Spin Filter Properties of Armchair Graphene Nanoribbons with Substitutional Fe Atoms

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The spin-dependent transmission properties of (0,8) graphene nanoribbons (GNRs) with Fe atoms at substitutional sites have been studied by use of the non-equilibrium Green's function (NEGF) method in conjunction with density functional theory (DFT). The emphasis of this presentation is placed on the effectiveness of these nanomaterials as spin filters. Several configurations of the type *n*Fe-aGNR, with n =1, 2, were analyzed in terms of the magnetocurrent ratio (MCR) as a function of the bias. For both single and double substitution, the results are seen to vary sensitively with the number and the substitutional sites of the atomic impurities. A further parameter of relevance for the case of double substitution is the relative orientation of the magnetic moments of the two impurities. MCR values exceeding 80 percent were recorded for both single and double substitution. In particular, high spin polarization efficieny is found for an arrangement involving two Fe atoms substituted at bulk sites along the aGNR length coordinate. This effect is seen to diminish with increasing distance between the impuritiy atoms.

Qualitative explanations of the oberserved spin polarization effects can often be given in terms of the transmission spectrum at zero bias in combination with total and partial density-of-states distributions. For adequate description of the current-voltage profiles, however, taking into account the bias dependence of the transmission function proves to be imperative.