Electronic and transport properties of graphene due to its functionalization using dopants, chemical groups or metallic clusters

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Graphene exhibits extraordinary structural and electronic properties and is thus a promising candidate for various fields in nanotechnology such as nanoelectronic devices, gas sensing or even as a catalytic substrate (when its atomic structure is modified). The goal of the present work consists in investigating using first-principles techniques how the properties of graphene can be tuned using chemical functionalization or when its surface is decorated with metallic nanoclusters.

At first, the quantum transport properties of graphene nanoribbons have been calculated in presence of hydroxide (OH-) and hydrogen (H+). The quantum conductance is found to be altered by these chemical groups which play the role of scattering centers. Indeed, some specific conduction drops can be observed either at the right or at the left of the Fermi energy, depending on the nature of the impurities. Consequently, our calculations suggest the possible use of these graphene-based devices as pH nanosensors.

Secondly, the interaction of small gold clusters with defected graphene (including vacancies) has been studied ab initio in order to check the modification of their catalytic properties. Small gold clusters are known to preferentially adopt a planar structure in free space, but their atomic structure is not reported in presence of a planar substrate. The role of the vacancy defect consists in pinning the gold cluster at the graphene surface. Our ab initio calculations predict that these small clusters conserve their stable planar configuration on top of the graphene sheet. The only gold atom actively participating in the bonding is located above the carbon vacancy, thus linking the gold cluster to the hexagonal carbon network. An important electronic charge is found to be localized on that gold atom and the three connected first-nearest neighboring carbon atoms. This important charge transfer observed in gold nanoclusters on graphene could induce an enhancement of their catalytic activity when compared to conventional freestanding clusters.