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Transport properties of molecular wires from ab initio calculations 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 focus on the transport properties of molecular wires bridged between metallic electrodes, especially on the effects of contacts to electrodes and on the dependence of the length of molecular wires on transport properties. 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. 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 well separated for the long molecular wires. We will present detailed data of electronic states at contacts to metallic electrodes under strong electronic fields and will discuss the polarization, screening effect, and potential barrier formation at contacts on the transport properties of molecular wires, comparing them with those of metallic atomic wires.

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