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Localization of inserted species inside single walled carbon nanotubes bundles: experimental and *ab initio* study. NEDJMA BENDIAB, LPS-Univ J Fourier-Grenoble, A. MARCO SAITTA, IMPMC-Univ Pierre et Marie Curie-Paris 6, ROBERT ALMAIRAC, RAYMOND AZNAR, JEAN-LOUIS SAUVAJOL, LCVN-Univ Montpellier II, ISABELLE MIREBEAU, LLB-CEA Saclay — The aim of this work is to understand the structural organization of inserted alkali atoms inside single walled carbon nanotube bundles. First of all, we present X-rays and neutrons diffraction results obtained on rubidium inserted carbon nanotubes (n-doping). The results of X-rays and neutrons diffraction experiments are surprising and in apparent contradiction, and will be discussed in connection with the debated question of the lattice expansion of the hexagonal tubes framework under insertion. The possible insertion sites of the rubidium atoms in the nanotube bundle will be discussed in terms of their effects on the diffraction spectra. The experimental results will be compared to diffraction simulations and ab initio DFT calculations. The main outcome of our combined experimental and theoretical study is that: i) up to saturation, the spectra show no lattice expansion; ii) the extinction of the (10) peak is only compatible with Rb insertion inside the tubes; iii) DFT calculations show that at constant lattice parameter the insertion within the tubes is energetically favored with respect to insertion between the tubes.

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