

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Distinct properties of single-wall carbon nanotubes with sidewall chemical functionalization JIANPING LU, HYOUNGKI PARK, Univ. of North Carolina at Chapel Hill, JIJUN ZHAO, Washington State University — *Ab initio* calculations reveal distinct electronic properties associated with side wall functionalization of SWNTs. The metallic tubes are found to be more reactive than the semiconducting ones. The hybridization between the addend and the tube induces unique impurity states near the Fermi level. For semiconducting tubes the state is localized near the functionalized site with a characteristic length of 15 Å. In contrast, the impurity state is extended and acts as a strong scattering centre in metallic tubes. This effect greatly hinders the ballistic transport of electrons along the metallic nanotubes. The characteristic dependence of the electronic states and the conductance on functional molecules provides possible pathways for chemical sensor applications and the band structure engineering.

Jianping Lu
Univ. of North Carolina at Chapel Hill

Date submitted: 16 Jan 2006

Electronic form version 1.4