

## **FUNCTIONALISED CARBON NANOTUBES FOR INTEGRATED NANO-ELECTRONIC SENSORS**

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Despite an exponentially increasing interest for using carbon nanotubes (CNTs) as sensors in industrial or medical environments, most of the efforts carried out so far still have to address the issue of recording and analysing a signal coming from a very small number of sensing elements. The unreliable contact interfaces between the CNTs and the rest of the electrical circuit are also greatly hindering progresses in this field. Moreover a better theoretical understanding of the transport phenomena responsible for signal generation and transduction inside the CNTs is clearly needed.

The SANES (Self-Adjusting Nano-Electronic Sensors) project aims at designing, building, and characterising multifunctional nanotube-based sensor micromodules, which will have to monitor simultaneously several factors, e.g. temperature, pressure, gas concentration, in various conditions. These modules will be integrated into a matchbox-sized electronic device which will hopefully be produced industrially afterwards. Potential applications range from security to medicine, covering communication and environmental issues as well.

In this project, the sensing unit is made of functionalised CNTs. Our objective is to provide the experimentalists with a valuable insight into the electronic properties of these CNTs, and to speed-up the process of selection of the functional molecules. Our calculations thus focus on the transport properties of single functionalised metallic and semi-conducting CNTs. In a first series we study the contact between a CNT and different metallic pads. In a second series we compare the influence of a large number of potentially interesting functional groups when the system is exposed to various gases. We investigate the effects of the presence of water as well.