KEY ELECTRONIC PROPERTIES OF GRAPHENE NANO-RIBBONS

Armchair-edge GNRs

The nearest-neighbor π-orbital tight-binding model indicates that armchair-edge GNR (A-GNR) with $N + 1 = 3q$ should be metallic (or nearly metallic if more sophisticated models are used). Here N is the number of atoms in zigzag dimer chain across A-GNR, and q is a positive integer. A-GNRs with $N + 1 \neq 3q$ are predicted to be semiconducting. For A-GNR its metallic or semiconducting nature is determined purely from geometrical considerations: A-GNR width equals the integer number of half-wave lengths in the transversal direction. The wave functions in metallic A-GNRs corresponding to a single channel conductance window with energies lying near the Fermi level (E_F) are evenly spread across the A-GNR. That means the edge imperfections (missing or extra edge atoms) have a strong influence on the wave function and result in a strong backscattering. One may also think of an extra or missing edge atoms as of small fragments of semiconducting A-GNRs incorporated into originally metallic ribbon. Therefore A-GNRs with edge imperfections have mobility band gap: even though there are energy states near E_F the transmission in the single channel window can be very low (Ref. [1]). This statement is illustrated in Fig. 1 depicting the conductance, G, of a perfect (green line) and corresponding edge-disordered (black line) 1 μm long, 6.40 nm wide (N = 53), metallic armchair-edge strip. The *only* form of disorder present in the imperfect armchair-edge strip is a 10% concentration of edge defects as it is illustrated for a short segment in the insert.

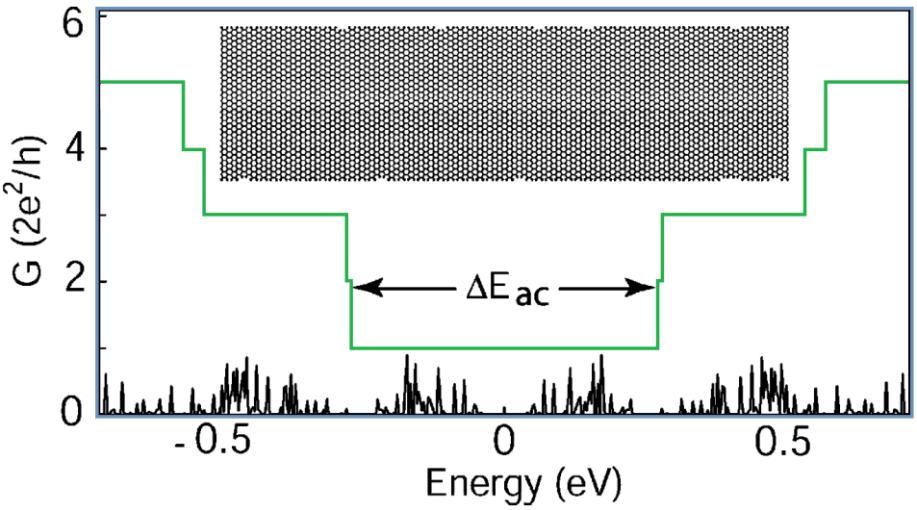

Figure 1

Zigzag-edge GNRs

The nearest-neighbor π-orbital tight-binding model without spin polarization indicates that zig-zag-edge GNRs (Z-GNRs) are metallic for any ribbon width. Figure 2 dispersion plots for Z-GNRs with 20 and 64 carbon atoms in the unit cells are presented.

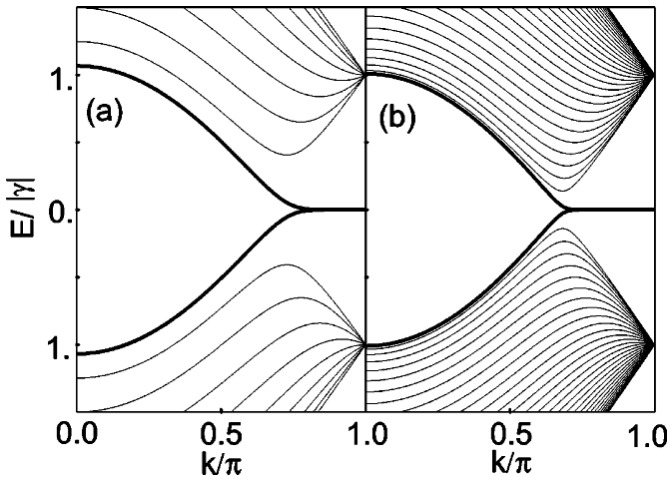

Figure 2

However, the flat portion of the dispersion curve nearest to the E_F suggests that simple π-orbital model is insufficient. There are several counterbalancing terms in the Density Functional Theory (DFT) expression for the total energy. The first major term called exchange-correlation energy (E_{xc}) always decreases with increasing spin polarization. The second major term is called Band Energy and denoted as E_B. It is a sum of energies of all single-electron states. E_B can be obtained by integrating over wave number k all dispersion curves multiplied with the Fermi function. In the spin unpolarized system Fermi energy E_F^0 is the same for spin-up and spin-down states. If the number of, let us say spin-up electrons prevails, then, according to the Pauli's principle, the spin-up electrons have to occupy states higher than E_F^0, and spin-down electrons empty the states with the energies below E_F^0. That would increase E_B (for simplicity we assume that for spin polarized state the band structure remains the same). In most materials it appears that the gain in E_B has greater absolute value than the E_{xc}, and hence it is energetically unfavorable for the material to be in a spin polarized state. The exceptions are the materials with nearly flat half-filled band (cf. Fig. 2), because changing occupancies of spin-up and spin-down bands does not change E_B (energies of occupied and unoccupied states are nearly the same). That makes spin-polarization energetically favorable and hence an extra term should be added to a conventional tight-binding Hamiltonian. As it is explained in Ref. [2], combination of π-orbital nearest-neighbor tight-binding and the Hubbard capture all necessary physics and yields the correct band structure. Figure 3 presents the band structure of Z-GNR with 40 atoms in the unit cell in the presence of spin polarization.

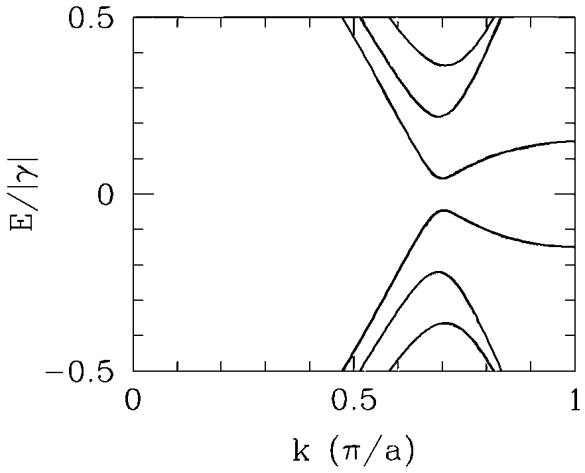

Figure 3

At non-zero temperature the spin polarization is not continuous. Figure 4 presents possible spin distribution in Z-GNR (bottom). Simulation results were obtained for self-consistent spin-polarized model from initially random spin distribution (top).

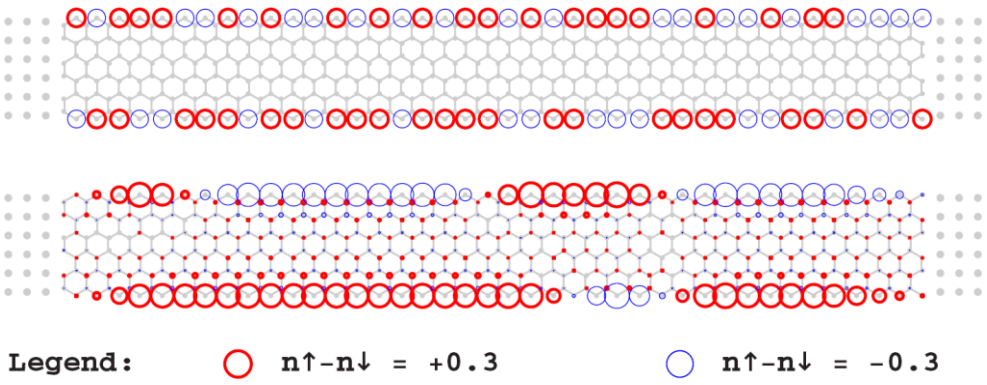

Figure 4

Simulations presented in Ref. [2] demonstrate that passing an electric current along the strip can switch it from spin-polarized state (Fig. 3) to spin unpolarized state (Fig. 2). The critical voltage, at which such transition occurs, depends on the ribbon length and contacts quality. The shorter is the ribbon and the better is the contact, the lower is the threshold voltage. The band gap collapse can be recognized by the abrupt current increase, which makes the experiment conceptually simple. Plotted in Fig. 5 is the I-V curve of the 22-atoms-wide Z-GNR 6.4 nm long. The contact coupling was matched to correspond to experimentally measured contact resistance of 60 kΩ.

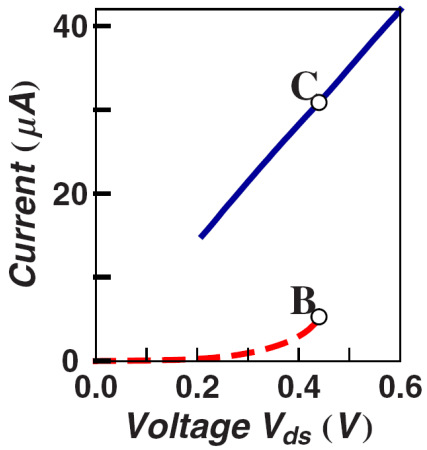

Figure 5

So far all experimentally observed graphene nano-ribbons (GNRs) exhibited semiconducting behavior. The GNR type (zigzag or armchair) in most experiments is unknown. The GNR length is usually tens of nanometers and applied voltages are below (length-dependent) threshold.

Therefore the spin-induced band gap collapse has neither been experimentally confirmed nor proven impossible. This topic still awaits experimentalists to say their "final word".

Another interesting property of Z-GNR is discussed in Ref. [3]. It appears that Z-GNR 60° turns are highly reflective and 120° are virtually transparent. The computations assumes no spin-polarization. If the effect will be observed experimentally, the transmission differences between 60° and 120° turns are expected to be less pronounced due to the spin-induced band gap.

[1] D.A. Areshkin, D. Gunlycke, C.T. White, "Ballistic Transport in Graphene Nanostrips in the Presence of Disorder: Importance of Edge Effects", NANO LETTERS v.7, p.204 (2007)

[2] D.A. Areshkin, B.K. Nikolic, "I-V curve signatures of nonequilibrium-driven band gap collapse in magnetically ordered zigzag graphene nanoribbon two-terminal devices", PRB v.79, 205430 (2009)

[3] D.A. Areshkin, C.T. White, "Building blocks for integrated graphene circuits", NANO LETTERS, v.7, p.3253 (2007).