

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic Structure of Metal-covered Semiconducting Carbon Nanotubes WENGUANG ZHU, Harvard University, EFTHIMIOS KAXIRAS, Harvard University — Carbon nanotube field-effect transistor (CNFET) are regarded as potential building blocks for future nanoelectronics. The interaction between a carbon nanotube and metal contacts and the resulting electronic structure effects are crucial for device properties. In this talk, we present recent results on the properties of semiconducting single wall carbon nanotubes in contact with Pd, in a fully covered geometry that resembles experimental setups. We use first-principles calculations to determine the electronic structure, charge transfer effects, electrostatic potential and Fermi level alignment at the interfaces between the metal contact and various semiconducting single-wall carbon nanotubes.

Zhenyu Zhang
ORNL & The University of Tennessee

Date submitted: 06 Dec 2005

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