Magnetic zigzag graphene nanoribbons from carbon nanotubes

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Recently, zigzag graphene nanoribbons (ZGNR) has been proposed as a new type of carbon based magnetoresistive device due to their remarkable electronic properties**[1]**. The appearance of flat bands at the Fermi energy associated with edge states leads to magnetic moments localized at the edges**[2,3]**. The resistance of the whole structure strongly depends on the relative orientation of these magnetic moments and usually decreases when this orientation goes from antiparallel to parallel by applying an external magnetic field.

So far, experimental research on ZGNRs has been hampered due to difficulties in the fabrication of ribbons with well-defined and controlled edges. Recent work **[4,5]** shows the possibility of fabrication of these nanodevices by chemically unzipping metallic (n,n) carbon nanotubes (CNTs) (see figure). Here we study the emergence of magnetism and the relation between conductance and spin order for these unzipped CNT's using density functional theory (DFT) calculations and compare with results obtained with the Hubbard model**[6]**. It is, however, an open question whether or not magnetism survives since this is dependent on the specific chemical saturation of the open edges. We address this question for both hydrogen and oxygen saturated edges. We use the Landauer formalism with the Green's function approach for the conductance calculation.

We also explore the magnetoresistive properties of CNT's and ribbons with non-magnetic edges after doping with hydrogen. It is known that a single hydrogen atom on top of a carbon atom in graphene has a magnetic moment. In the case of a low concentration of hydrogen dopants, it is believed that the ground state features local moments with zero total spin. We show that an application of a strong enough magnetic field can spin polarize the system and reduce the resistance.

References:

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Figures: