Quantum transport in N-doped graphene and in atomic carbon chains

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The incorporation of foreign atoms into graphene has been widely investigated in order to modify its electronic and chemical properties. In contrast with conventional materials, the effect of foreign atoms in a 2D material is expected to depend significantly on the position and the local environment of each atom due to the quantum confinement of the electrons. When a nitrogen source is introduced during the CVD growth of graphene, the nitrogen incorporation exhibits a preferential accommodation within one of the two triangular sublattices that compose the honeycomb network [1]. *Ab initio* STM images and computed local density of states reveal specific signatures for each type of nitrogen defects, which are then correlated with experimental STM/STS measurements, thus confirming such a unbalanced sublattice N-doping in graphene (although not hitherto understood). Electronic structure and transport properties of N-doped graphene with a single sublattice preference are then investigated using both first-principles techniques and a real-space Kubo-Greenwood approach [2]. Such a breaking of the sublattice symmetry leads to the appearance of a true band gap in graphene electronic spectrum even for a random distribution of the N dopants. 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 carrier at the conduction band edge present outstanding transport properties including long mean free paths, high mobilities and conductivities. Such a transport behavior can be explained by a non-diffusive regime (quasi-ballistic transport behavior at the conduction band edge), and originates from a low scattering rate [2]. The presence of a true band gap along with the persistence of carriers traveling in an unperturbed sublattice suggest the use of such N-doped graphene in G-FET applications, where a high I_{ON}/I_{OFF} ratio is expected. The present *ab initio* simulations should encourage more investigation and specific transport measurements on N-doped graphene samples where such an unbalanced sublattice doping is observed.

Carbyne, the sp^1-hybridized phase of carbon, is still a missing link in the family of carbon allotropes. Despite many efforts in synthetic chemistry, bulk phases of carbyne remain elusive, and this type of carbon material is believed to be unstable. However, in recent years the elementary constituents of carbyne, i.e., linear chains of carbon atoms, have been observed in the electron microscope. Hence, isolated atomic chains exist and are highly interesting one-dimensional conductors that have stimulated considerable theoretical work. Because of the challenge involved in the controlled synthesis and characterization of carbon chains, experimental information is still very limited. Recently, detailed electrical measurements and first-principles electronic transport calculations have been performed on monoatomic carbon chains [3-4]. When the 1D system is under strain, the current-voltage curves exhibit a semiconducting behavior, which corresponds to the polyyne structure of the atomic chain with alternating single and triple bonds. Conversely, when the chain is unstrained, the ohmic behavior is observed in agreement with the metallic cumulene structure with double bonds. This confirms a recent theoretical prediction, namely that a metal-insulator transition can be induced by adjusting the strain. The key role of the contacting leads is also scrutinized by *ab initio* quantum conductance calculations, explaining the rectifying behavior measured in monoatomic carbon chains in a non-symmetric contact configuration.

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