Tight Binding Model of Nanopatterned Graphene

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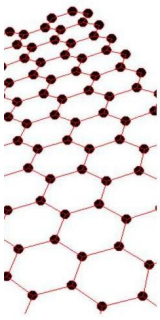
Motivation: *Carbon electronics*

- A single layer of carbon atoms arranged in an hexagonal motif is called graphene (a multilayer arrangement being called graphite).

- In 2004 graphene was prepared on a surface of silicon carbide by the group of Walter de Heer at Georgia Tech [Ber2004] opening the possibility of using conventional lithographic techniques to pattern the surface.

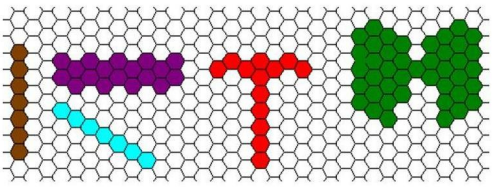
- In our research we theoretically explore the behavior of graphene sheets patterned in various shapes of future devices. In particular we explore the tunable bandgap of carbon nanoribbons and the ballistic transport of electrons on the graphene surface.

- We also explore the effect of an external electric field (applied through a gate) and we are working on including a magnetic field as an additional perturbation.



Designing the device

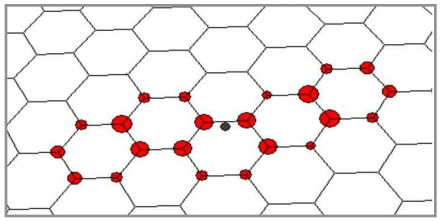
- The simulation programs allow the user to hand select the atoms of the graphene lattice that will form the device.
Patterns that could be tried include nanoribbons, "T"s, pairs of reservoirs, interconnects of various kinds and even nanowires.



Injection of electrons and their evolution

- The program allows the user to choose a point of injection of electrons that are subsequently monitored to observe their evolution.

- This part of the simulation is crucial to understand these novel devices because they depart from the traditional electronic devices that are based on bulk notions of diffusion and mobility, while on graphene quantum mechanics dominates.

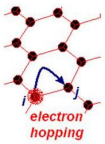


Tight binding model

- It is a simple approach to study the quantum mechanical behavior of electrons. It was already considered for carbon by Wallace in his seminal work on the band theory of graphite [Wal1947].

- It considers a hopping energy for electrons to move from atom to another.

- If only nearest neighbors are considered there is only one parameter in the Hamiltonian:



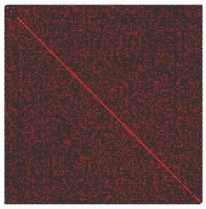
$$H_{if} = \begin{cases} V_o & \text{if atoms } i \text{ and } j \text{ are nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

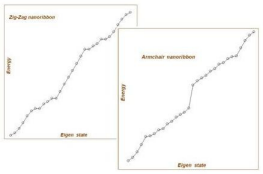
- For a given device made out of graphene this means that the Hamiltonian matrix will be sparse, which makes it easy to diagonalize using standard mathematical techniques such as the Jacobian method.

Calculating the Hamiltonian and diagonalizing the matrix

-Our programs use the device designed by the user to generate a Hamiltonian matrix that contains all the nearest neighbor potentials.

- The matrix so generated is diagonalized using the Jacobian method. This procedure has the option of showing the progress as a graphical depiction of the matrix elements.





The eigen-energies obtained from diagonalization show the expected semiconducting gap in the case of armchair ribbons and gapless distribution for zigzag cases.

We also obtain the eigenvectors that describe the evolution of the electrons when they move on the lattice.

Outlook

The addition of electric and magnetic fields to observe the effect of their perturbations is planned as the next step in these studies. Also the presence of thermal energy will be considered. This way more realistic devices will be simulated

References

Ber2004 Ultrathin epitaxial graphite: 2D electron gas properties and a route towards graphene-based nanoelectronics. C. Berger et al. J. Phys. Chem. B 108, 19912 (2004)

Wal1947 The Band Theory of graphite. P. R. Wallace, Physical Review 72, (9) 622-634 (1941)

Acknowledgements

This research was inspired in the simulation programs written by Dr. Walter de Heer to study the behavior of carbon nanotubes and nanoribbons in the years 2000 and 2001.

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