Topological insulator graphene by heavy atom adsorption: Impact of segregation

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Since the prediction of the existence of topological insulators in 2005 [1,2], graphene has been considered a promising platform for their observation. However, due to the extremely weak intrinsic spin-orbit coupling, realizing a topological phase in pristine graphene is experimentally unattainable. There are several recent proposals to artificially increase the spin-orbit coupling by chemical modifications of graphene or the realization of hybrid structures. In particular, the adsorption of heavy adatoms has been predicted to introduce locally strong spin-orbit coupling [3]. This would allow the engineering the topological phase and the observation of the quantum spin Hall regime in graphene. However, all experimental attempts to confirm such a new possibility have remained unsuccessful to date. Here, we illustrate how this failure might be determined by adatom segregation, which is experimentally unavoidable. Moreover, we show that the adsorbate clustering can induce bulk extended states of original nature.

In the present contribution, we consider thallium adatoms randomly distributed (non-segregated or clustered) over graphene, see fig.1. Thallium adatoms place above the center of carbon hexagons and induce an effective spin-orbit coupling between the carbon atoms of the involved plaquettes ($\mathcal{R}$). The system is described by a standard effective tight-binding model [1-3]

$$\mathcal{H} = -\gamma \sum_{\langle ij \rangle} c_i^\dagger c_j + \frac{2i}{\sqrt{3}}\lambda \sum_{\langle\langle ij \rangle\rangle \in \mathcal{R}} c_i^\dagger \vec{s} \cdot (\vec{d}_{kj} \times \vec{d}_{ik}) c_j - \mu \sum_{i \in \mathcal{R}} c_i^\dagger c_i + \sum_i V_i c_i^\dagger c_i$$

where γ =2.7 eV is the nearest-neighbor coupling, λ=54 meV the spin-orbit coupling, μ=270 meV the local energy shift and we considered the possible presence of a superimposed potential *V*. We investigate transport in both a two-terminal configuration (by using the Green's function formalism) and a 2D configuration (by using the Kubo-Greenwood approach).

Our results for non-segregated adatoms confirm the onset of a topological phase with the observation of a quantum spin-Hall regime, where the two-terminal conductance is quantized to $2e^2/h$ in the region of the topological gap and spin-polarized currents flow at the ribbon edges, see figs.2(a,b). Upon segregation of adatoms into islands with radius between 2 and 3 nm, the conductance is no more quantized in the region of the topological gap, where it becomes higher and fluctuating, see fig.2a. This breakdown of the spin-Hall phase can be understood by looking at the local density-of-states of the injected electrons reported in fig.2(c). Contrary to the case of scattered adatoms, electrons flow through the bulk. The explanation of such a behavior is that the induced spin-orbit coupling vanishes in the region between the islands, where electrons can flow as in a normal conductor. The distance between the islands, though short, does not allow the proximity effect observed for non-segregated atoms to take place. We can conclude that segregation has a detrimental effect on the quantum spin Hall phase and leads to the failure of its observation [4].

When considering the conductivity of a two-dimensional system, we observe the transition from topological insulator (for non-segregated adatoms) to a metal (for clustered adatoms) with a minimum conductivity at the charge neutrality point of about $4e^2/h$, see fig.3(a). The value of the minimum conductivity is stable in the presence of long-range disorder of different strengths, and, more importantly, the quantum diffusion coefficient does not undergo localization, see fig.3(b), thus indicating the extended nature of the states.

References

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[3] C. Weeks, J. Hu, J. Alicea, M. Franz, and R. Wu, Phys. Rev. X, **1** (2011) 021001.
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Figures

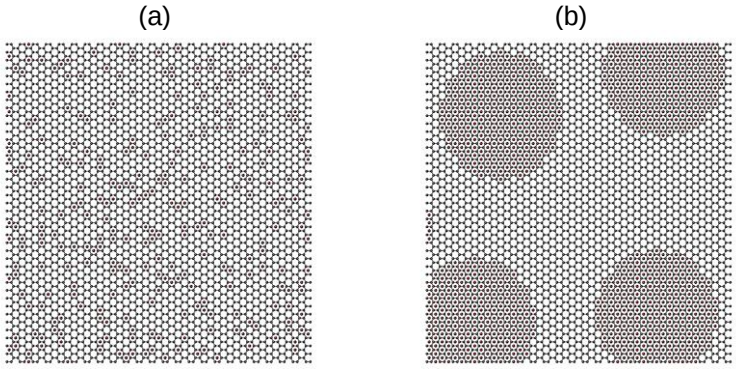

Figure 1: (a) Non-segregated thallium adatoms adsorbed over graphene. (b) Thallium adatoms clustered into islands with a radius of 2 nm. For given adatoms density, the distance between the islands increases as their radius increases.

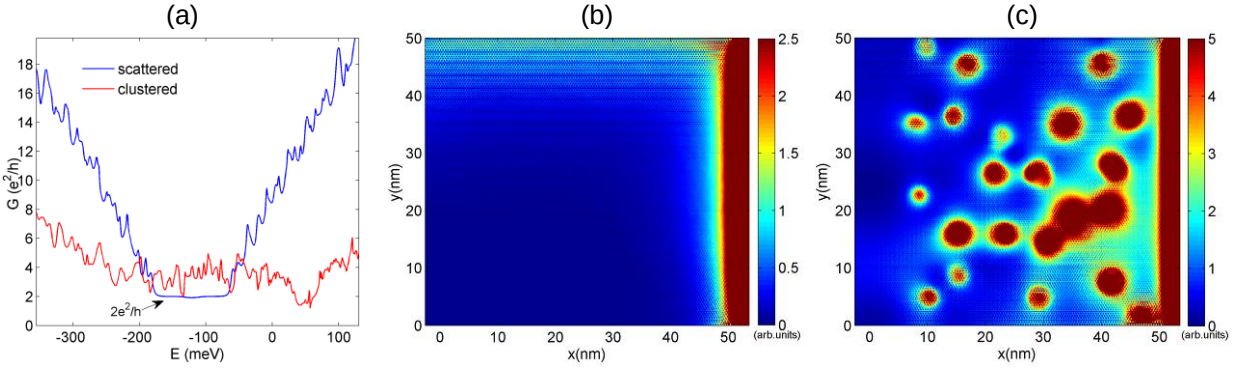

Figure 2: (a) Zero-temperature differential conductance of a graphene ribbon of width 50 nm with a section of length 50 nm functionalized with a density n=15% of scattered or clustered (with island radius between 2 and 3 nm) thallium adatoms. (b) Local density-of-states for spin down electrons injected from the right contact at energy -100 meV. Spin-down electrons flow along the top edge. Spin-up electrons, not shown here, flow along the bottom edge. Such a spatial chirality gives rise to a quantum spin-Hall phase. (c) Same as (b) for clustered adatoms.

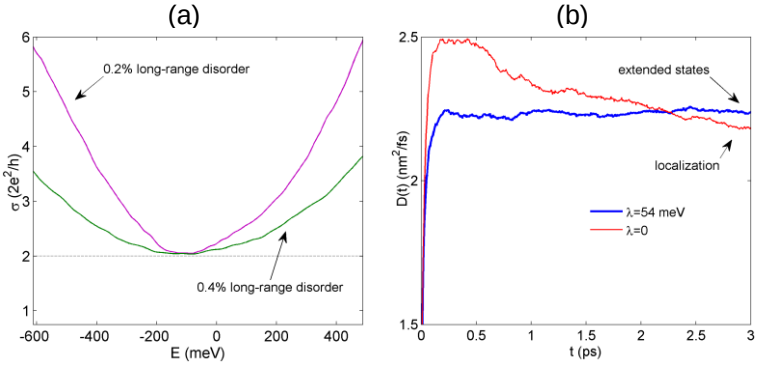

Figure 3: (a) Kubo-Greenwood conductivity for 2D graphene with thallium adatoms segregated into islands with radius up to 3 nm. Different concentrations of long-range disorder (with strength Δ=2.7 eV) have been considered. Note the minimum conductivity of about $4e^2/h$. (b) Time-dependent diffusion coefficient when spin-orbit coupling is active or inactive in the system. Extended states are observed in the presence of spin-orbit coupling.