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Defects in carbon nanotubes RODRIGO G. AMORIM, ANTÔNIO J. R. DA SILVA, A. FAZZIO, Instituto de Física, Universidade de Säo Paulo, ALEX ANTONELLI, Instituto de Física "Gleb Wataghin", UNICAMP — It is a consensus that defects can alter in a significant way the mechanical properties of carbon nanotubes. We here will investigate, using ab initio total energy density functional theory calculations, some defects and their properties, such as: 1) an interstitial carbon atom right besides a vacancy that can connect tubes in bundles or in multi-wall nanotubes; 2) two vacancies that can connect tubes in bundles; 3) a variety of configurations for two vacancies in one nanotube, and how their energies vary with separation. In particular, we will compare the formation energies of the 5-8-5 and 555-777 two-vacancy defects as a function of nanotube diameter.

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