Designing multifunctional chemical sensors using metal doped carbon nanotubes

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We demonstrate a bottom up approach to the computational design of a multifunctional chemical sensor [1,2]. General techniques are employed for describing the adsorption coverage and resistance properties of the sensor based on density functional theory (DFT) and non-equilibrium Green's function methodologies (NEGF), respectively. Specifically, we show how Ni and Cu doped metallic (6,6) single-walled carbon nanotubes (SWNTs) may work as effective multifunctional sensors for both CO and NH_3.

References

[1] J. M. García-Lastra, D. J. Mowbray, K. S. Thygesen, A. Rubio, and K. W. Jacobsen, Physical Review B, **82** (2010) 245429.
[2] D. J. Mowbray, J. M. García-Lastra, K. S. Thygesen, A. Rubio, and K. W. Jacobsen, Physica Status Solidi B, **247** (2010) 2678.

Figures

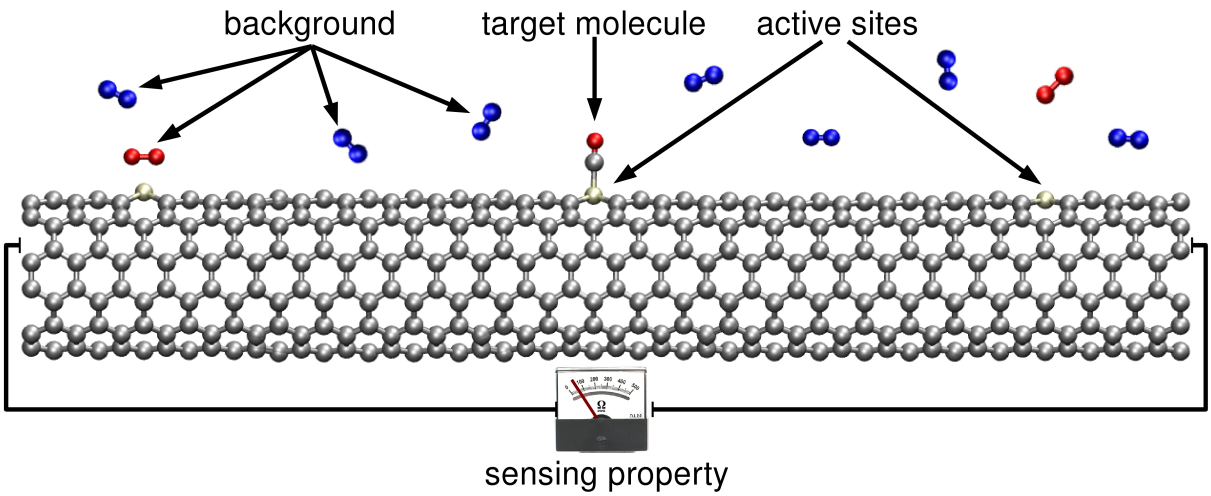

Figure 1: Schematic of a chemical sensor consisting of active sites (metal dopants in a (6,6) carbon nanotube), a target molecule (CO), a background (atmospheric air), and a sensing property (resistance).