Arrangement and electronic structure of the fluorinated SWNT produced by HiPco method

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Single-wall carbon nanotubes (SWNT) produced by HiPco technique were fluorinated using a volatile mixture of BrF3 and Br2 at the room temperature. Transmission electron microscopy showed the fluorination did not destroy the ropes of nanotubes. The content of fluorinated material estimated by X-ray photoelectron spectroscopy is about C4F. The C1s line has two maxima corresponded to the fluorinated carbon and bare one. Electronic structure of pristine material and fluorinated one was studied by X-ray fluorescent and optic absorption spectroscopy. To interpret the changes observed in the measured spectra the models of carbon nanotubes with different distribution of fluorine atoms were calculated by semiempirical quantum-chemical MNDO method.