Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Ab initio Calculation of Contact Effects on Transport Properties of Carbon Nanotubes Connected to Metallic Electrodes NOBUHIKO KOBAYASHI, Nanotech Res Inst, AIST, JAPAN, TAISUKE OZAKI, Res Inst Comp Sci, AIST, JAPAN, KENJI HIROSE, Fund Env Res Lab, NEC, JAPAN
— Recently, a number of studies have been performed to make carbon nanotube devices. One of the important issues in the developments of the carbon nanotube devices is the control of contact effects of the electrodes. To detect electric signals through nanotubes, electrodes must be connected to the nanotubes. Contact with the electrodes sensitively influences the transport properties. Therefore, it is important to discuss the transport properties on the basis of the detailed electronic state calculation that includes the effect of contact with the electrodes. We have developed a first-principles method of analyzing quantum transport in nanometer-scale systems between electrodes. The electronic states are calculated using a numerical atomic orbital basis set in the framework of the density functional theory, and the conductance is calculated using the Green's function method. We apply the method to calculating transmission spectra of carbon nanotubes connected to metallic electrodes, and discuss the contact effect of the electrodes on the transport properties in the finite size of metallic and semiconducting nanotubes.

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Date submitted: 30 Nov 2005 Electronic form version 1.4