Quantum spin transport in carbon chains with graphene-like contacts.

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Linear carbon chains (or carbynes) have been recently synthesized via electronic irradiation of graphene inside a transmission electron microscope [1, 2, 3], showing experimental evidence of carbon chains terminated on graphitic fragments, as suggested in previous works about amorphous carbyne-rich pure carbon films produced via supersonic cluster beam deposition [4, 5]. The connections between carbon chains and graphitic nanofragments have the twofold effect of stabilizing the chain [6] and providing contacts for measurements, suggesting a possible use in nanoelectronics. In addition, the monatomic C chain can be considered as the smallest possible interconnect in all-carbon nanodevices [7].

To validate the latter applications, first-principles and non-equilibrium Green's functions methods are used to investigate the spin-polarized electronic transport properties of monatomic carbon chains covalently connected to graphene-like contacts as graphene nanoribbons (GNR). This study [8] reveals that a net spin polarization is always present on odd chains [Fig. 1], while even chains are not spin polarized. Besides, quantum electron conductance of the chain-GNR system is characterized by narrow resonant states resulting from the simultaneous presence of open conductance channels in the contact region and on the chain atoms. Such a behavior could be suggested as the physical mechanism underlying the observed on/off switching of graphene nanodevices [9]. Most interestingly, the magnetic and electronic properties of the complex chain-GNR structures can be tuned by tailoring graphene edges shape and chain parity to achieve any combination of spin polarization and electrical conductivity as semiconducting non spin-polarized, metallic spin-polarized, and even semiconducting spin-polarized systems, opening the way for the design of a new kind of spintronic nanodevices with tunable magnetic and conducting properties.

References

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Figures

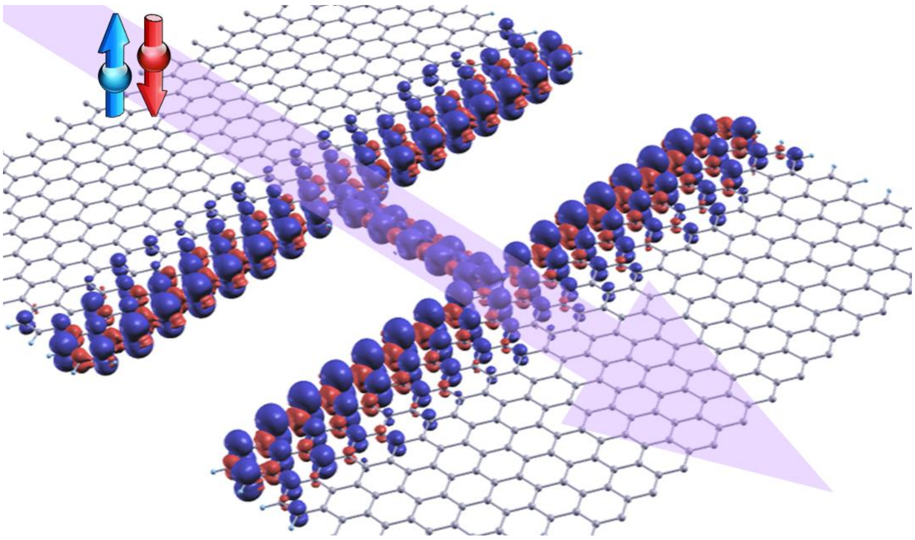

Figure 1. *Spin density ($\rho\uparrow - \rho\downarrow$) on the C_9 monatomic carbon chain between armchair graphene nanoribbon (A-GNR) contacts. Blue and red correspond to positive and negative isodensities of $\rho\uparrow - \rho\downarrow$. The lilac arrow indicates the spin-transport direction. [Z. Zanolli, et al., ACS Nano **4** (2010) 5174–5180].*