CONTRIBUTED TALK

Aspects of graphene nanoribbon device simulations

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Graphene nanoribbons (GNRs) have been considered as strong candidates for electronics, since they incorporate some of the remarkable properties from graphene while presenting a band gap [1]. These structures can be fabricated nowadays with a high control on the edge structure with the so-called bottom-up approaches [2]. Together with these experimental breakthrough a major effort has been devoted to the theoretical and computational methods developments. In this talk I will show some challenging features found when simulating GNRs based devices, such as: 1. The effects on the transport properties of 4-terminal crossed GNRs devices when varying the structural parameters determining the crossing; 2. The effect of substitutional chemical defects on the transmission channels and the importance of a proper description of the electrostatics in quasi 1-dimension systems.

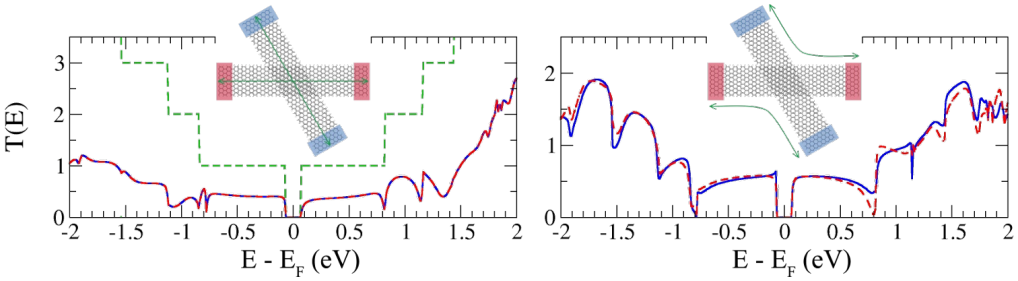

Figure 1: Direct (left) and inter-ribbon (right) transmissions at V=0 in a crossbar system with 60˚ rotation angle.

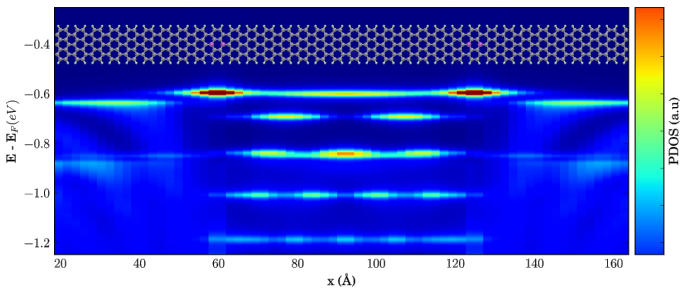

Figure 2: Project density of states from a substitutional boron-doped armchair graphene nanoribbon.

[1] L. Yang *et al.*, Phys. Rev. Lett. **99**, 186801 (2007).
[2] J. Cai *et al.*, Nature **466**, 470-473 (2010).