DFT study of the graphene nanoribbon quantum dots

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Low-energy electrons in graphene behave like massless particles and obey the two-dimensional Dirac-like equation[1] due to the gapless linear band structure of the material near the charge neutrality point. The confinement of such particles by the external electrostatic potential is excluded because of a perfect transmission through potential barriers at normal incidence (the Klein tunneling [2]). There exists several methods to open the gap. One of those methods is to use the finite strips of the graphene called nanoribbons [3]. It has been shown both theoretically [3] and experimentally[4] that such structures exhibit a band gap and therefore the confinement by the external potential is now possible.

In this work we present a DFT study of the quantum dots defined within the graphene nanoribbon with armchair edges only. The quantum dot is defined by the electrostatic potential defined at the center of the sample. We evaluate the one-electron results as obtained by the standard tight-binding method for the p_z orbitals located on the carbon sites. From the one-electron spectrum we select a certain number of the valence and conduction band states near the charge neutrality point and use them for calculations of the electron-electron interactions as introduced by the DFT method. Using the restricted space allows us to make calculations for the quite large structures (up to 15 thousands carbon sites). We discuss charging the quantum dot induced inside the ribbon by electrons and holes, conditions for stability of confined electron system and the charge localized within the quantum dot as a function of the Fermi energy and the quantum dot potential depth, as well as transport gaps open by top and back gate potentials For a neutral system the modification of the lateral confinement - with introduction of the flake into the ribbon – does not induce formation of a localized charge puddle. Nevertheless, the excess electrons – when present within the system – get localized within the flake already in the absence of the external potential. A good qualitative correspondence with the transport gaps observed in Ref. [4] as functions of the back gate and the top gate potentials is found.

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References

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