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Investigation and Application of Zig-zag and Armchair Edged Graphene Nanoribbons in Nanoscale Electronic Devices

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Abstract **–** This study investigates the roles of the edge and substrate effects of zig-zag and armchair graphene nanoribbons on atomic and electronic structures of graphene. Graphene is a two-dimensional flat monolayer of carbon atoms packed into a honeycomb lattice. It is made out of carbon atoms arranged in hexagonal structure. Graphene has a high electronic mobility and high charge carrier concentrations. Series of simulations with Zig-zag and Armchair nanoribbons are made using Gold, Copper, and Indium. The electron-electron interactions of the nanoribbons' molecules are calculated with generalized gradient approximation (GGA) through Perdew-Burke-Ernzerhof (PBE) exchange correlation. The k-points are set to 1 x 1 x 50 for n_a, n_b, and n_c, respectively. The electron temperature of 300K is used. The C – C bond length between the carbon atoms in graphene nanoribbon is 1.24 Å. The superposition of the various orbitals in the nanoribbon leads to the variation in the Density of States (DOS). The Projected Density of States (PDOS) on the edge is mainly consistent around Fermi level. Electron Density calculations show regions with large electron density, which are found around the atoms, and their bonds. The observed nanotubes may have great potential for the application in nanoscale electronic devices fabrication and can be used as gate in the FET transistors.

Keywords**:** density of states, projected density of states, electron density, graphene nanoribbon, brillouin zone, fast-speed FET, nanoscale electronic device