

DFT calculation of spin-dependent transport properties of Z-shaped graphene nanoribbons

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The recent fabrication of single layer graphene has promoted huge expectations in the field of all-carbon nanoelectronics and spintronics. The possibility to pattern graphene nanoribbons (GNRs) with widths of few tens of nm, has enabled band-gap engineering and the development of efficient GNRs-based spin filters. The lateral confinement of the 2DEG in GNR induces finite bandgap in semi-metallic graphene. It has been predicted that the electrical properties of GNR can be tuned from perfectly metallic, for zig-zag edge ribbons, to semiconducting behaviour, for armchair ribbons. In this later case, the gap varies with the ribbon width, length and topology [1].

We performed density-functional theory (DFT) based calculations to obtain electronic structure of armchair/zig-zag/armchair Z-shaped GNRs [2] with a large variation of geometrical parameters. The spin-dependent exchange-correlation potential is approximated within the generalized gradient approximation (GGA) using the QuantumWise toolkit ATK, which employs local numerical double-zeta polarized basis orbitals. The spin-dependent transport properties of the electrode-device-electrode geometry were calculated by means of non-equilibrium Green's function formalism as implemented in ATK [3].

The GNR lateral asymmetry produces strong spin-dependent behavior resulting in a large spin polarisation effect. It is shown by analyzing the GNR transmissivities. Our results endorse that for the generation of spin-polarized currents, formation of spin-ordered edge-localized states along the zigzag edges is the key mechanism [4, 5]. In the case of antiferromagnetic spin orientation at the opposite GNR edges spin dependent transmissivities appear when zigzag edges are long enough (Fig. 1). We analyzed the influence of the GNR width and of the lengths of arm-chair and zig-zag parts (Fig. 2). The first calculations of gate electrode influence is performed as well (Figs3, 4). Since GNRs have long spin-correlation lengths and good ballistic transport characteristics they can be considered as a promising active material of spintronic devices without the need of ferromagnetic electrodes or other magnetic entities [6]. The spin filtering structure could be prepared by the nanolithography of GNR.

References

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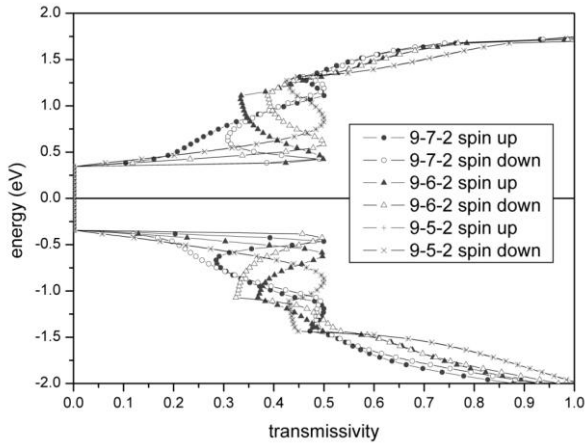


Fig 1.

Transmissivities of Z-shaped GNR with the width of 9 carbon atoms, two arm-chair segments with length of 2 carbon atoms and middle zig-zag part with length of 7, 6, and 5 carbon atoms for electrons with spin up and spin down orientations. No spin polarisation appears for the GNR with the shortest arm-chair part.

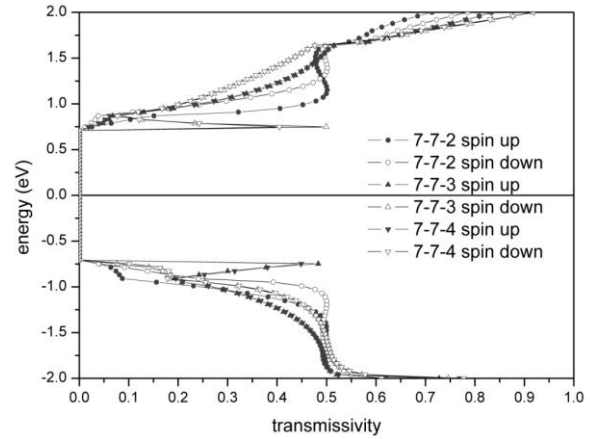


Fig. 2

Transmissivities for spin up and spin down of Z-shaped GNR with the width of 7 carbon atoms, two arm-chair segments with length of 2, 3 and 4 carbon atoms and middle zig-zag part with length of 7 carbon atoms. The GNRs with 3 and 4 carbon atoms in arm-chair segments show almost the same behavior.

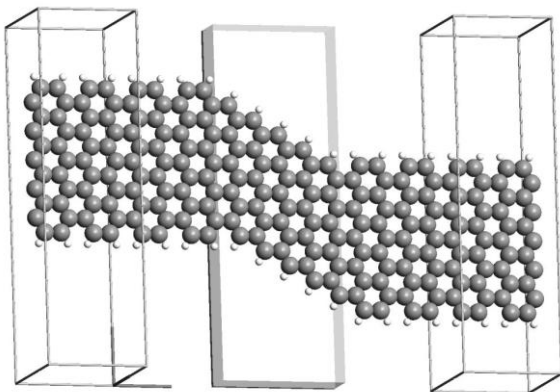


Fig. 3

Structure of Z-shaped GNR with the width of 11 carbon atoms, two arm-chair segments with length of 2 carbon atoms and middle zig-zag part with length of 7 carbon atoms and the gate beneath the zig-zag part.

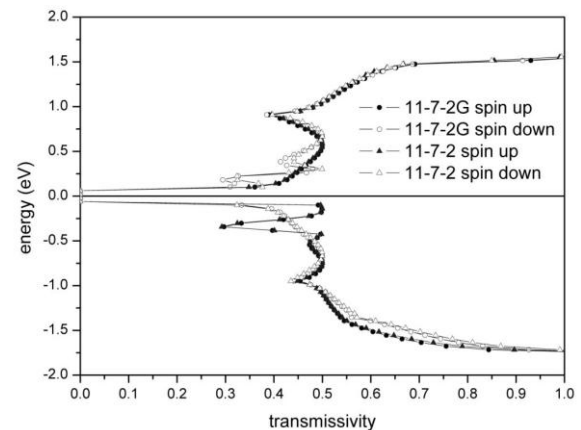


Fig. 4

Transmissivities for spin up and spin down of Z-shaped GNRs from Fig. 3 with (G) and without the gate beneath the zig-zag part. The gate potential is the same as at the both electrodes. The transmissivities are almost the same for this gate potential.