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Ab initio RTM/NEGF method for Electron Transport through Single Molecules KENJI HIROSE, Fund.Res.Labs., NEC Corp., NOBUHIKO KOBAYASHI, Dept. of Applied Physics, Univ. of Tsukuba — Using the RTM/NEGF method, which is an ab initio calculation method based on the density-functional formalism with use of accurate scattering waves combined with non-equilibrium Green's function method, we study the transport properties between metallic electrodes through single molecules. Especially, we investigate how the atomic-scale contacts to electrodes affect quantum transport. We find that transport behaviors change significantly due to the contacts. For fairly good contacts, transport properties are determined by the HOMO-LUMO states by resonant tunneling processes. However, as the contacts to one electrode becomes worse, I-V characteristics are mostly determined by tunneling condition with strong non-linear behaviors and molecular states are hard to be observed in the conductance data. Furthermore, we find that negative differential resistance appears at some distances between single molecules and one of the electrodes. We will clarify the mechanisms for these anomalous transport behaviors and show the relationship of HOMO-LUMO resonant states and tunneling vs. ballistic transport with various contact conditions to electrodes.

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