

Abstract Submitted
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Carbon nanotube conditioning: ab initio simulations of the effect of defects and doping on the electronic properties of carbon nanotube systems.¹ MATIAS SOTO, ENRIQUE BARRERA, Rice Univ — Using carbon nanotubes for electrical conduction applications at the macroscale has proven to be a difficult task, mainly, due to defects and impurities present, and lack of uniform electronic properties in synthesized carbon nanotube bundles. Some researchers have suggested that growing only metallic armchair nanotubes and arranging them with an ideal contact length could lead to the ultimate electrical conductivity; however, such recipe presents too high of a cost to pay. A different route and the topic of this work is to learn to manage the defects, impurities, and the electronic properties of carbon nanotubes present, so that the electrical conduction of a bundle or even wire may be enhanced. We used density functional theory calculations to study the effect of defects and doping on the electronic structure of metallic, semi-metal and semiconducting carbon nanotubes in order to gain a clear picture of their properties. Additionally, using dopants to increase the conductance across a junction between two carbon nanotubes was studied for different configurations. Finally, interaction potentials obtained via first-principles calculations were generalized by developing mathematical models for the purpose of running simulations at a larger length scale using molecular dynamics.

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