Electronic and magnetic structure of zigzag graphene nanoribbons: quantum chemical calculations

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Zigzag graphene nanoribbons (zGNR) due to their unique and peculiar edge states are one of the most interesting graphene nanostructures from the fundamental point of view. They are promising also for applications [1]. Therefore, thorough quantitative information about their structure is needed. To gain this information we have performed quantum chemical calculations of zGNRs using well tested for carbon systems semiempirical molecular orbital PM3 method [2]. Our calculations have been done for one-dimensionally periodic infinite nanoribbons of different width using Born–von Karman boundary conditions. We have calculated antiferromagnetic (AFM) and ferromagnetic (FM) ground states of zGNRs. The AFM state of 4zGNR (consisting of four zigzag carbon chains) is found to be lower in energy by 0.3 eV/atom than FM state. These states differ in their geometrical structures considerably. Calculations of electron energy band structures of FM and AFM states of zGNR show that AFM state is a semiconductor with the band gap decreasing with the number N of carbon chains in NzGNR, while FM state is a semimetal. The conductivity of the FM state of zGNR is localized in edge states.

[1] Graphene and its fascinating attributes / Eds. S.K. Pati, T. Enoki, C.N.R. Rao (New Jersey: World Scientific, 2011) 270 p.
[2] J.J.P. Stewart. J. Comp. Chem., 10 (2), 209–264 (1989).

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Electrical Conductivity of Single-Wall Carbon Nanotubes Films

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We report results of experimental investigations of electrical conductivity of carbon nanotubes films fabricated from single-wall carbon nanotubes (SWCNTs) bundles comprising individual nanotubes of different length (in the range from 150-300 nm up to 2 μm).
The samples were prepared by spraying of the isopropanol-SWCNTs suspension or water-sodium dodecyl sulfate (SDS)-SWCNT suspension onto substrates with 4 parallel Pd electrodes with length of 5 mm and width of 5 μm. SWCNTs produced by arc-discharged method or by gas-phase catalysis (HiPCO process) with diameter of 1.2-1.5 nm were used as pristine nanotubes for preparation of homogeneous SWCNTs dispersions. The substrates were heated during spraying to rapidly evaporate at temperature 120 ^{0}C.
Temperature dependencies of the resistance R(T) and IV-characteristics were measured in the temperature range 2-300 K in close-cycled refrigerator Cryogenics in order to determine charge transport mechanisms in the samples. Carbon nanotubes films obtained from isopropanol-SWCNT suspension show negative temperature coefficient of resistance ($dR/dT<0$) in the whole investigated temperature range. A crossover between metallic ($dR/dT>0$) and non-metallic ($dR/dT<0$) temperature dependence of the resistance was observed for SWCNT films prepared from water-SDS-SWCNT suspension. Nonlinear IV- characteristics observed for all types of samples with nonlinearity rising as the temperature decreased.

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