Electronic study of the doped carbon nanotube

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Abstract

By inserting carbon chains, the geometry and electronic properties of carbon nanotubes (CNTs) will change dramatically. Much research has been done to experimentally discover the effect of inserting the carbon chain into carbon nanotubes. In this work, theoretically studies through the Density Functional Theory (DFT) the geometry of carbon chains inserted in carbon nanotubes, doped and with vacancy, and analyzes the mechanism of structural changes and electronic conductivity after the insertion of carbon chains. The results show that carbon chains and their impurities in the nanotube are an effective way to change the electrical properties of carbon nanotubes, leading to electron redistribution and therefore a change in the conductivity of the resulting configuration.

References

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[3] © 2016 Macmillan Publishers Limited. All rights reserved, DOI: 10.1038/NMAT4617.
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Figures

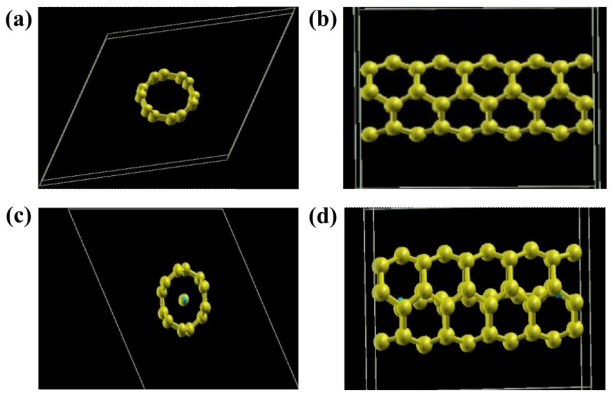

Figure 1: This figure shows the structural part of the Carbon Nanotube. In figure (a) pure nanotube front. (b) pure nanotube side (c) carbon nanotube with front carbon chain insert (d) carbon nanotube with side carbon chain insert