Electronic and transport properties of unbalanced sublattice N-doping in graphene

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The incorporation of foreign atoms into the carbon honeycomb lattice has been widely investigated in order to modify the electronic and chemical properties of graphene [1,2]. In contrast with conventional materials, the effect of foreign atoms in a 2D material, such as graphene, is expected to depend significantly on the position and surrounding of each atom due to the quantum confinement of the electrons [2]. Recent scanning tunneling microscopy and spectroscopy studies of nitrogen doped graphene have revealed how the incorporation of this foreign atom into the sp^2 lattice occurs. Joucken and coworkers showed that the exposure of graphene to a nitrogen plasma flux after synthesis leads to an homogeneous distritution of substitutional atoms [3]. However, when a nitrogen source is introduced during the CVD growth of graphene, the nitrogen incorporation exhibits a preferential accomodation within one of the two triangular sublattice that compose the honeycomb lattice [4,5]. This wayward incorporation of nitrogen atoms into graphene is not hitherto understood. Nevertheless, the consequences of this peculiar atom arrangement on the electronic and transport properties of graphene are adressed in this work.

Electronic structure and transport properties of nitrogen-doped graphene with a single sublattice preference are investigated using both first-principles techniques and a real-space Kubo-Greenwood approach. Such a break of the sublattice symmetry leads to the appearance of a true band gap in graphene electronic spectrum. A band gap opening due to an ordered superlattice of dopants has already been discussed [6,7]. However, such a periodic doping configuration is rather difficult to envisage experimentally. In this work, we demonstrate the robustness of the band gap opening for the case of a random distribution of dopants in the same sublattice. In addition, a natural spatial separation of both types of charge carriers at the band edge is observed, leading to a highly asymmetric electronic transport. For such N-doped graphene systems, the carriers at the conduction band edge present outstanding transport properties with long mean free paths, high conductivities and mobilities. This phenomena is explained by a non-diffusive regime, and originates from a low scattering rate. The fact that corresponding electrons reside mainly in the unaltered sublattice explains such low scattering rate.

The presence of a true band gap along with the pesistence of carriers traveling in an unperturbed sublattice suggest the use of such doped graphene in GFET applications, where a high I_{ON}/I_{OFF} ratio is needed. The present simulations should encourage more investigation and specific measurements on N-doped graphene samples where such an unbalanced sublattice doping has been observed.

References

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Figures

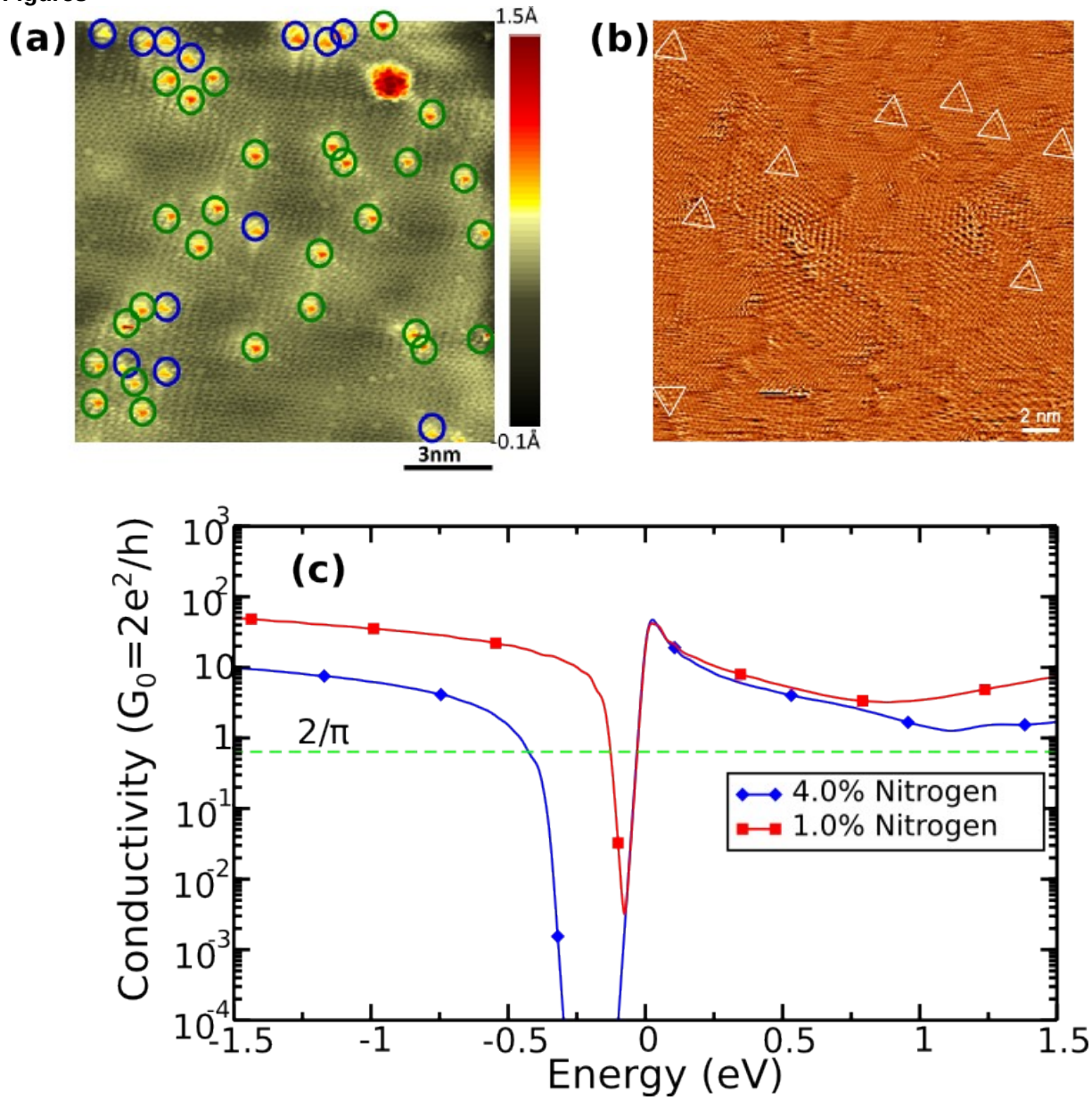

Figure 1. STM images of nitrogen doped graphene obtained by incorporation of N during growth: (a) single substitution [4], and (b) double substitution [5]. (c) Calculated semiclassical conductivities in graphene for various concentrations of N dopants randomly distributed in one sublattice [8].