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DFT COMBINED WITH NEGF BASED TRANSPORT PROPERTY CALCULATION OF DISTORTED 2,2 ZIGZAG GRAPHENE NANORIBBONS

Engineering

KEYWORDS : Graphene nanoribbons, density functional theory, transport property calculation

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ABSTRACT

Because of the extraordinary versatility of nanomaterials which reveal a rich polymorphism of various allotropes exhibiting each possible dimensionality: fullerene molecule (0D), nanotubes and graphene ribbons (1D), graphite platelets (2D), and nano-diamond (3D) exhibiting different physical and chemical properties, carbon nanostructures are playing an important role in nanoscience and nanotechnology. Graphene ribbons were originally introduced as a theoretical model by Mitsutaka Fujita and co-authors to examine the edge and nanoscale size effect in graphene. Graphene nanoribbons (also called nano-graphene ribbons), often abbreviated GNRs, are strips of graphene with ultra-thin width (<50 nm). Transport calculations are carried out within the framework of density functional theory (DFT) combined with nonequilibrium Green's function (NEGF) method as implemented in the Atomic level virtual tool kit software package (trail version). A narrow ribbon with chiral indices (2, 2) corresponding to a zigzag graphene nanoribbon, 8 carbon atoms wide have been design using the builder tool of ATK. The parameters are: Aligned unit cell vector C with n=2, m=2 zigzag edge 8 atom wide with bond length 1.42086A⊕. The Stone–Wales defect by rotating a bond 45⊕, 90 and 135 have been created and the resultant transmission spectra shows a sharp scattering region .15eV above fermi level in comparision to the graphene nanoribbons without distortion.

INTRODUCTION

High electron mobility and long coherence length make graphene a subject of great interest for nanoscale electronic applications, even for the realization ofroom-temperature ballistic (dissipation-free) electronics. However, a major setback in the development of graphene-based field-effect transistors is the inability to electrostatically confine electrons in graphene, because a single layer of graphite remains metallic even at the charge neutrality point. In order to overcome this problem, a way to open a gap in the electronic structure of graphene has to be found. A straightforward solution is to pattern the graphene sheet into narrow ribbons. Thanks to recent progresses in preparing single graphite layers on conventional device setups, graphene nanoribbons (GNRs) with varying widths have been synthesized and characterized experimentally [1,2,3].

EXPERIMENTAL DETAILS

In this work ZGNR(Zigzag Graphene Nanoribbons) with n=2 and m=2 with 12 C axis repetition has been design. After building 2,2ZGNR the rotation angle of two center carbons has been changed to 45° , 90° 135° and the transport calculations were done. The details of building the ZGNR and electrode device is as follows.under the generalized gradient approximation (GGA).

COMPUTATIONS

Transport calculations are carried out within the framework of density functional theory (DFT) combined with nonequilibrium Green's function (NEGF) method as implemented in the Atomistix ToolKit (ATK) software package [3]. The two probes molecular device includes three regions: the left electrode, the right

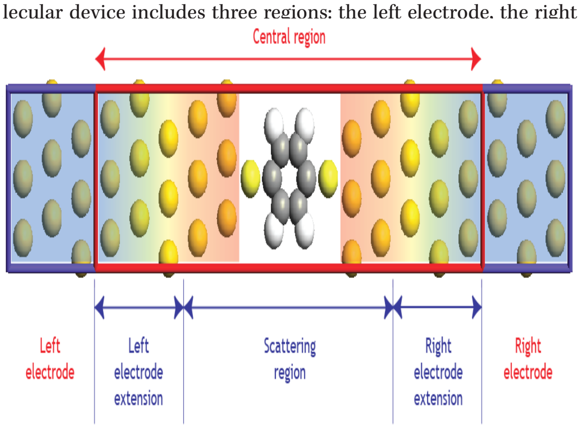


Figure 1: The scattering region plus an extension copy of the two electrodes forms the central region.

The **scattering region** is the part of the central region which is different from the electrodes. In the picture above it's obvious that the molecule form is most important ingredient of the scattering region. However, also the two outermost layers of the metal surfaces are in the scattering region, and are allowed to undergo reconstruction. The easiest way to build a device is usually to define the central region as a periodic extension of the intended electrode materials, then modify the scattering region (possibly inserting additional atoms, molecules, layers, etc), and finally extract the electrodes. The device geometry can then be optimized.

BUILDING THE TRANSPORT SYSTEM Narrow ribbon with chiral indices (2,2), corresponding to a ZGNR, 8 carbon atoms wide have been design using the builder tool of ATK. The parameters are: Aligned unit cell vector C with n=2, m=2 zigzag edge 8 atom wide with bond length 1.42086A°

In order to have a long enough ribbon to form the central region, we need to repeat the NR unit cell in the Z direction. The Stone–Wales defect by rotating a bond 45°, 90° and 135° have been created and the resultant GNR are as shown below (**Fig.2.1 to Fig.2.6**).

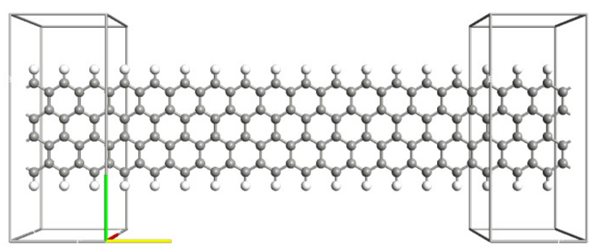


Figure 2.1:2,2ZGNR with C-C bond distortion of 0°

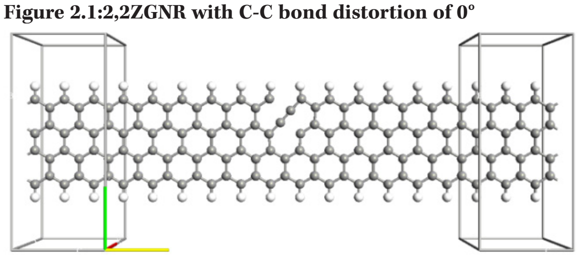


Fig.2.2 2,2ZGNR with C-C bond distortion of 45°

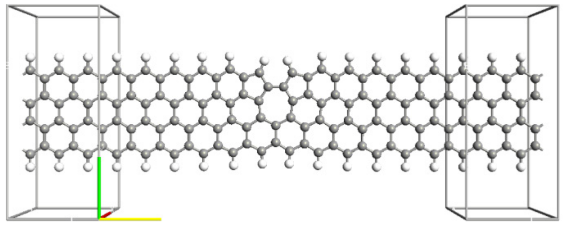


Fig.2.3 2,2ZGNR with C-C bond distortion of 90°

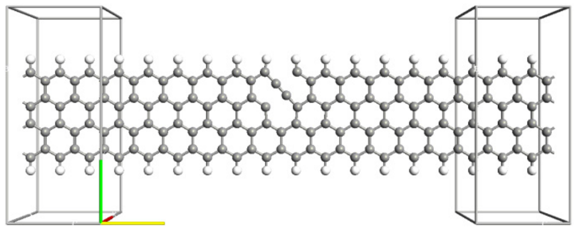


Fig.2.4 2,2ZGNR with C-C bond distortion of 135°

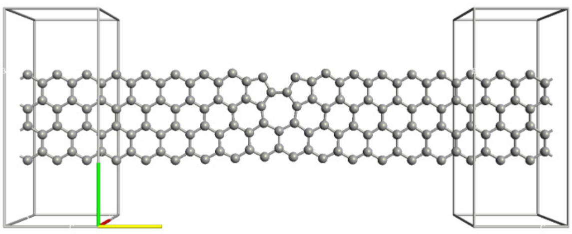


Fig.2.5 Both edge Hydrogen terminated 2,2ZGNR with C-C bond distortion of 90°

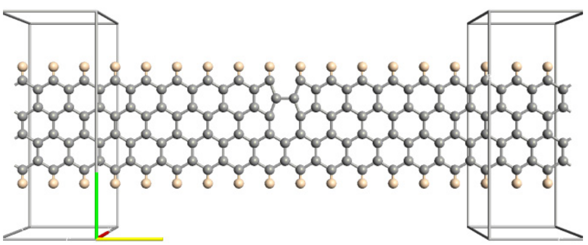


Fig.2.6 Both edge Si doped 2,2ZGNRwith C-C bond distortion of 90°

The Builder will automatically try to detect the periodicity of the region closest to the edges of the central region, and suggest possible electrodes. In order for this to work, there should be at least one full period plus one additional layer of the electrode present in the central region.

The suggestion 7.38 Å generates a reasonable electrode for this system (3 periods of the nanoribbon cell), so click OK to create the device geometry.

OPTIMIZING THE GEOMETRY

Although the geometry at this point resembles the desired structure, the Stone–Wales defect was just created by rotating the bond. In reality, the bond length also changes, to accommodate the new double-pair of pentagons and heptagons which are formed when the bond is rotated.

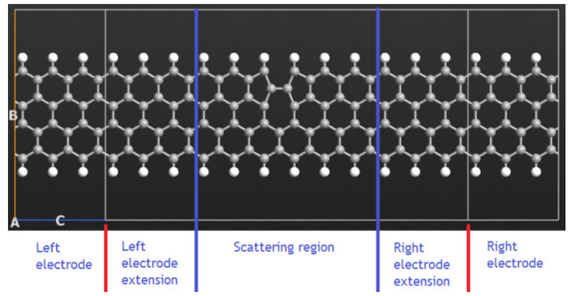
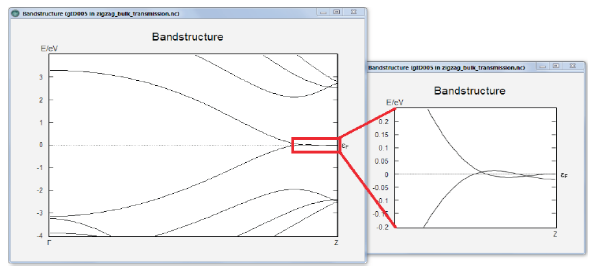


Figure 3.1: Final geometry of GNR

If you inspect the geometry carefully, you will find that it now has precisely the structure as depicted in the figure in the beginning of this chapter. In the figure (**Fig. 2.7**) below, the various regions are indicated for the GNR. The final geometry optimization and further computation of the transmission spectrum will be set up in the **Script Generator.**Figure 3.1: Band structure of the zigzag ribbon



ANALYZING THE RESULTS

Running the calculation, by dropping the script on the **Job Manager** (or send it to there from the Script Generator). It should take just a few minutes to finish. When it finishes, locate the NetCDF file in the file browser. Note that in addition to the analysis quantities, there are three configurations stored in the file; the first one is the original geometry calculated with the Brenner potential, the second one is the optimized geometry, also calculated with the Brenner potential, and the third one is the converged Hückel transport calculation.

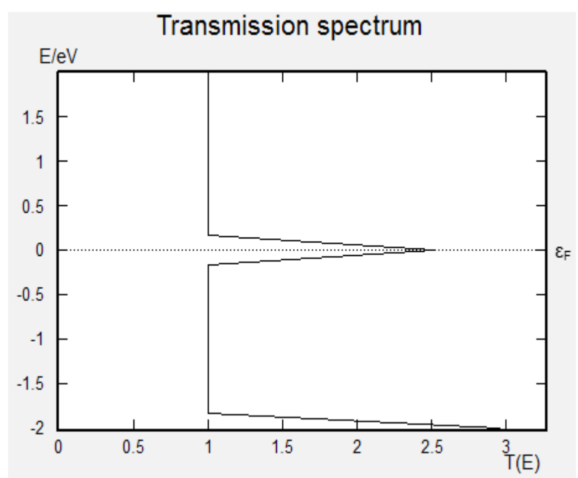


Figure 3.2: 2,2ZGNR (C-C bond distortion of 0°)

For a perfect zigzag graphene nanoribbon, i.e. if you had not introduced the defect, you would see perfect, integer transmission at all energies [4,5]. But in the system with the Stone–Wales defect the transmission is suppressed quite a lot, indicating strong scattering from the defect. The most prominent feature of the plot is the enhanced transmission around the Fermi level. This is due to a peculiarity in the band structure of the zigzag ribbon (Fig.3.1), and interestingly the enhancement is retained even if the ribbon is distorted [6] at least in the way that will be investigated.

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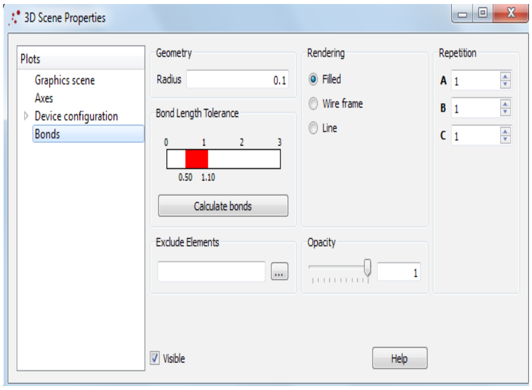

Figure 3.3: 3D Scene Properties

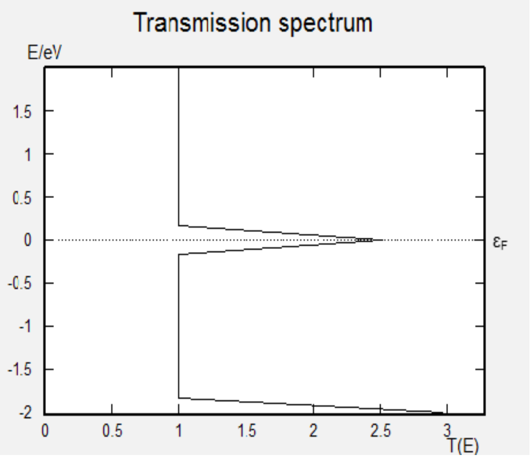

Figure 3.4: 2,2ZGNR C-C bond distortion of 45°)

Specifically, there is a very noticeable dip in the spectrum (C-C bond distortion of 90°) at about 0.15 eV above the Fermi level, where the transmission is almost completely blocked. That is why this energy was selected for the second transmission pathway; it will now be interesting to see how the electron propagates at this energy (**Fig.3.2 to 3.8**).

Next view is the transmission pathways. When it is ready the volume of each arrow indicates the magnitude of the local transmission between each pair of atoms, the arrow and the color designates the direction of the electron flow. The positions of the atoms are quite obviously deducible, but we can also add them explicitly by dropping the Device Configuration with id gID002 onto the plot. The bonds hide the arrows, however, so the best option is to plot them as lines.

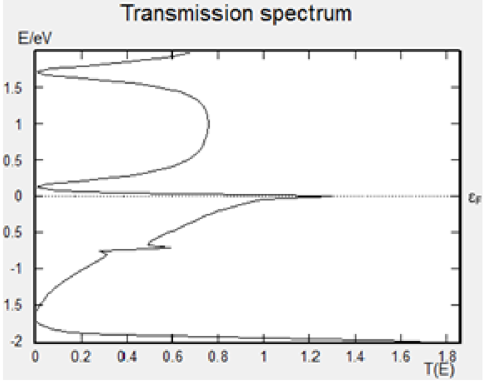

Figure 3.5: 2,2ZGNR (C-C bond distortion of 90°)Figure 3..6: 2,2ZGNR (C-C bond distortion of

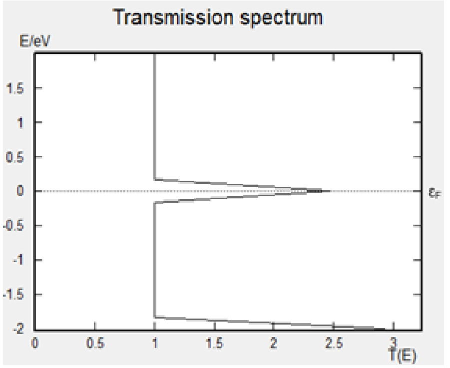

Figure 3..6: 2,2ZGNR (C-C bond distortion of 135°)

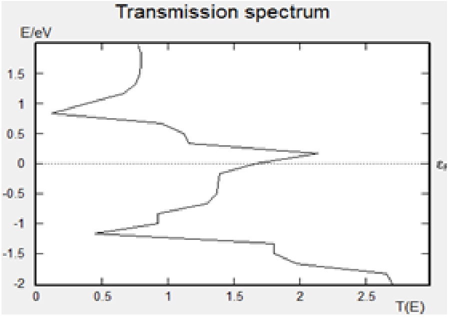

Figure3.7: 2,2ZGNR H-terminated (C-C bond distortion of 90°)

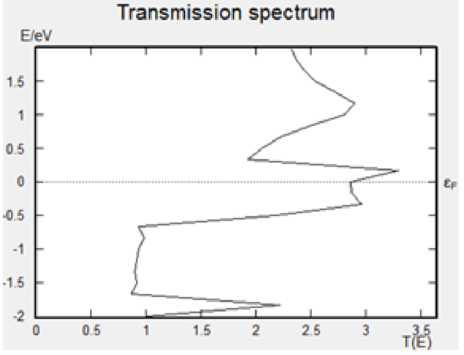

Figure 3.8: 2,2 ZGNR Si-doped (C-C bond distortion of 90°)

The final rendering of the transmission pathways at the two energies, zoomed in around the defect, will look as below:

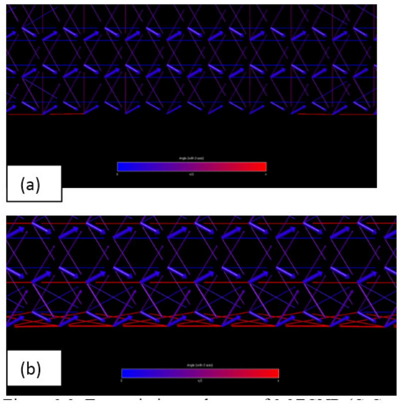

Figure 3.9: Transmission pathways of 2,2ZGNR (C-C bond distortion of 0°) at (a) Fermi level &. (b) Energy 0.15 eV above the Fermi level.

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CONCLUSION

To conclude, because of their remarkable electronic properties and structural physical properties GNRs are expected to play an important role in the future of nanoscale electronics [7,8]. They are mechanically very stable and strong and their carrier mobility is equivalent to that of good metals, suggesting that they would make ideal interconnects in nanosized devices.

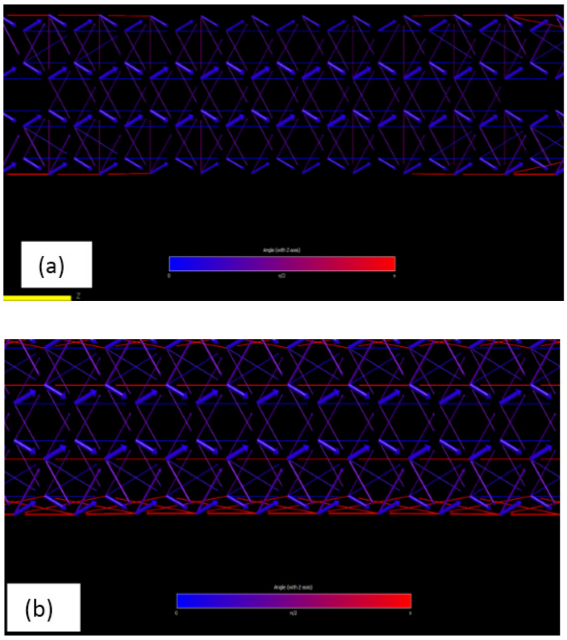


Figure 3.10: Transmission pathways of 2,2ZGNR (C-C bond distortion of 45°) at (a) Fermi level &. (b) Energy 0.15 eV above the Fermi level.

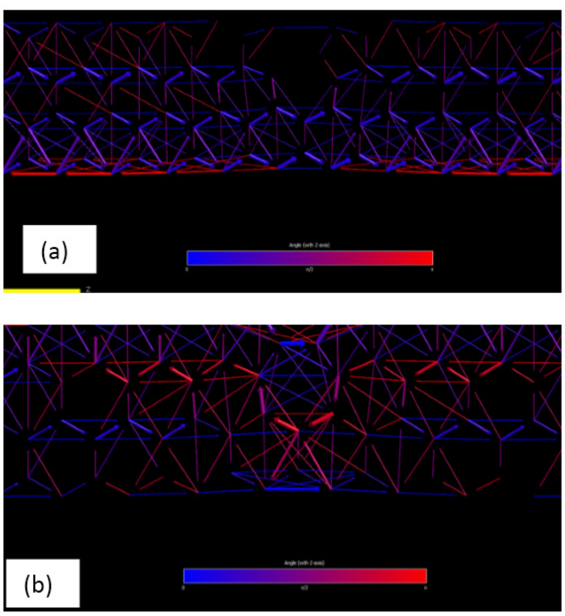


Figure 3.11: Transmission pathways of 2,2ZGNR (C-C bond distortion of 90°) at (a) Fermi level &. (b) Energy 0.15 eV above the Fermi level.

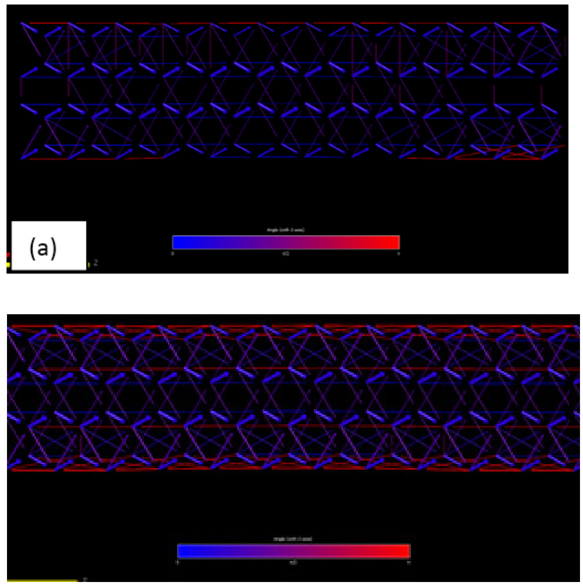


Figure3.12: Transmission pathways of 2,2ZGNR (C-C bond distortion of 135°) at (a) Fermi level &. (b) Energy 0.15 eV above the Fermi level.

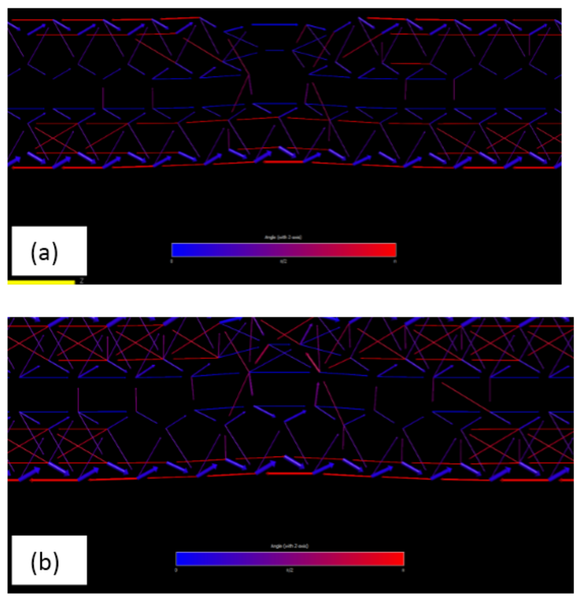
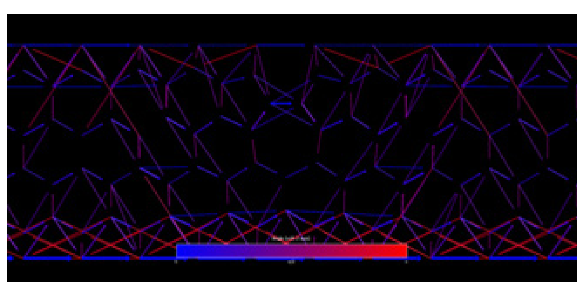


Figure 3.13: Transmission pathways of 2,2ZGNR H-terminated (C-C bond distortion of 90°) at (a) Fermi level & (b) energy 0.15 eV above the Fermi level.



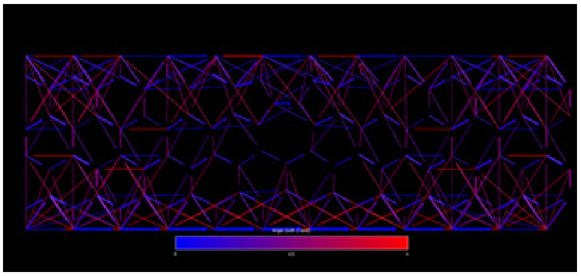


Figure 3.14: Transmission pathways of 2,2ZGNR Si-doped (C-C bond distortion of 90°) at (a) Fermi level (b) energy 0.15 eV above the Fermi level.

Further, the intrinsic semiconducting character of other nanoribbons, as controlled by their topology, allows us to build logic devices at the nanometer scale, as already demonstrated in many laboratories. Similarly the combination of 2D graphene for interconnects together with graphene nanoribbons for active field effect transistor devices could allow completely carbon-made nanoelectronics.

REFERENCE

1. X. Li, X. Wang, L. Zhang, S. Lee, H. Dai, Science 319, 1229 (2008) 2. L. Tapaszto, G. Dobrik, Ph. Lambin, L. Biro, Nat. Nano.3, 397 (2008) 3. K. Nakada, M. Fujita, G. Dresselhaus, M.S. Dresselhaus, Phys. Rev. B 54, 17 954 (1996) 4. V.M. Galitski, S. Adam, S. Das Sarma, Phys. Rev. Lett. 76, 245405 (2007). 5. A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, A.K. Geim, Rev. Mod. Phys. 81, 109 (2009). 6. M.Y. Han, B. Ozylmaz, Y. Zhang, P. Kim, Phys. Rev. Lett. 98, 206805 (2007). 7. L. Tapaszto, G. Dobrik, Ph. Lambin, L. Biro, Nat. Nano.3, 397 (2008). 8. K. Nakada, M. Fujita, G. Dresselhaus, M.S. Dresselhaus, Phys. Rev. B 54, 17 954 (1996).