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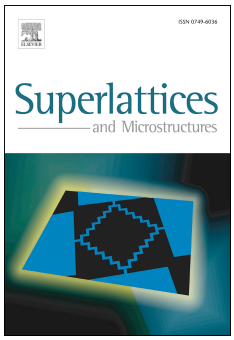

Structural analysis, electronic properties, and band gaps of a graphene nanoribbon: A new 2D materials

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Structural Analysis, Electronic Properties, and Band Gaps of a Graphene Nanoribbon: A New 2D Materials

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Abstract

Graphene nanoribbon (GNR), a new 2D carbon nanomaterial, has some unique features and special properties that offer a great potential for interconnect, nanoelectronic devices, optoelectronics, and nanophotonics. This paper reports the structural analysis, electronic properties, and band gaps of a GNR considering different chirality combinations obtained using the p_z orbital tight binding model. In structural analysis, the analytical expressions for GNRs have been developed and verified using the simulation for the first time. It has been found that the total number of unit cells and carbon atoms within an overall unit cell and molecular structure of a GNR have been changed with the change in their chirality values which are similar to the values calculated using the developed analytical expressions thus validating both the simulation as well as analytical results. Further, the electronic band structures at different chirality values have been shown for the identification of metallic and semiconductor properties of a GNR. It has been concluded that all zigzag edge GNRs are metallic with very small band gaps range whereas all armchair GNRs show both the metallic and semiconductor nature with very small and high band gaps range. Again, the total number of subbands in each electronic band structure is equal to the total number of carbon atoms present in overall unit cell of the corresponding GNR. The semiconductors GNRs can be used as a channel material in field effect transistor suitable for advanced CMOS technology whereas the metallic GNRs could be used for interconnect.