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MS-2-P-3464 Dopants as Morphology Promoters: A Fundamental Study of the Role of Boron and Sulfur in the Formation of MWCNT Junctions

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Doping of carbon nanotubes has proven to be an invaluable tool to modify their physical and chemical properties [1]. In this work, we demonstrate that by using minute amounts of both boron and sulfur as codopants it is possible to synthesize 3-Dimensional arrays consisting of carbon nanotube interconnections. The materials were produced using a spray-assisted chemical vapor deposition experiment, in which small amounts of boron and sulfur sources were added to a solution containing a carbon source and an iron-based catalyst. The resulting structures consisted of nano- and micron-size fibers decorated with radially grown multi-walled carbon nanotubes resembling "nanotentacles." These novel structures were extensively characterized by SEM, HRTEM, and XRD. Spectroscopic techniques have also been used to determine the doping amount and binding environment, such as EELS, XPS, and Raman Spectroscopy. Quantification of EELS spectra shows that boron has a higher concentration on the tips of the radially grown nanotubes. Ab initio calculations were performed in order to understand the role of boron and sulfur as promoters of the negative curvature regions that are necessary to form covalent nanotube junctions. Our calculations show both boron and sulfur incorporation in the graphitic nanotube lattice is more stable when located in curved areas of the nanotube, with boron having a marked preference for negative curvature while sulfur is stable in both negatively and positively curved areas. Due to their high surface area, these synthesized structures have also been tested as electrodes in Li-ion batteries and supercapacitors. Finally, we will demonstrate that these tentacles behave as excellent electron field emitters, maintaining high currents over time at low operating voltages.

[1] B. Sumpter, et al. Int. J. Quant. Chem., Vol 109, 97-118 (2009)

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