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First-principles study of effects of metallic electrode contacts on transport properties of carbon nanotubes NOBUHIKO KOBAYASHI, Inst Appl Phys, Univ Tsukuba, Japan, TAISUKE OZAKI, Res Inst Comp Sci, AIST, Japan, KENJI HIROSE, Fund Env Res Lab, NEC, Japan — Towards a development of constructing nanometer-scale devices, considerable effort has been made in experiments using carbon nanotubes for fabricating nanoscale field-effect transistors. To detect electric signals, electrodes must be connected to the conductors. Contact with the electrodes sensitively influences the transport properties. Therefore, we have studied the transport properties on the basis of the detailed electronic state calculation that includes the effect of contact with the electrodes. We have investigated quantum transport in carbon nanotubes bridged between metallic 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 have analyzed transport properties of the finite size of carbon nanotubes bridged between Al, Au, Pt, Pd metallic electrodes, and discuss the contact effect of the electrodes on the transport properties. We reveal their dependency on the electrode materials.

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