Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Bundling up carbon nanotubes through Wigner defects ANTÔNIO J. R. DA SILVA, ADALBERTO FAZZIO, Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970, São Paulo, SP, Brazil, ALEX ANTONELLI, Instituto de Física "Gleb Wataghin", UNICAMP, CP 6165, 13083-970, Campinas, SP, Brazil
— We show, using *ab initio* total energy density functional theory, that the so-called Wigner defects, an interstitial carbon atom right besides a vacancy, which are present in irradiated graphite can also exist in bundles of carbon nanotubes. Due to the geometrical structure of a nanotube, however, this defect has a rather low formation energy, lower than the vacancy itself, suggesting that it may be one of the most important defects that are created after electron or ion irradiation. Moreover, they form a strong link between the nanotubes in bundles, increasing their shear modulus by a sizeable amount, clearly indicating its importance for the mechanical properties of nanotube bundles.

Antônio J. R. da Silva
Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970, São Paulo, SP, Brazil

Date submitted: 01 Dec 2004 Electronic form version 1.4