Graphene with enhanced spin-orbit coupling: Multiple quantum phases

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Abstract

Functionalization with heavy atoms has been predicted to locally enhance the spin-orbit coupling in graphene [1] and turn it into a topological insulator [2]. For graphene ribbons, this would result in a quantum spin Hall phase, with polarized edge channels and a $2e^2/h$ quantized conductance in the energy region of the topological gap. However, at present, any experimental confirmation of such a phenomenon is critically lacking.

In this contribution, we focus on the case of thallium adatoms and show how their clustering might be responsible for this failure. Our numerical codes based on the Landauer-Büttiker and Kubo-Greenwood approaches, allow us to simulate both edge (in graphene ribbons) and bulk (in 2D graphene) electronic transport for samples of realistic size. Adatom clustering is shown to have a detrimental effect on the formation of the topological phase (see Fig.1), since it leaves large areas of graphene uncovered, where the effective spin-orbit coupling vanishes. Very intriguingly, we report a transition from the quantum spin Hall phase to the spin Hall effect upon thallium segregation [3], with a residual spin accumulation at the sample edges (see Fig.2). Such a phenomenon is related to the rise of local currents around the clusters, whose chirality depends on the spin orientation and that result in low-energy bulk extended states, as evidenced by a robust minimum conductivity $\sim 4e^2/h$ (see Fig.3).

References

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[2] C. Weeks et al, Phys. Rev. X **1** (2011) 021001.
[3] A. Cresti, D. Van Tuan, D. Soriano, A.W. Cummings, and S. Roche, Phys. Rev. Lett. **113** (2014) 246603.

Figures

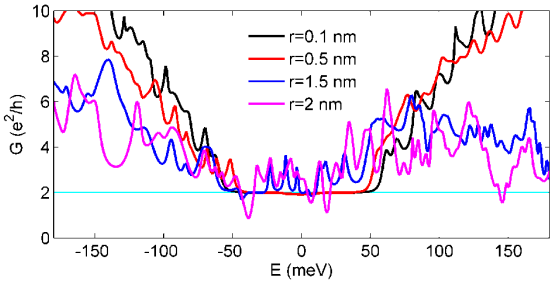

Fig.1: Conductance as a function of the electron energy *E* for a 50 nm wide and 50 nm long graphene ribbon with doped contacts and a 15% of thallium adatoms in clusters with radius *r* from 0.1 nm to 2 nm. Note the detrimental effect of clustering on the conductance plateau in the region of the topological gap (from about -50 meV to 50 meV).

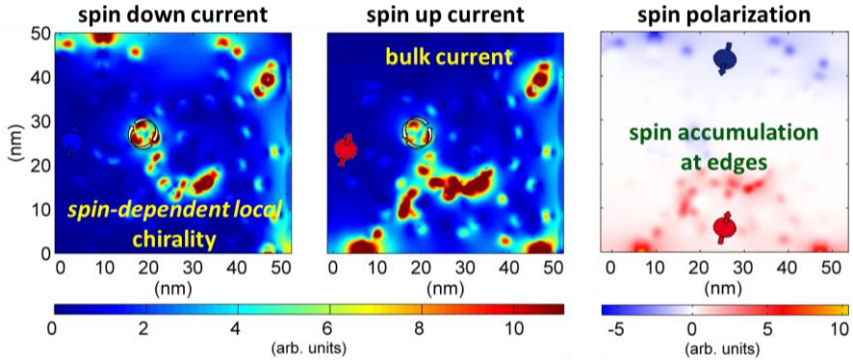

Fig.2: Local distribution of spin-resolved spectral current and polarization in the ribbon described in Fig.1 for *r*=1.5 nm at *E*=15 meV. The current flows through the bulk (breakdown of the topological gap) and forms spin-dependent chiral currents around the clusters (the indicated arrows are an example). The local spin polarization shows accumulation at edges resulting from a spin Hall effect.

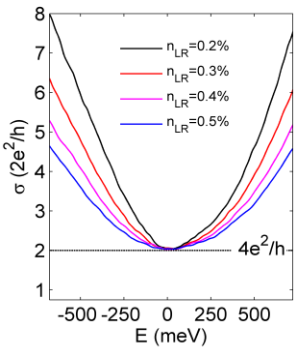

Fig.3: Conductivity of 2D graphene with a 15% of clustered thallium atoms and different densities of long-range impurities.