Carbon nanotube sensors and electronic properties of carbon chains

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The remarkable electronic and transport properties of carbon nanotubes (CNTs) make them very promising for a wide variety of applications in nanoelectronics and spintronics. In particular CNTs could be used as detection element for gas sensing nanodevices thanks to their high surface-to-volume ratio and to the high sensitivity of their physical properties to external perturbations. However, the response of pristine CNTs to gases is weak due to the intrinsically inert sp^2 carbon network that characterizes their sidewalls. In this talk, I will show how *ab initio* simulations can help to predict that CNT containing defects and decorated with various metal catalytic particles exhibit an extraordinary sensitivity and selectivity to gas molecules [1-4].

As strings of monoatomic thickness, chains of *sp*-hybridized carbon atoms constitute the logical one-dimensional phase of carbon. These 1D systems have been proposed theoretically for a long time until they were observed in electron microscopy studies. However, electrical measurements on these monoatomic chains have not been feasible. Now, by using a measuring system with an STM tip in a TEM specimen stage, carbon chains are not only produced but their electrical properties are also measured. Ab initio simulations (confirmed by MBPT calculations) reveal that strain has a decisive influence on the bandgap of the chain, thus determining its conductivity [5].

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