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Spin channels in functionalized graphene nanoribbons GIOVANNI CANTELE, CNR-INFM and University of Napoli "Federico II", YOUNG-SU LEE, Korean Institute of Science and Technology, DOMENICO NINNO, University of Napoli "Federico II", NICOLA MARZARI, Massachusetts Institute of Technology
— Graphene nanoribbons have attracted lot of interest, due to high potentiality in technological applications, mostly in graphene-based nanoelectronics. Electronic and transport properties may strongly be influenced by the crystallographic orientation as well as by the presence of defects and different chemical functionalizations. Among the possible edges, the zigzag ones deserve special attention, because it has been shown that magnetic ordering is obtained in the ground state, so as half-metallicity and spin-filtering behavior could in principle be observed under suitable experimental conditions. Here we show how the chemistry of the ribbon edge and surface may strongly affect the transport properties. Quantum conductance is calculated, with ab-initio accuracy, by combining a maximally localized Wannier function approach and the Landauer formula. We show that proper functionalization of the edges may strongly modify the electronic properties. Chemical species adsorbed on the nanoribbon surface can, on the other hand, significantly affect the spin channels, giving rise in some cases to an almost perfect spin-filtering behavior.

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