Transport properties of hydrogen-passivated graphene systems

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The transport properties of graphene nanoribbons as described by the p_z tight binding theory and its Dirac low-energy approximation predict metallic dispersion relation for zigzag and armchair nanoribbons with 3n+2 atoms across the channel. For these ribbons formation of perfectly conducting channels is predicted by the theory [1]. In fact, the transport experiments resolve a finite transport gap [2, 3] near the neutrality point for all types of nanoribbons. The finite band gaps originate from quantum confinement, edge disorder effects, and/or passivation [4, 5, 6] of the dangling bonds at the edges of the ribbon. Formation of energy gaps is reported by the ab-initio calculations [5, 6] for the dispersion relation of the nanoribbons.

In this paper we study the transport properties of nanoribbons with hydrogen-passivated edges and discuss the effects of the passivation for the systems based on nanoribbons as electron scatterers. We use the tight binding approach using three p/d orbitals per atom [6] and develop a version of quantum transmitting boundary method [7] to study the transport with the Landauer approach. We confront the results obtained for the passivation model agains the results of a single-p_z tight binging model. Our study involves graphene nanoribbons perturbed by external potentials and quantum point contact of various geometries.

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