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**Ab initio transport calculations of molecular wires with electron-phonon couplings** KENJI HIROSE, NEC Corp., NOBUHIKO KOBAYASHI, Univ. of Tsukuba — Understanding of electron transport through nanostructures becomes important with the advancement of fabrication process to construct atomic-scale devices. Due to the drastic change of transport properties by contact conditions to electrodes in local electric fields, first-principles calculation approaches are indispensable to understand and characterize the transport properties of nanometer-scale molecular devices. Here we study the transport properties of molecular wires between metallic electrodes, especially focusing on the effects of contacts to electrodes and of the electron-phonon interactions. We use an ab initio calculation method based on the scattering waves, which are obtained by the recursion-transfer-matrix (RTM) method, combined with non-equilibrium Green's function (NEGF) method including the electron-phonon scatterings. We find that conductance shows exponential behaviors as a function of the length of molecular wires due to tunneling process determined by the HOMO-LUMO energy gap. From the voltage drop behaviors inside the molecular wires, we show that the contact resistances are dominant source for the bias drop and thus are related to local heating. We will present the electron-phonon coupling effects at contact on the inelastic scattering and discuss on the local heating and local temperature, comparing them with those of metallic atomic wires.

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