

Introdução às simulações computacionais em Grafeno

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Resumo

This research project addresses the graphene and their properties. Having learned how to calculate the distribution of electric charge density on the graphene network and how to represent them graphically intended to deepen the study and analysis of the effects of changes in the distribution of electron cloud in monolayers of graphene due to different types of disorder which Professor Dr. Ana Luiza C. Pereira, guiding this project, has researched in recent years using the tight-binding model. Among the studied defects we can mention the vacâncias¹⁻³ and defects at the edges.

Palavras Chave: Graphene, Disorders, Simulations.

Introdução

In last years the research and findings on graphene has had breakthrough. This new material obtained in the first time in 2004⁴, contains only one atom thick, consisting solely of carbon atoms linked in a two-dimensional hexagonal lattice. Besides being a two-dimensional material it exhibits a number of outstanding characteristics such as high mechanical strength, suppleness and flexibility. At room temperature, no other known material has higher electron mobility (It has the highest mean free path).

Resultados e Discussão

In all simulations, we used the tight - binding model to emulate the graphene network because this approach allows the various forms of disorders cited and a wide range of geometries. We can thus calculate energy spectra and densities of states (DOS).

By simulating several times with the same disorder network of sites it was possible to densify enough data to build the histograms in Figure 1.

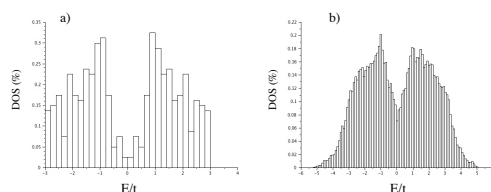


Figura 1. Histograms for networks with twenty to twenty carbon atoms with the sites disorder, one realization (a) and eight hundred realizations (b). Some simulations of ground states were done to assist in the understanding of the network geometry and the degenerated states.

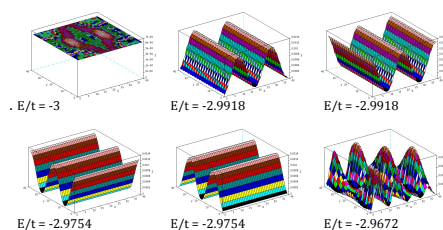


Figura 2. Graphical representations of electrical charge density in the six lower energy states of a 40X40 network carbon atoms with boundary conditions and without disorders. The x and y axes represent the network area while the z-axis electrical charge density.

Conclusões

In Figure 1 (b) it was possible to better characterize the histogram of the network and bring it closer to the numerical result, besides spending less time than simulate a larger network in order to get the same amount of data. In Figure 2, it was noticed that the lower energy waves get along parallel edges Zique-Zaque edges and degenerated states hapen in $E = -2.9918$ and $E = -2.9754$.

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¹ D. A. Bahamon, A. L. C. Pereira, P. A. Schulz, "Tunable resonances due to vacancies in graphene nanoribbons". *Physical Review B* 82, 165438 (2010).

² A. L. C. Pereira and P. A. Schulz, "Additional levels between Landau bands due to vacancies in graphene: towards a defect engineering", *Phys. Rev. B* 78, 125402 (2008).

³ A. L. C. Pereira and P. A. Schulz, "Graphene in the Quantum Hall Regime: Effects of Vacancies, Sublattice Polarization and Disorder", *Int. Journal of Mod. Phys. B* 12, (2009).

⁴ K. S. Novoselov et al., *Science* 306, 666 (2004).