

Single-Molecule Sensing Using Carbon Nanotubes Decorated with Magnetic Clusters

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Since their discovery, Carbon Nanotubes (CNTs) have constantly attracted growing interest in the scientific community due to their remarkable electronic and quantum transport properties that make them potentially useful for applications in nanoelectronics, spintronics and gas sensing devices. Thanks to their high surface-to-volume ratio and being one-dimensional nanosystems, CNTs are considered as exceptional nanodetectors since their properties are extremely sensitive to external perturbations. Moreover, CNTs decorated with transition metal magnetic nanoparticles are also good candidates for spin-dependent transport applications.

In this work, first-principles techniques and non-equilibrium Green's function approaches are used to investigate magnetism and spin-polarized quantum transport in carbon nanotubes (CNT) decorated with transition metal magnetic nanoclusters (NC). For small cluster sizes (< 1 nm), *ab initio* calculations predict a considerable local magnetic moment that induces spin polarization in the host CNT due to a strong mutual interaction with the magnetic NC. Such a huge local magnetic perturbation can be tailored by molecular adsorption on the metallic NC, thus modifying both the magnetization and the spin-dependent conductance of the hybrid CNT–NC system. The adsorption of benzene on Ni- or Pt-decorated metallic CNTs has been investigated as a test case. The *ab initio* simulations demonstrate that the magnetization change due to the absorption of a single benzene molecule should be large enough to be detected experimentally using either magnetic-AFM or SQUID magnetometer. Consequently, the present research suggests a novel approach for single molecule gas detection, based on local magnetic moment measurements in CNT–NC hybrid systems [1].

[1] Z. Zanolli, J.-C. Charlier, ACSNano 6 (2012) 10786–10791.