Spin Transport Properties of Armchair Graphene Nanoribbons with Substitutional Transition Metal atoms

Frank Hagelberg

Department of Physics and Astronomy, East Tennessee State University,
Johnson City, TN 37614, USA

Abstract

The spin-dependent transmission properties of (0,8) graphene nanoribbons with *n* substitutional transition metal ™ atom impurities (*n*TM–aGNRs, *n* = 1,2) have been studied by use of the non-equilibrium Green's function (NEGF) method in conjunction with density functional theory (DFT). Emphasis is placed on the spin-filtering activity of transmission elements based on these structures. In particular, it is shown that the limit of half-metallicity is approached by (0,8) GNRs with one or two substitutional Fe atoms, where the spin polarization of the current traversing the GNR is controlled by the bias across the device. This effect is rationalized by means of bandstructure and partial-density-of-states (PDOS) analysis. An occupied spin minority state, induced by the Fe-atom moiety and close to the Fermi energy of *n*Fe–aGNR, accounts for the predominance of minority spin polarization. Comparison with nanosystems derived from *n*Fe – aGNRs, involving vacancies rather than impurities, or both types of defects, reveals that substantial degrees of current spin polarization prevail across a wide variety of device types.