

Abstract Submitted
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Effect of Strain and Defects on Transport Properties of Carbon Nanotubes YAO HE, University of Florida, CHUN ZHANG, Georgia Technology Institute, CHAO CAO, HAI-PING CHENG, University of Florida — Strain dependence of electronic transport properties of carbon nanotubes has been studied using first-principles calculations. We have found that the quantum conductance decreases monotonically with increasing strain, due to the strain-dependent contribution of molecular orbitals. Transport properties are also affected by the presence of defects. Our results have demonstrated that the electronic transport properties of a nano-scale device are closely related to the nature of the band structure of the metallic lead and the details of chemical bonding in the scattering region. Acknowledgement: DOE/BES under grant FG02-02ER45995

Hai-Ping Cheng
University of Florida

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