Half-metallicity in strained graphene nanoribbon devices with vacancies

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Spin-filtering devices, used to generate currents with well-defined net spin populations, are of major interest for spintronics. These elements are exemplified by *half metals*, materials that are metallic for one spin orientation, while acting like semiconductors or insulators for the other. This contribution deals with transport properties of zigzag Graphene Nanoribbons (zGNRs) which are studied by density functional theory (DFT) in conjunction with Green's function analysis. In particular, spin transport through longitudinally strained zGNR (12,0) devices is investigated under the condition of ferromagnetic coordination of the ribbon edges. Several configurations with two vacant sites in the edge and the bulk region of the zGNR device are derived from this system. ZGNR devices with vacancies in the edge regime turn out to exhibit half-metallic behavior, acting as perfect spin filters for well-defined choices of the strain and the bias. In the alternative structure, characterized by vacancies in the bulk regime, spin currents with majority orientation prevail. Magnetocurrent ratios are calculated for these systems. With respect to both the sign and the size, these quantities depend sensitively on the device parameters, i.e. the vacancy locations, the bias, and the amount of strain. These results are interpreted in terms of density-of-states distributions, transmission spectra, and transmission operator eigenstates.