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First-principles calculations of effects of metallic electrode contacts on transport properties of carbon nanotubes NOBUHIKO KOBAYASHI, Institute of Applied Physics, University of Tsukuba, TAISUKE OZAKI, Research Center for Integrated Science, Japan Advanced Institute of Science and Technology, KENJI HIROSE, Nano-Electronics Research Laboratories, NEC Corporation — Recently, considerable effort has been devoted to developing carbon nanotube devices. One of the important issues in the developments of 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 their electronic structures and transport properties. Therefore, it is important to discuss the transport properties on the basis of the detailed electronic state calculations that include 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 metallic electrodes, and discuss the contact effect of the electrodes on the transport properties. We reveal their dependency on the length and the electrode materials.

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