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Electronic, magnetic and transport properties of graphene nanoribbons[1]

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The recent fabrication of a single graphite layer opens a new possibility in the area of nanoelectronics. These experimental findings motivated us to study a novel one dimensional nanomaterial – a graphene nanoribbon (GNR). Based on a first-principles approach, we have established the scaling rules for electronic energy bandgaps as a function of ribbon width. Both armchair and zigzag edged GNRs, with homogeneous edges passivated with hydrogen, are shown to have bandgaps, differing from the results of simple tight-binding calculations or solutions of the Dirac's equation based on them. Our *ab initio* calculations show that the origin of energy gaps for GNRs with armchair shaped edges arises from both quantum confinement and the crucial effect of the edges. The variations in energy bandgap of GNRs with armchair shaped edges exhibit three distinct family behaviors. For GNRs with zigzag shaped edges, gaps appear because of a staggered sublattice potential on the hexagonal lattice due to edge magnetizations. Based on electronic structure calculations on GNRs, we present two novel phenomena in GNRs and GNR nano-constrictions. First, our calculations show that the magnetic properties of nanoribbons can be controlled by electric fields. In particular, half-metallicity is predicted in GNRs if in-plane homogeneous electric fields are applied across zigzag shaped edges of these systems. Such asymmetric electronic structure for each spin originates from the fact that the spatially separated spin polarized states with opposite spin orientations in the semiconducting GNRs are shifted oppositely in energy by the applied fields. This closes the gap associated with one spin orientation and widens the other. Second, in GNR nano-constrictions with armchair shaped edge, conductances are shown to depend on the family behavior of energy gap of GNRs forming nano-constrictions. Depending on the width of nano-constriction, the incoming electrons from GNR leads are shown to experience perfect transmissions or nearly complete reflection in a wide range of energy. This work has been collaborated with M. L. Cohen and S. G. Louie.

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