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Ab initio studies of mechanical, electric, and magnetic properties of functionalized carbon nanotubes[1] KAROLINA MILOWSKA, MAGDALENA BIROWSKA, JACEK A. MAJEWSKI, University of Warsaw — We present results of extensive theoretical studies of mechanical, electric, and magnetic properties of functionalized carbon nanotubes (CNTs). Our studies are based on the ab initio calculations in the framework of the density functional theory. We have performed calculations for various metallic and semiconductor single wall CNTs, functionalized with simple organic molecules such as OH, COOH, NH_n, CH_n and metals, Al, Fe, Ni, Cu, Zn, and Pd. We have determined the stability of the functionalized CNTs, their elastic moduli, conductance, and magnetic moments (in the case of CNTs decorated with magnetic ions). These studies shed light on physical mechanisms governing the binding of the adsorbed molecules and also provide valuable quantitative predictions that are of importance for design of novel composite materials and functional devices. In particular, we find out that the Young's modulus of functionalized CNTs is smaller than in the case of bare CNTs, however it is large enough to provide a strong enforcement of composites. The functionalization with molecules leads also to the metallization of semiconducting CNTs, being relevant in the context of CNT interconnects, whereas the functionalization with metals might be used to cut CNTs into ribbons.

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Jacek A. Majewski
University of Warsaw

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