Ab initio studies of graphene and BN nano-ribbons

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We present a theoretical study of structural and electronic properties of graphene and boron nitride nano-ribbons. The study is based on the *ab initio* calculations in the framework of the density functional theory. We determine the morphology of the zig-zag and armchair nanoribbons of various widths and further calculate their band structure and density of states. These studies shed light on the physical mechanisms leading to the opening of the band gap in armchair graphene nanoribbons and the role of edge states in this process. In particular, the studies provide theoretical predictions concerning the magnitude of the band gap energy as a function of the ribbon's width in the armchair graphene and all types of boron nitride nanoribbons and confirm the metallic character of zig-zag graphene nanoribbons. Further, the morphology and electronic structure of multilayers consisting of graphene and boron nitride nanoribbons has been examined. The performed electronic structure calculations provide the spontaneous spin polarization of the structures and allow also for the studies of magnetic properties of the investigated systems. At the end, we investigate the electronic structure of graphene nanoribbons doped with B and N, and compare it to the correspondingly doped two-dimensional systems.

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