Stability of Functionalized Carbon Nanotubes

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Functionalization of carbon nanotubes (CNTs) with simple organic molecules plays an important role in applications of CNTs, either as electrical sensors of chemical and/or biological substances or as an enforcement of weak materials (like polymers) to obtain strong composite materials. Recently it has been observed a lot of research activity in these fields. We have performed extensive studies to determine the stability of the functionalized CNTs with simple organic molecules such as CH_n, NH_n, OH, and COOH. We discuss the dependence of the cohesive energies of functionalized CNTs, its deformations, and changes in the electronic structure on the density of the adsorbed molecules. All these factors influence the electrical and mechanical properties of the functionalized CNTs and are important for reliable description of the sensor electrical characteristics and also for modeling composite materials. Our studies are based on the *ab initio* calculations in the framework of the density functional theory. We use the generalized gradient approximation (GGA) for the exchange-correlation density functional and supercell geometry within the numerical package SIESTA.

Our studies reveal physical mechanisms of the binding of the studied groups to the CNTs. Generally, the stability of the functionalized CNTs is weakly dependent on the diameter of the CNTs, whereas the stability strongly decreases with the density of the adsorbed groups. In particular, we find that the NH_n and CH_n groups with n larger than two do not bind to the CNTs. In particular, it turns out that practically only CH_2 groups make reasonably strong bonds to the CNTs (CH_3 groups bind, but extremely weakly with bond length of 1.56 Å). In the case of CH_4 groups, we observe their dissociation into CH_2 and H_2 dimer placed in the surrounding of CNT; CH_2 binds to the CNTs, whereas H_2 remains unbound. The functionalization of CNTs with NH_n causes practically no deformation of the CNTs, whereas the CH_n groups attached to the CNTs cause reconstruction of the CNTs.