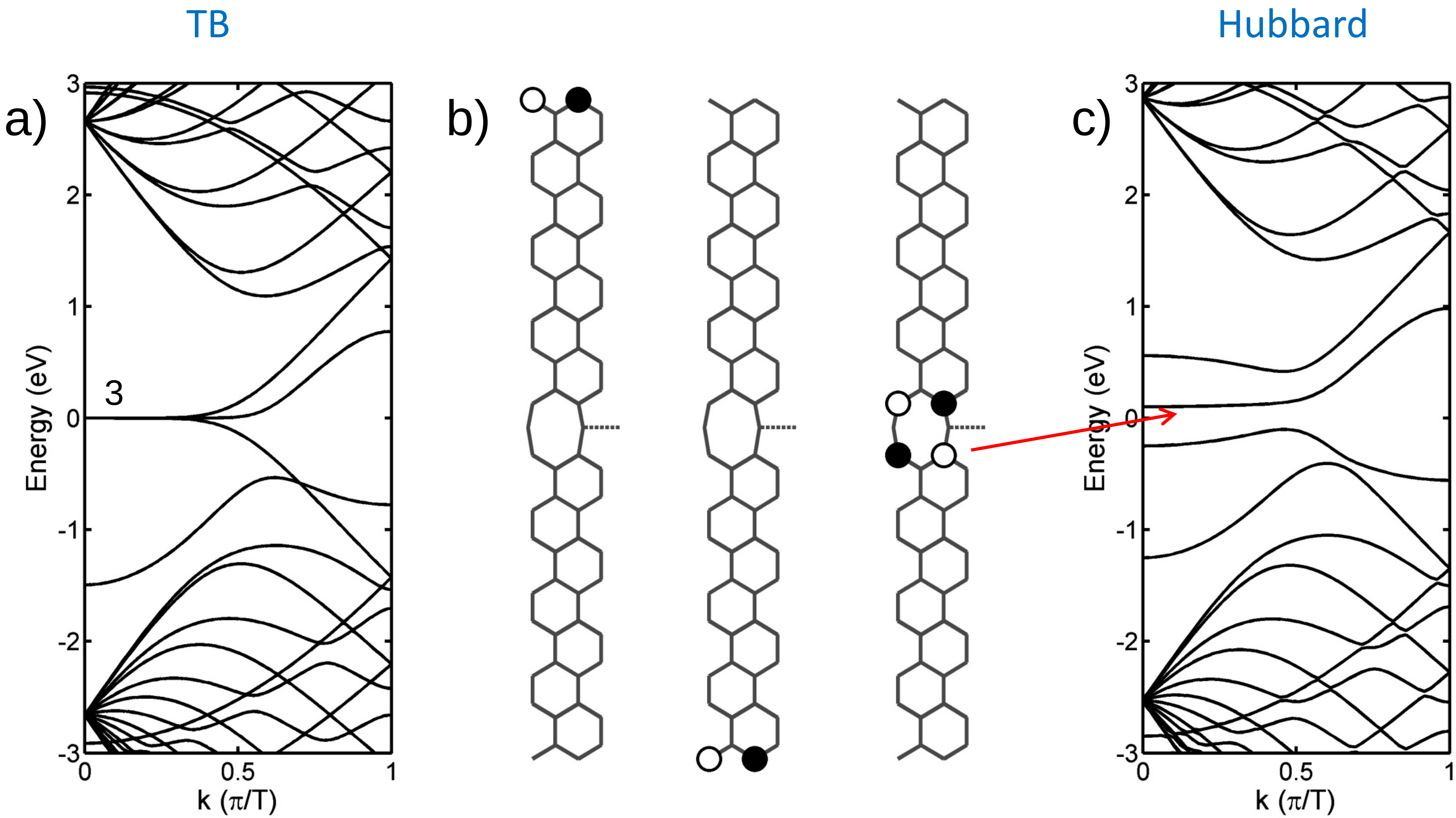

character of the resonance between two states belonging to the inner zigzag edges confining the line of defects all the calculated flat bands

can be obtained *without calculations*

by applying our rules introduced in 2011

for finding edge-states in graphene nanoribbons;

however, the presence of octagons,

which do not mix graphene sublattices

is responsible for localization just at the Fermi energy

Conclusions

- octagonal defect lines in graphene structures lead to state localization with energies close to the Fermi level
- the localization happens independently on the sublattice mixing
- some of the investigated structures reveal spontaneous magnetization
- the appearance of localized flat bands at octagonal defects can be explained using simple rules introduced in our previous work, but octagons are responsible for the localization just at Fermi energy