Metal doped carbon nanotube interacting with vitamin C: ab initio study

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Carbon nanotubes – characterized for the first time in 1991 by Iijima [1] – have attracted much attention in terms of both fundamental science and technology because of their unique electrical, mechanical, and chemical proprieties [2]. Since the use of these nanoscale systems, pristine or functionalized, can collaborate to the development of new materials, where in interactions with biological molecules, as the case of vitamin C, could help the study of new routes in the delivery of drugs in the body [3]. In this work, we analyzed by first principles simulations based on Density Functional Theory (DFT) [4], using the SIESTA code [5], single-wall carbon nanotube doped with aluminum, iron, manganese and titanium interacting with acid ascorbic (vitamin C). We evaluated the structural and electronic properties of systems for each used dopants. The binding energies obtained for the interactions between the vitamin and carbon nanotube doped with aluminum, iron, manganese and titanium were 0.78, 0.82, 0.51, 0.97 eV, respectively. Although the systems do not form chemical bonds, the results show that it is possible to change the spin polarization of the systems. In addition, it is possible to change the conductance character of the nanotube, depending on the doping atom. This would be of great relevance to the application of these systems in spintronics and in the development of new materials for nanotechnological applications.

Keywords: Carbon nanotube, density functional theory, metal, doping.


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