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

Supplementary Material: Bandgap evolution in nanographene assemblies

F. Crasto de Lima[1,*] and A. Fazzio[1,†]

[1] *Brazilian Nanotechnology National Laboratory CNPEM, C.P. 6192, 13083-970, Campinas, SP, Brazil*

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ASSEMBLIES

Studied assemblies atomic geometry, with the unit cell marked in red and band structure. The label name is just for reference.

Ha

Structure with label "Ha" presenting 108 carbon atoms in the hexagonal unit cell, intermolecule bond density $\eta = 3.0$, and TB predicted energy gap of 1.89 eV.

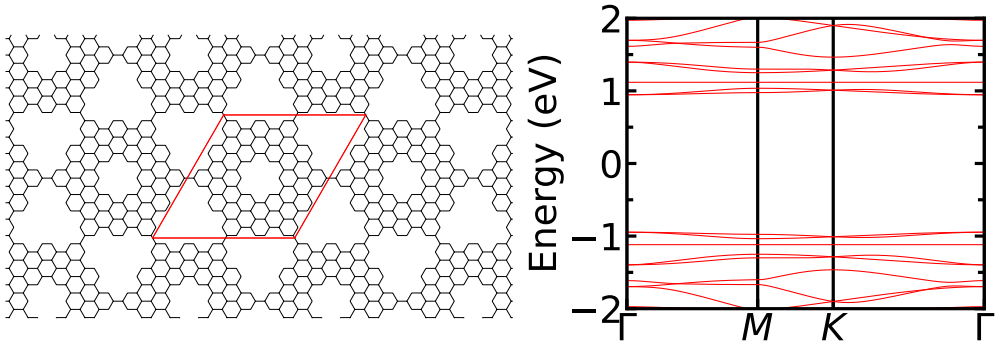

FIG. S1. Ha.

Hb

Structure with label "Hb" presenting 108 carbon atoms in the hexagonal unit cell, intermolecule bond density $\eta = 9.0$, and TB predicted energy gap of 1.22 eV.

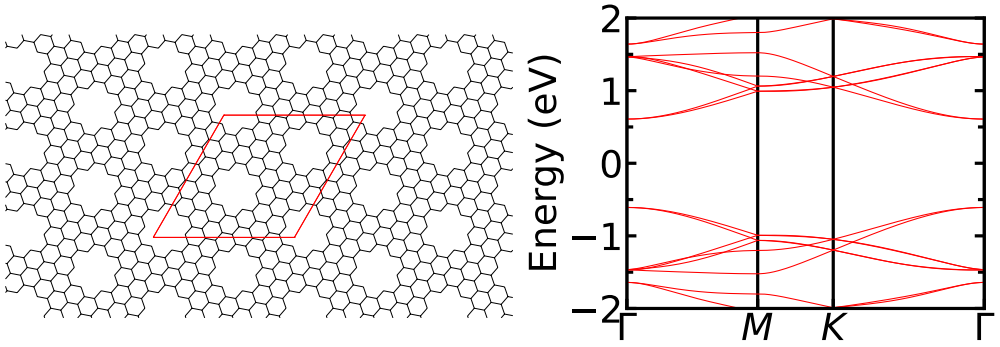

FIG. S2. Hb.

Hc

Structure with label "Hc" presenting 108 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 15.0$, and TB predicted energy gap of 0.44 eV.

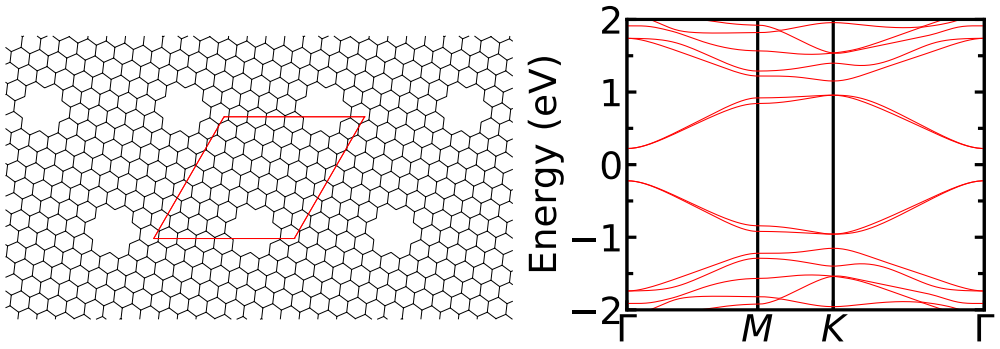

FIG. S3. Hc.

Hga

Structure with label "Hga" presenting 216 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 1.5$, and TB predicted energy gap of 1.95 eV.

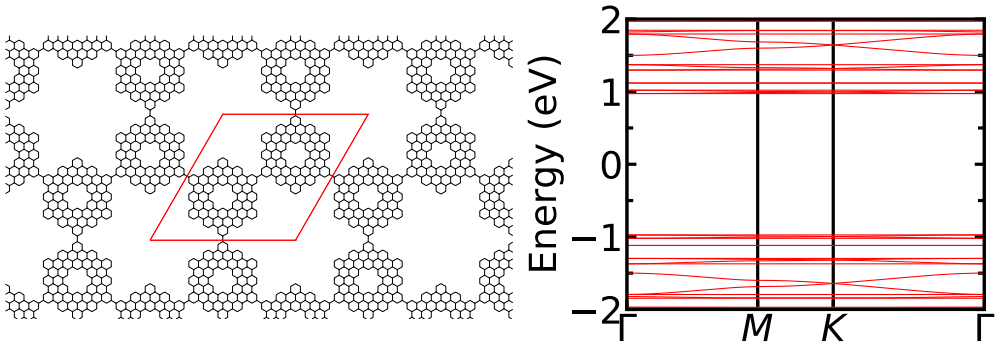

FIG. S4. Hga.

Hgb

Structure with label "Hgb" presenting 216 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 4.5$, and TB predicted energy gap of 1.57 eV.

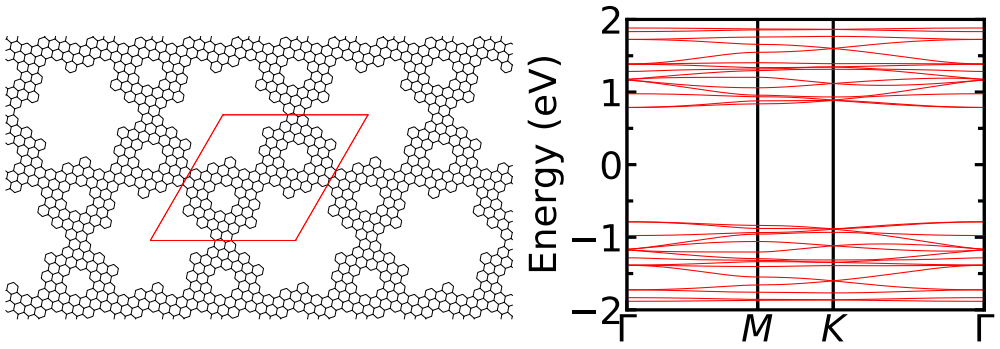

FIG. S5. Hgb.

Hgc

Structure with label "Hgc" presenting 216 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 7.5$, and TB predicted energy gap of 1.26 eV.

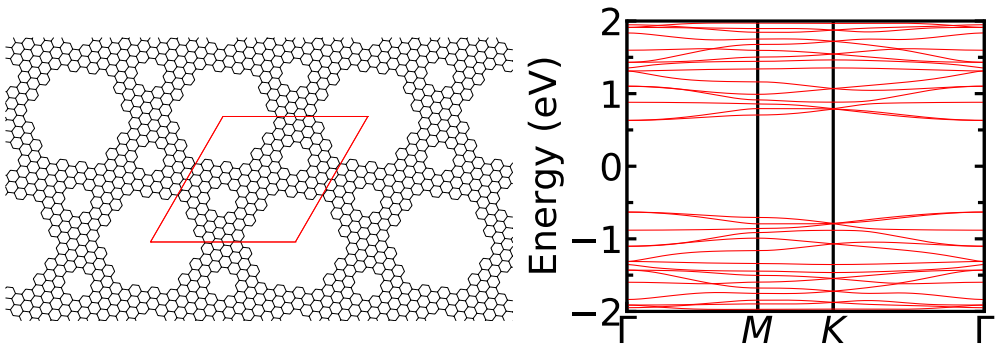

FIG. S6. Hgc.

Hka

Structure with label "Hka" presenting 324 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 2.0$, and TB predicted energy gap of 1.92 eV.

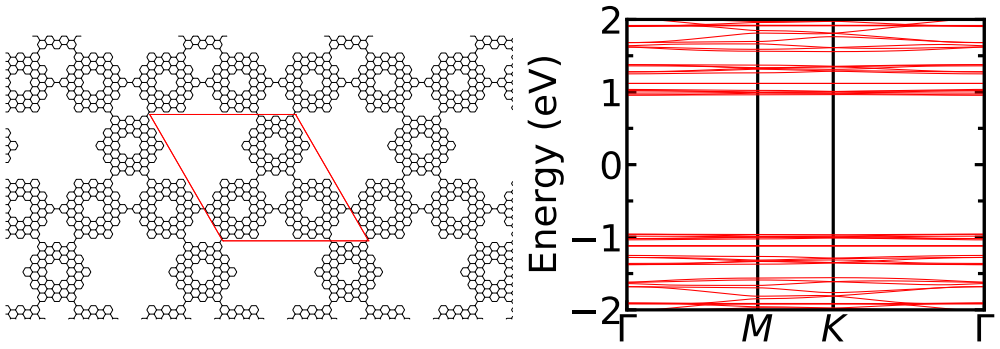

FIG. S7. Hka.

Hkb

Structure with label "Hkb" presenting 324 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 6.0$, and TB predicted energy gap of 1.44 eV.

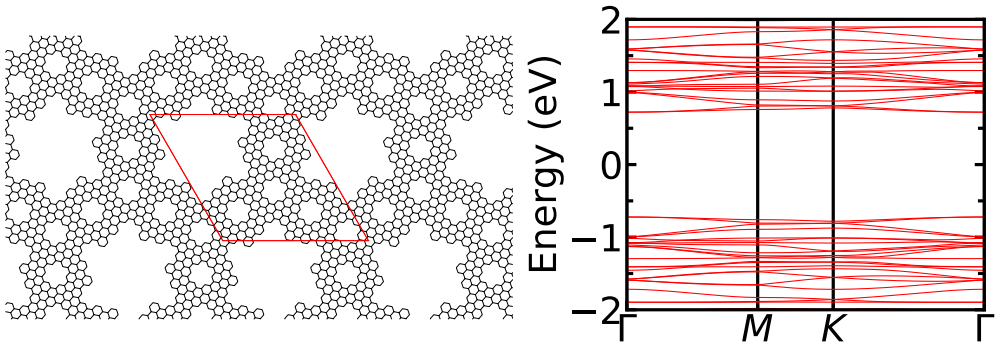

FIG. S8. Hkb.

Hkc

Structure with label "Hkc" presenting 324 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 10.0$, and TB predicted energy gap of 1.01 eV.

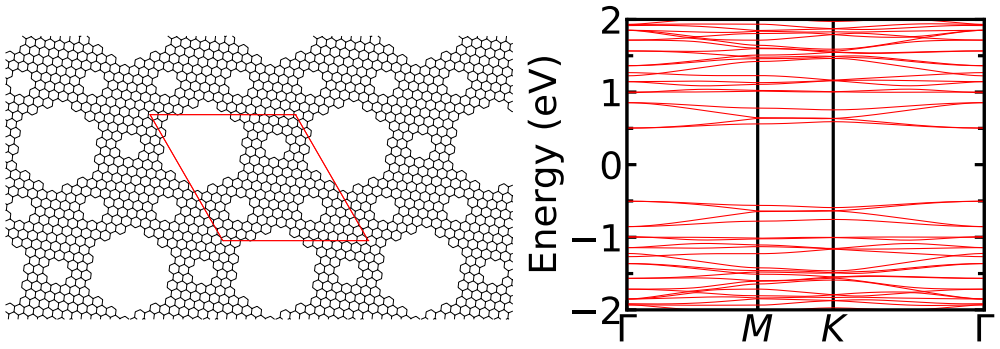

FIG. S9. Hkc.

Htka

Structure with label "Htka" presenting 324 carbon atoms in the tetragonal unit cell, inter-molecule bond density $\eta = 2.0$, and TB predicted energy gap of 1.92 eV.

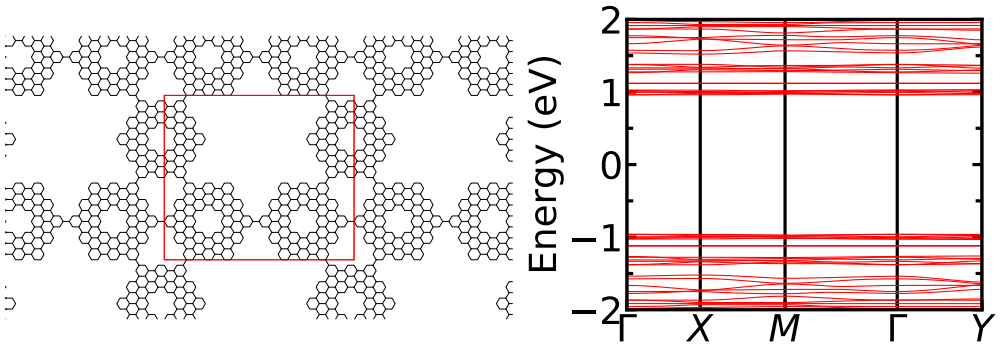

FIG. S10. Htka.

Htkb

Structure with label "Htkb" presenting 324 carbon atoms in the tetragonal unit cell, inter-molecule bond density $\eta = 6.0$, and TB predicted energy gap of 1.42 eV.

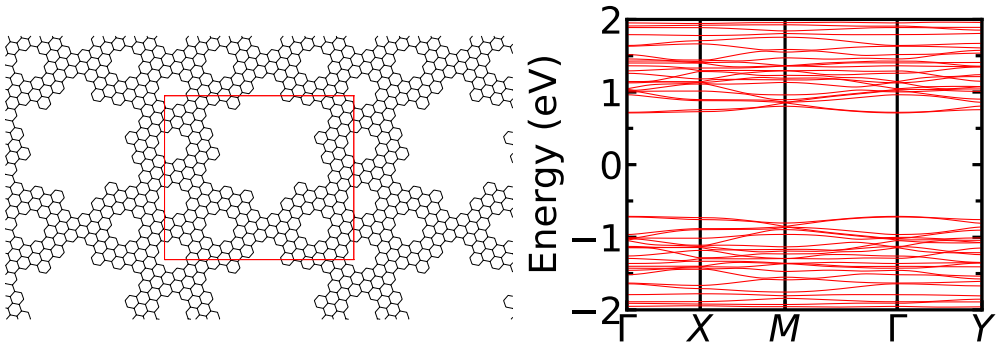

FIG. S11. Htkb.

Htkc

Structure with label "Htkc" presenting 324 carbon atoms in the tetragonal unit cell, inter-molecule bond density $\eta = 10.0$, and TB predicted energy gap of 0.93 eV.

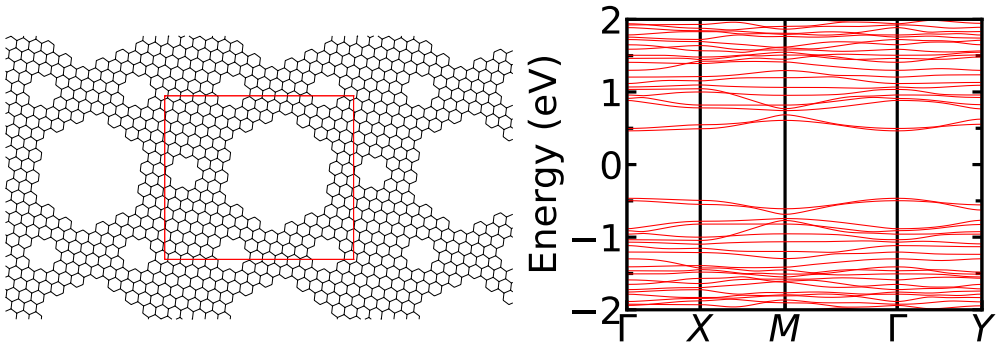

FIG. S12. Htkc.

H3a

Structure with label "H3a" presenting 864 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 2.625$, and TB predicted energy gap of 1.90 eV.

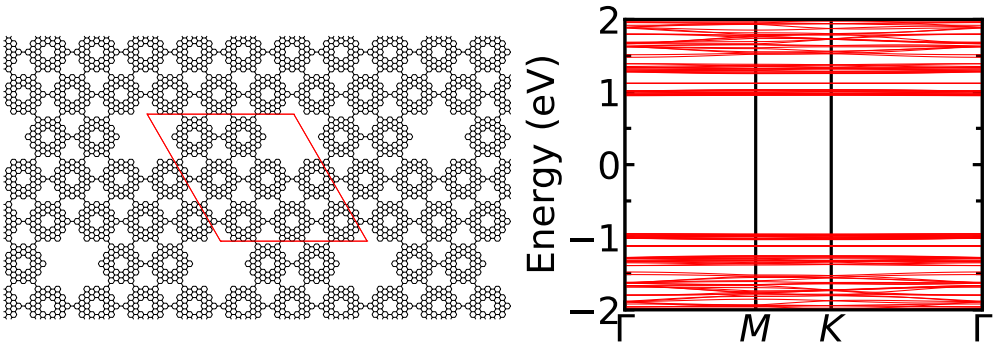

FIG. S13. Ha.

H3b

Structure with label "H3b" presenting 864 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 7.875$, and TB predicted energy gap of 1.28 eV.

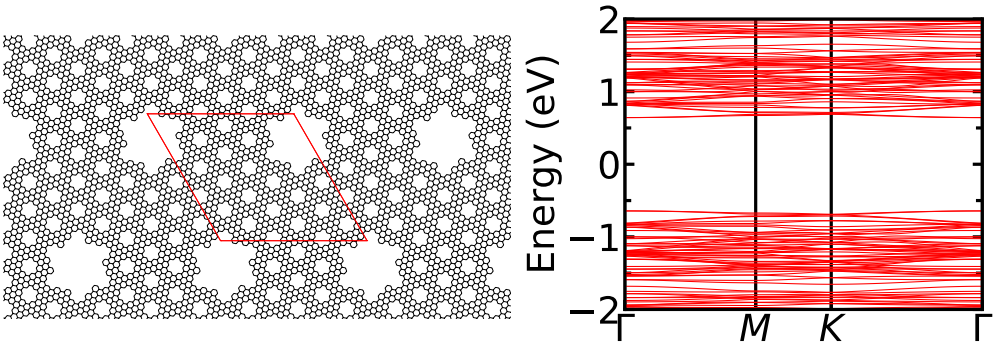

FIG. S14. H3b.

H3c

Structure with label "H3c" presenting 864 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 13.125$, and TB predicted energy gap of 0.62 eV.

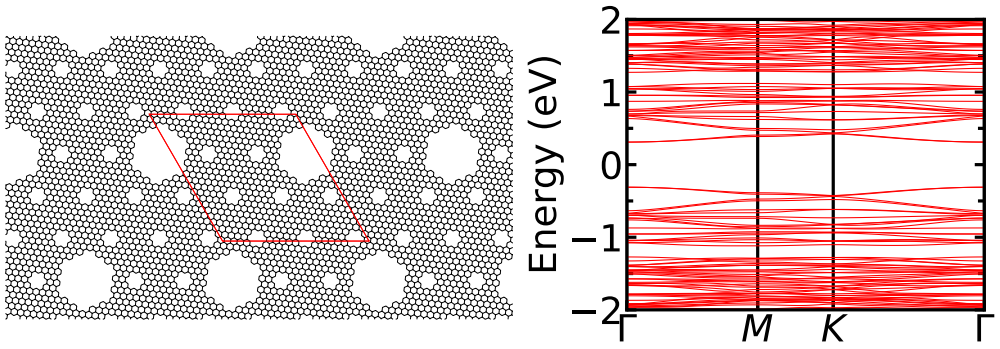

FIG. S15. H3c.

H4a

Structure with label "H4a" presenting 1620 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 2.8$, and TB predicted energy gap of 1.90 eV.

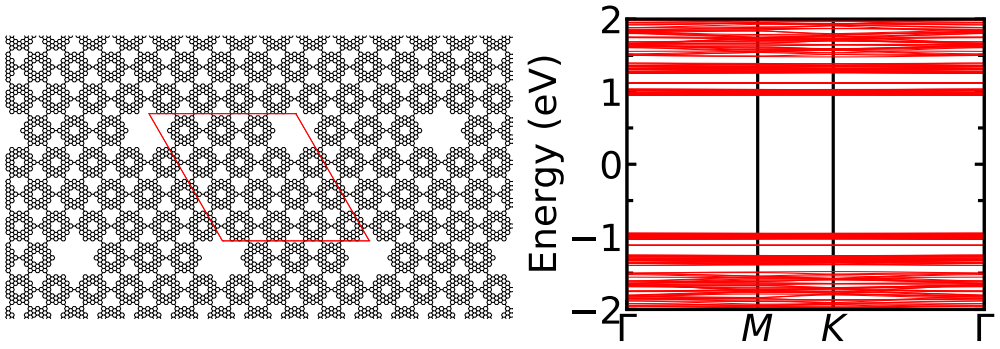

FIG. S16. H4a.

H4b

Structure with label "H4b" presenting 1620 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 8.4$, and TB predicted energy gap of 1.25 eV.

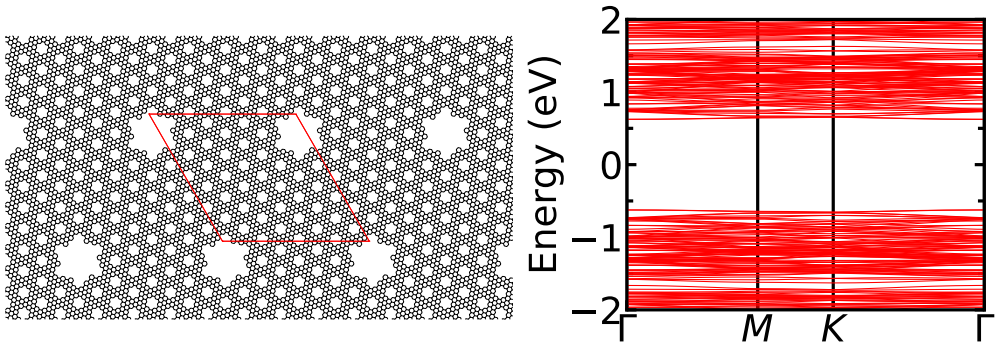

FIG. S17. H4b.

H4c

Structure with label "H4c" presenting 1620 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 14.0$, and TB predicted energy gap of 0.53 eV.

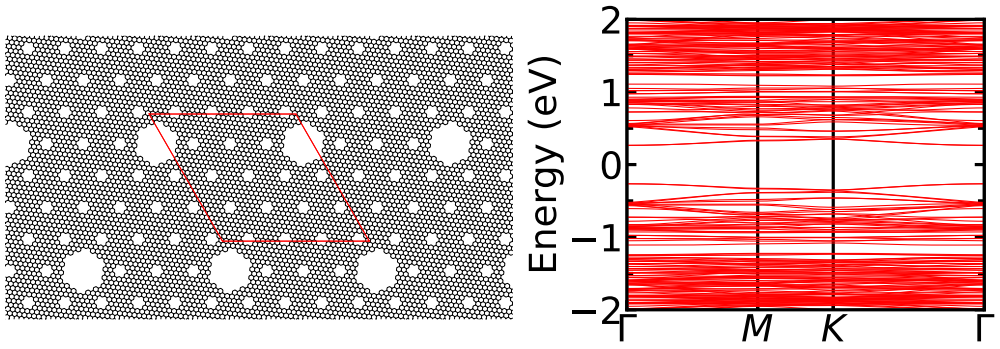

FIG. S18. H4c.

H6a

Structure with label "H6a" presenting 1512 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 1.9286$, and TB predicted energy gap of 1.92 eV.

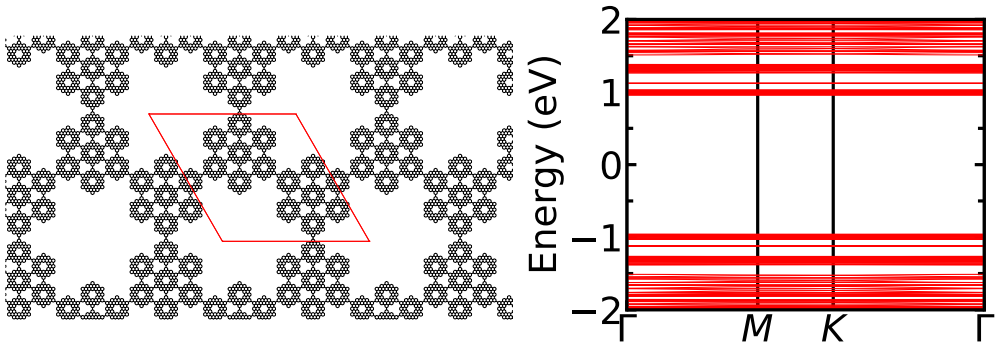

FIG. S19. H6a.

H6b

Structure with label "H6b" presenting 1512 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 5.7857$, and TB predicted energy gap of 1.39 eV.

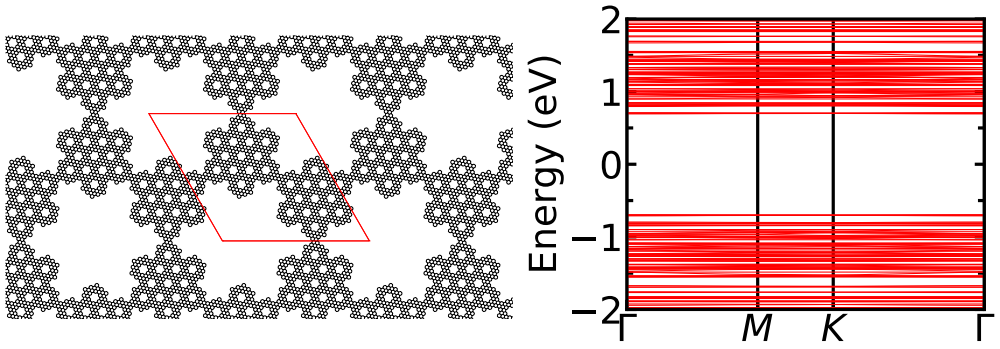

FIG. S20. H6b.

H6c

Structure with label "H6c" presenting 1512 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 9.6428$, and TB predicted energy gap of 0.86 eV.

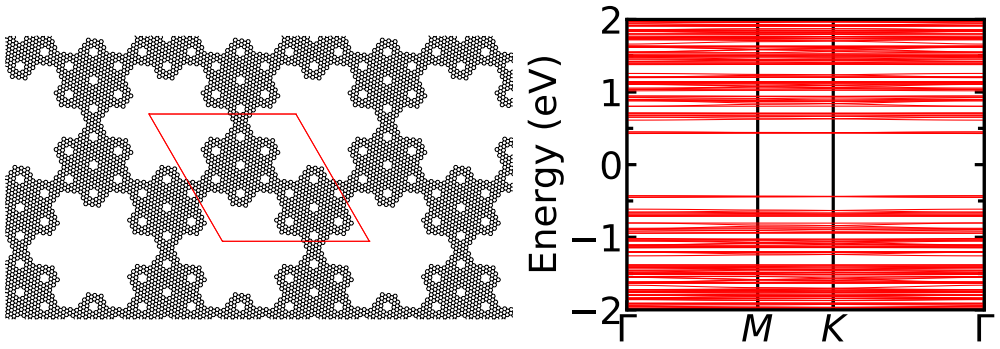

FIG. S21. H6c.

H6ga

Structure with label "H6ga" presenting 1296 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 1.25$, and TB predicted energy gap of 1.95 eV.

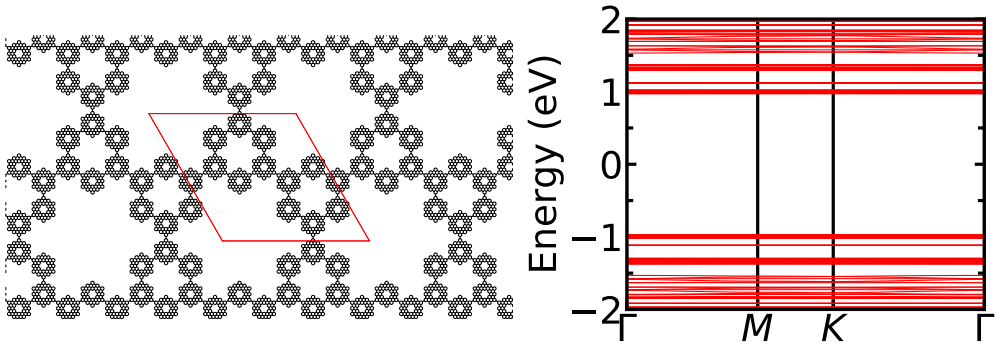

FIG. S22. H6ga.

H6gb

Structure with label "H6gb" presenting 1296 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 3.75$, and TB predicted energy gap of 1.61 eV.

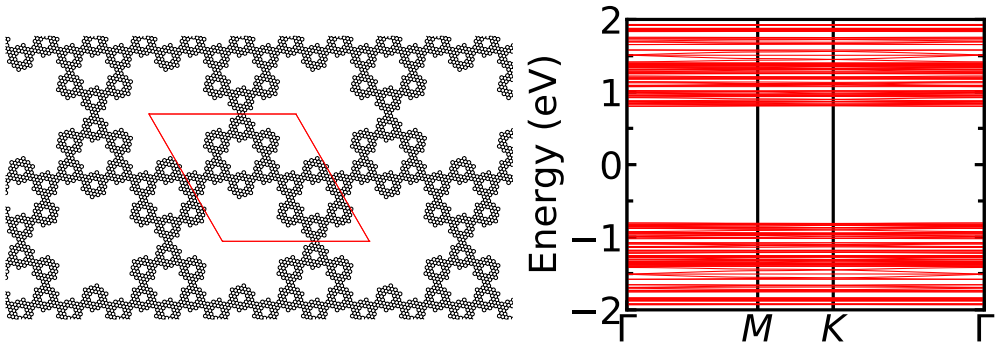

FIG. S23. H6gb.

H6gc

Structure with label "H6gc" presenting 1296 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 6.25$, and TB predicted energy gap of 1.32 eV.

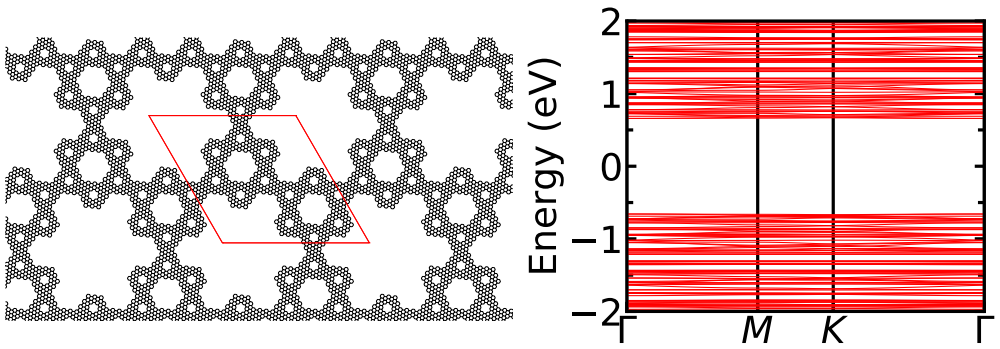

FIG. S24. H6gc.

Hsha

Structure with label "Hsha" presenting 648 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 2.5$, and TB predicted energy gap of 1.91 eV.

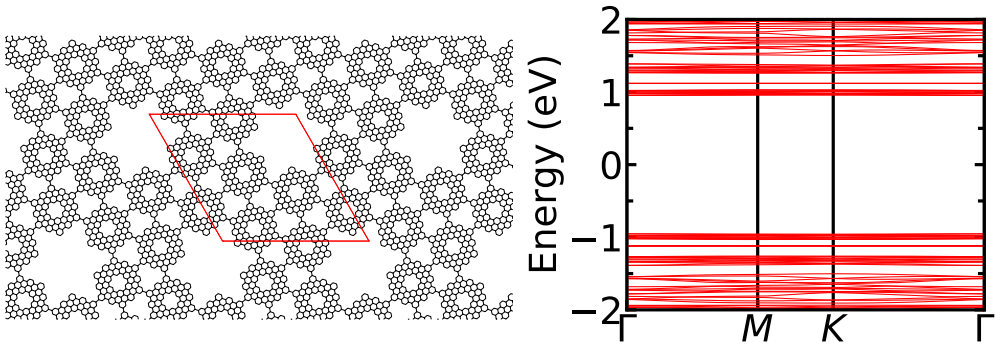

FIG. S25. Hsha.

Hshb

Structure with label "Hshb" presenting 648 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 7.5$, and TB predicted energy gap of 1.31 eV.

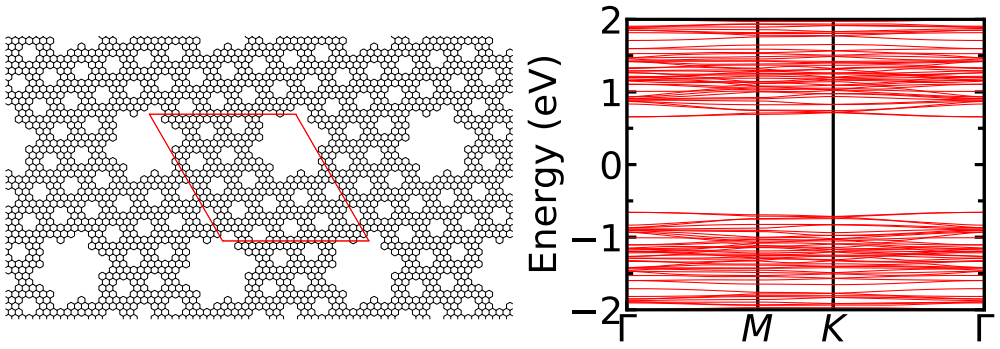

FIG. S26. Hshb.

Hshc

Structure with label "Hshc" presenting 648 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 12.5$, and TB predicted energy gap of 0.69 eV.

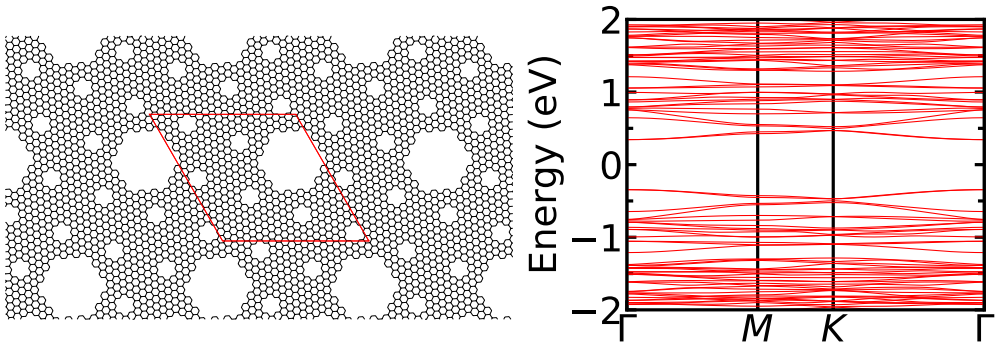

FIG. S27. Hshc.

Hs13a

Structure with label "Hs13a" presenting 1296 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 2.75$, and TB predicted energy gap of 1.90 eV.

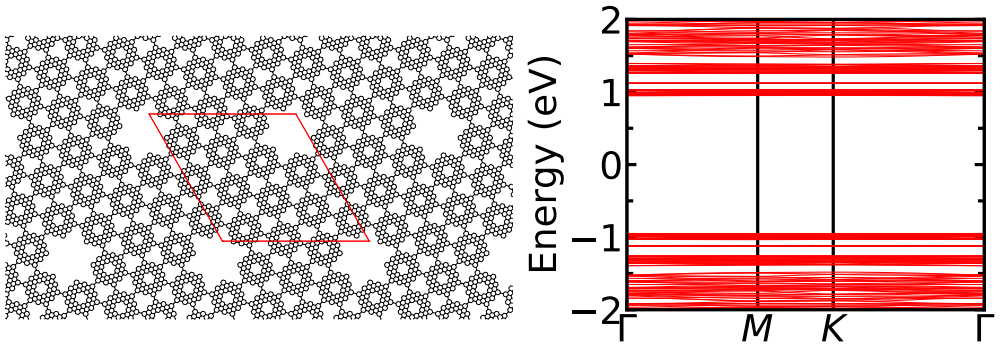

FIG. S28. Hs13a.

Hs13b

Structure with label "Hs13b" presenting 1296 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 8.25$, and TB predicted energy gap of 1.26 eV.

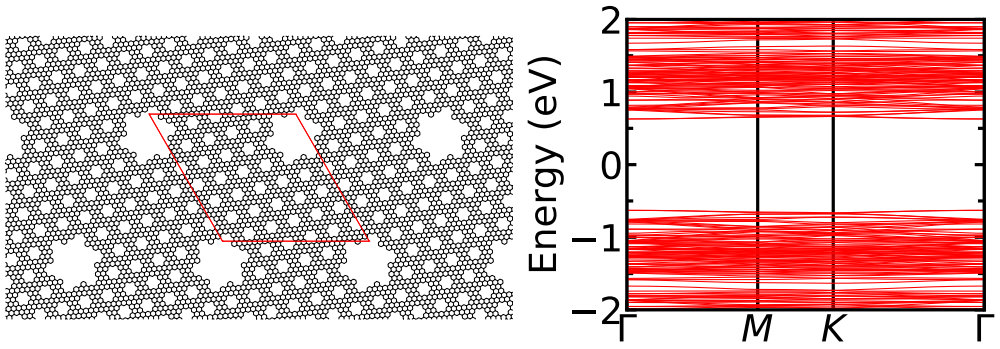

FIG. S29. Hs13b.

Hs13c

Structure with label "Hs13c" presenting 1296 carbon atoms in the hexagonal unit cell, inter-molecule bond density $\eta = 13.75$, and TB predicted energy gap of 0.55 eV.

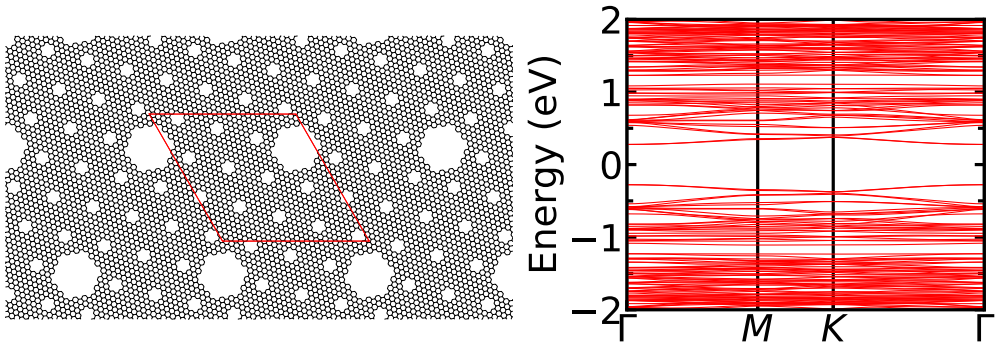

FIG. S30. Hs13c.

Ta

Structure with label "Ta" presenting 108 carbon atoms in the oblique unit cell, intermolecule bond density $\eta = 4.0$, and TB predicted energy gap of 1.64 eV.

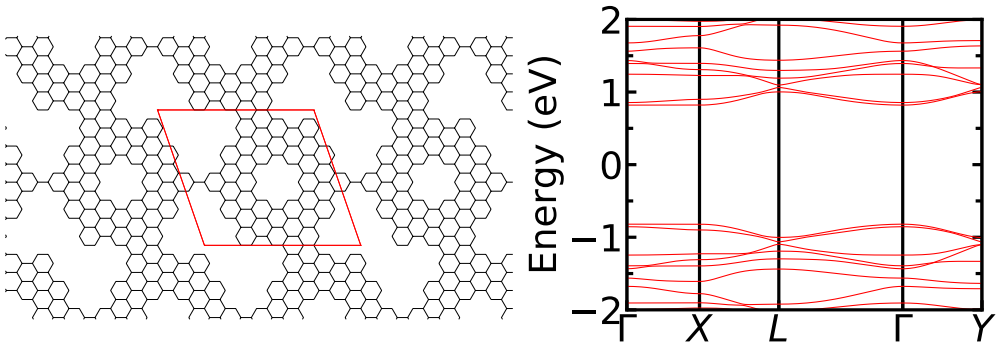

FIG. S31. Ta.

Tb

Structure with label "Tb" presenting 108 carbon atoms in the oblique unit cell, intermolecule bond density $\eta = 6.0$, and TB predicted energy gap of 1.39 eV.

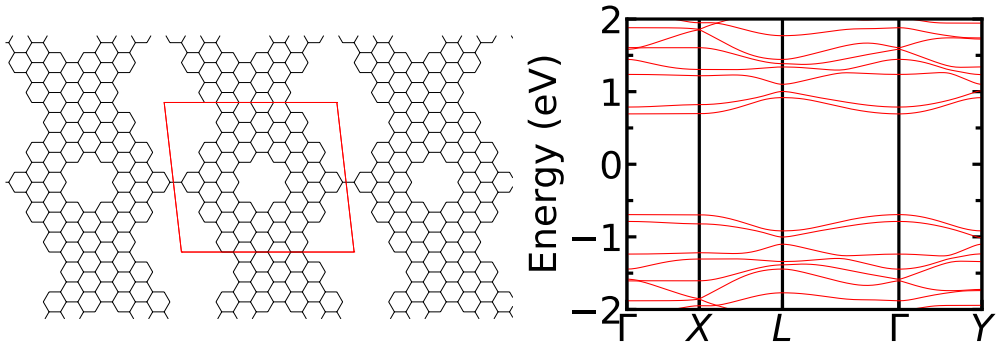

FIG. S32. Tb.

Tc

Structure with label "Tc" presenting 108 carbon atoms in the oblique unit cell, inter-molecule bond density $\eta = 8.0$, and TB predicted energy gap of 1.17 eV.

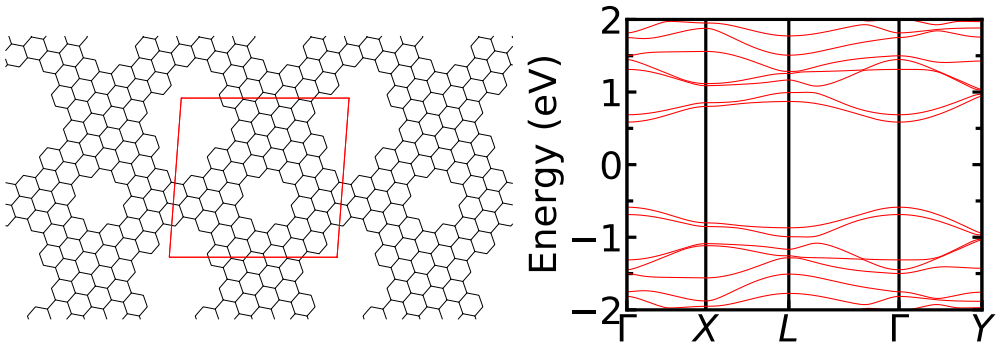

FIG. S33. Tc.

Td

Structure with label "Td" presenting 324 carbon atoms in the oblique unit cell, inter-molecule bond density $\eta = 2.67$, and TB predicted energy gap of 1.64 eV.

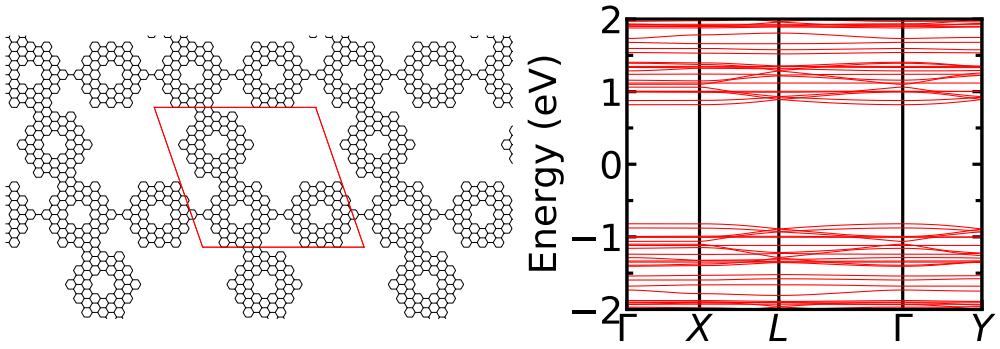

FIG. S34. Td.

Te

Structure with label "Te" presenting 324 carbon atoms in the oblique unit cell, intermolecule bond density $\eta = 4.0$, and TB predicted energy gap of 1.39 eV.

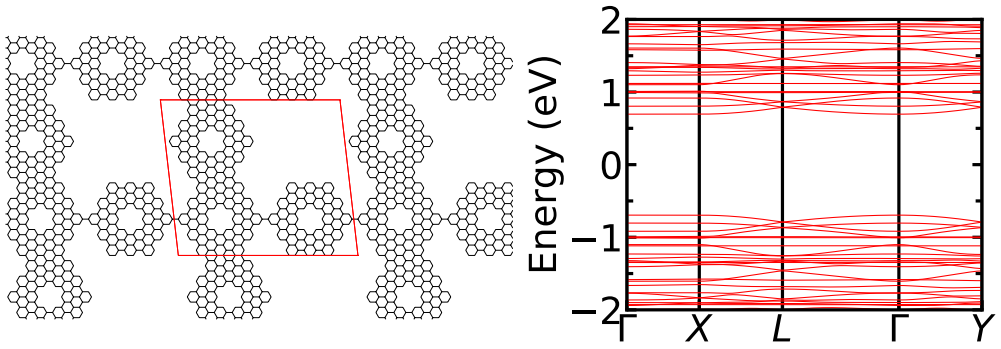

FIG. S35. Te.

Tf

Structure with label "Tf" presenting 324 carbon atoms in the oblique unit cell, intermolecule bond density $\eta = 5.33$, and TB predicted energy gap of 1.35 eV.

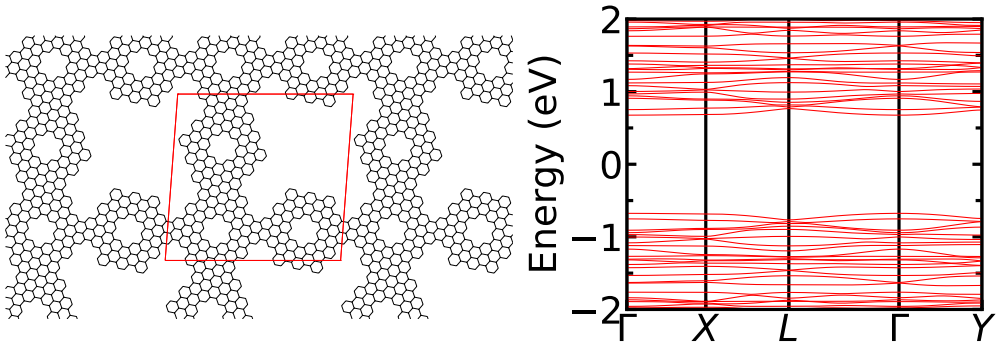

FIG. S36. Tf.

Ra

Structure with label “Ra” presenting 108 carbon atoms in the 1D unit cell, inter-molecule bond density $\eta = 1.0$, and TB predicted energy gap of 1.93 eV.

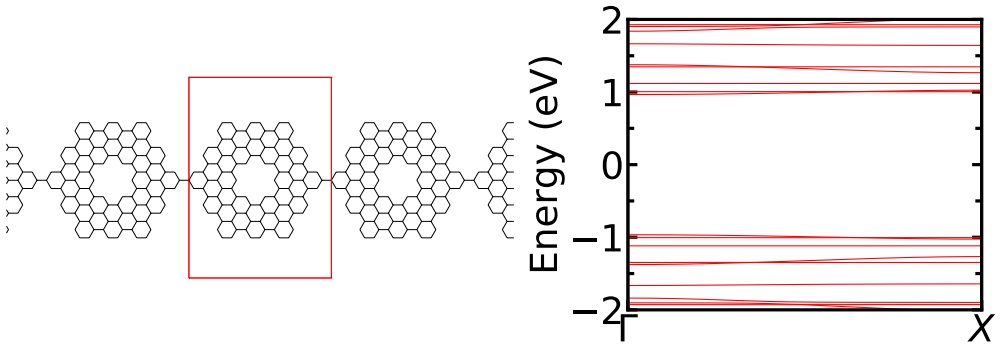

FIG. S37. Ra.

Rb

Structure with label “Rb” presenting 108 carbon atoms in the 1D unit cell, inter-molecule bond density $\eta = 3.0$, and TB predicted energy gap of 1.64 eV.

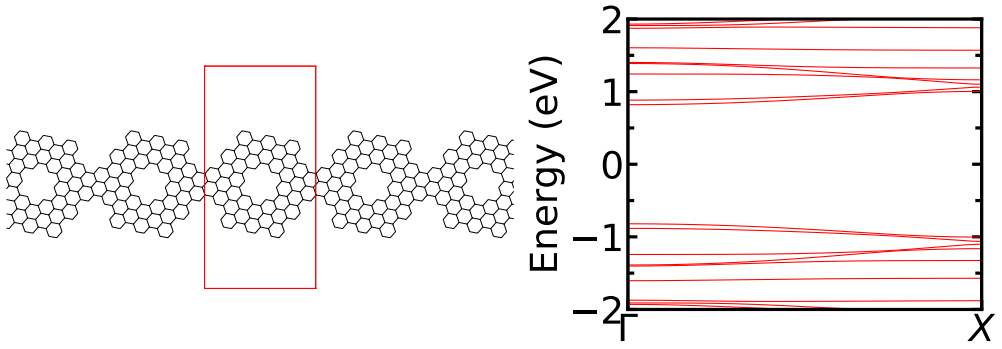

FIG. S38. Rb.

Rc

Structure with label "Rc" presenting 108 carbon atoms in the 1D unit cell, inter-molecule bond density $\eta = 5.0$, and TB predicted energy gap of 1.39 eV.

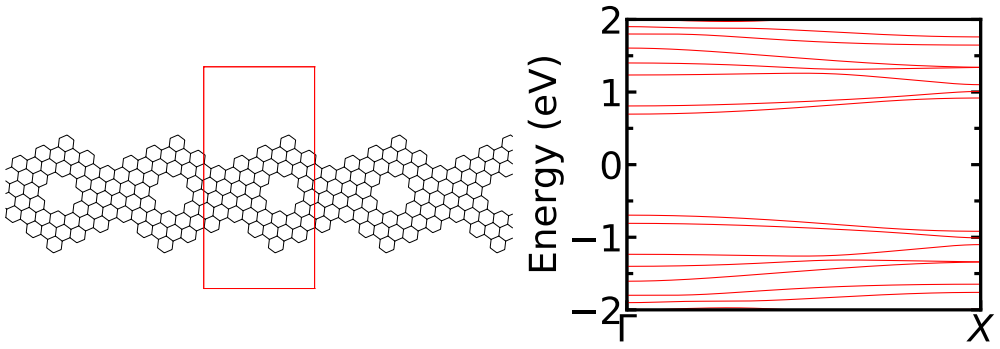

FIG. S39. Rc.

Rzb

Structure with label "Rzb" presenting 216 carbon atoms in the 1D unit cell, inter-molecule bond density $\eta = 3.0$, and TB predicted energy gap of 1.63 eV.

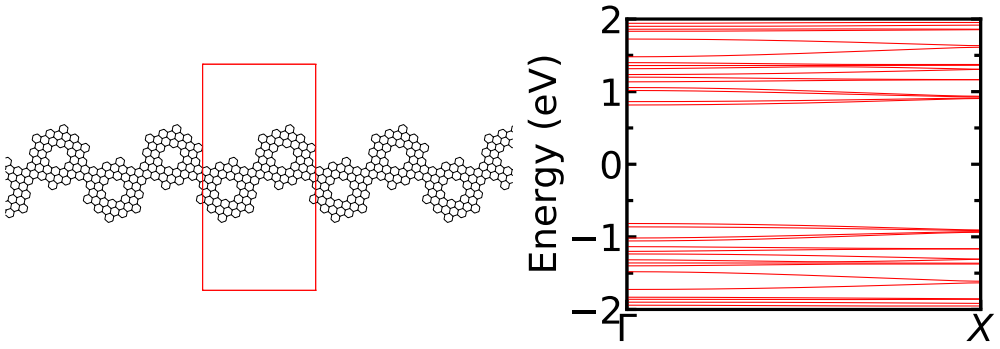

FIG. S40. Rzb.

Rzc

Structure with label "Rzc" presenting 216 carbon atoms in the 1D unit cell, inter-molecule bond density $\eta = 5.0$, and TB predicted energy gap of 1.34 eV.

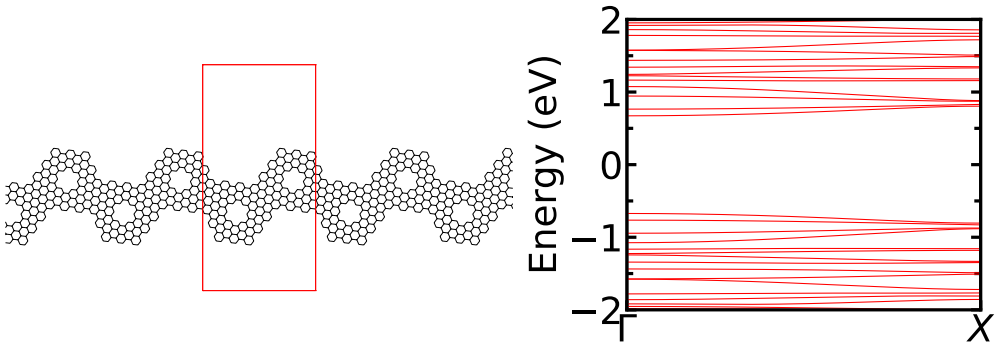

FIG. S41. Rzc.

* felipe.lima@lnnano.cnpem.br

† adalberto.fazzio@lnnano.cnpem.br