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Substitutional impurities in halfmetallic graphene/h-BN nanoribbons. ANDREA LATG, MARCIO COSTA, CARLOS LEON, Instituto de Fsica, Universidade Federal Fluminense, Niteri-RJ, Brazil — Zigzag graphene nanoribbons (ZGNRs) present a half-metallic response for a critical external electric field value-with possibilities for spin-filter applications. On the other hand, embedded ZGNRs in zigzag hexagonal boron nitride (ZBNNR) exhibit half-metallicity without the presence of an external field. In this work, we analyze electronic properties of a mixed nanoribbon system (ZBNR/ZGNR/ZBNR), using a Hubbard model Hamiltonian within a mean field approximation. Due to different electronegativities of the boron and nitrogen atoms, an electric field is induced across the ZGNR strip, breaking the spin degeneracy of the electronic band structure. Edge potentials as corrections for on-site energies are investigated, and also how they are affected due to the ZBNNR/ZGNR interfaces. Substitutional impurities are found as a mechanism to enhance half-metallic response. Here we analyze the effect of N and B impurities along the GNR and also through the interfaces. Energetic stabilities of the different configurations studied were included. We found that energy gap sizes may be properly engineered by controlling the spatial doping process and that binding energy impurity calculations may be used to study impurity diffusion processes along the mixed nanoribbons.

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