Energy structure of graphene quantum dots with edge relaxation

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The effect of strain inducing atoms' displacements is investigated in graphene quantum dots (GQDs) [1,2] and graphene nanoribbons (GNRs) [3-6]. The process of the edge relaxation affecting the band structures of GQDs and GNRs is studied. We investigate nanostructures of different shapes (hexagonal and triangular), sizes, and edge types (armchair and zigzag). For small systems, a comparison is made of simple tight-binding (TB) model to the case of the nanostructure geometry optimized within density functional theory (DFT) methods [7]. A change of the bond length between the atoms located at the edges produces variable hopping integral. We express hopping energy as a function of atomic distance in terms of Chebyshev polynomials [8]. We show that increasing with the lattice distance, hopping term accounts for the larger energy gap. An influence of hopping values variations on edge states in nanostructures with zigzag edges is investigated. We analyze the effect of hopping changes on the energy spectrum in a wide range of the hopping energies [8]. Our studies allow us to derive accurate TB model in order to investigate electronic properties of graphene nanostructures of sizes not accessible within DFT methods.

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