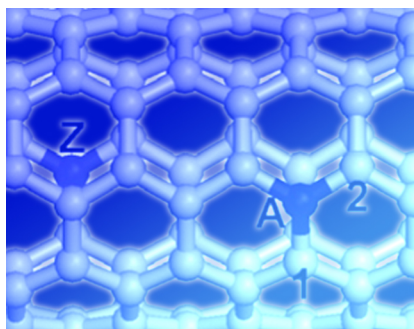


# CARBON NANOTUBES STUDIES— DOPING EFFECTS ON METALLIC & SEMICONDUCTOR SINGLE-WALL CARBON NANOTUBES



“The evaluation of the chemical modification effects and the comparison with the expected results allows one to save time and money.”

**Dr Francesco Buonocore**  
STMicroelectronics

## Module used

- Materials Studio - DMol<sup>3</sup>

## Industry sector

- Electronics

## Organization

- STMicroelectronics

Ultra large-scale integration (ULSI) technology is an expertise that has evolved in order to create chips which contain a complexity density of more than 10 million transistors / inch<sup>2</sup>. Demands from industry have led to memory devices requiring ultra-shallow junctions or nanojunctions.

A number of different solutions have been proposed, one amongst them is carbon nanotubes (CNTs). CNTs have been proven to reach figures of merit in field-effect devices even higher than those found in silicon technology. However a major limitation with the use of CNTs is the high contact resistance between metal and nanotube interface. A possible solution to exploit the use of CNTs in device nanojunctions is to control the electrical properties by doping with nitrogen or boron.<sup>1,2</sup>

Reporting in Philosophical Magazine, Dr Francesco Buonocore from STMicroelectronics has used Accelrys' density functional theory (DFT) code Materials Studio® DMol<sup>3</sup> to calculate the band structures of substitutive N- and B-doped (8,0) zig-zag single wall carbon nanotube (SWNT) and (5,5) armchair SWNT.<sup>3</sup>

The substitutive impurity is shown in Figure 1 for both the (5,5) and (8,0) SWNTs, two possible isomers, AZ and AA' were considered.

The results have shown that the calculated formation energies of the two isomers are very similar for any type of doping. However, upon further analysis into the band structures, differences between the isomers have been noticed.

For the (5,5) SWNT isomers, the band structure of AZ isomer is gapless and exhibits a crossing of fully occupied band and empty conduction band, whereas the band structure of AA' isomers exhibit an energy gap (0.4 eV within GGA) above the valence band. The joined analysis from the DOS and the density of charge concludes that the band crossing in the AZ isomer is due to the delocalisation of the density of charge and leads to metallic behaviour.

N- and B-doped (5, 5) SWNTs have equivalent electronic behaviours in the electron and hole descriptions, respectively. This finding is a direct consequence of the symmetry of the bands of the pure (5, 5) SWNT with respect to the Fermi energy.

In contrast to (5, 5) SWNT, the bands of pure (8, 0) SWNT are not symmetrical with respect to Fermi energy and N- and B-doped SWNTs show band structures with distinct features and different occupation. For N doped (8,0) SWNT the bands are just partially occupied and the isomers are metals, whereas in the B-doped case the Fermi energy is shifted downward to the top of the new valence band, and the doped SWNT exhibits a negligible indirect energy gap. However analysis of DOS has shown that both B-doped isomers are metals as well.

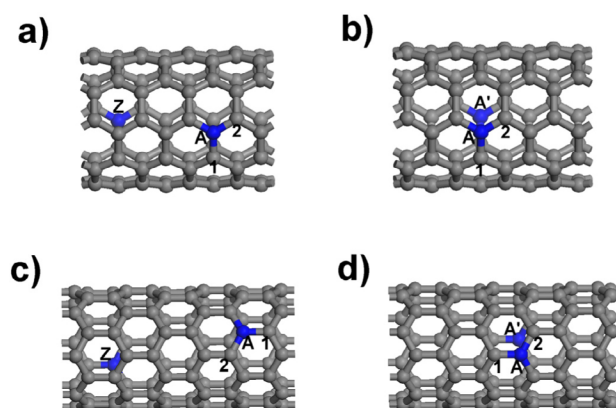
This work has been able to shed light on aspects of the electronic structures of doped SWNTs not documented in any previous studies.

Dr Francesco Buonocore said, "The modeling with Accelrys' tools let us to explore the properties of the materials before undertaking experiments in our laboratories. The evaluation of the chemical modification effects and the comparison with the expected results allows one to save time and money. Considering the computational models alongside experiments can also help drive processes and improve the understanding of results"

To learn more about Materials Studio by Accelrys, go to [accelrys.com/materials-studio](http://accelrys.com/materials-studio)

## REFERENCES

1. Lammert, P.E., Crespi, V.H., Rubio, A., Phys. Rev. Lett. **2001**, 87, 136402.
2. Nevidomskyy, A.H., Csanyi, G., Payne, M.C., Phys. Rev. Lett., **2003**, 91, 105502.
3. Buonocore, F., Philosophical Magazine, **2007**, 87, 1097.



**Fig. 1** The Unit cells of the N- or B-doped SWNTs. AZ and AA' isomers are shown for (5,5) SWNT in (a) and (b), respectively. AZ and AA' isomers are shown for (8,0) SWNT in (c) and (d), respectively.