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Contact Effects on Transport Properties through Single Molecules — ab initio RTM/NEGF method study KENJI HIROSE, Fund.Res.Labs., NEC Corporation, NOBUHIKO KOBAYASHI, NRI, National Institute of AIST — Recently much attention has been focused on the transport properties of single molecules sandwiched between electrodes, aiming at construction of ultimate functional devices with molecular electronics. Since the transfer of an electron through single molecules attached to electrodes is sensitivily affected by the atomic-scale contacts and also it is difficult at present to construct well-characterized nanostructures and to directly observe their atomic structures, theoretical approaches based on the ab inito calculations is indispensable to study the transport properties of molecular-scale devices. Using the ab initio RTM/NEGF method developed recently, we study the the transport properties through single molecules attached to electrodes. This method is based on the plane-wave basis sets and thus not dependent on the atomic positions, which enables us to treat accurate tails of wavefunctions in the tunneling regimes as well as those in the ballistic regimes on the same footing. We investigate especially atomic-scale contact effects on the I-V characteristics through single molecules, changing the distance to electrodes. We find strong non-linear behaviors appear in the I-V characteristics at some distances with and even without single molecules connected to electrodes. We clarify the relationship between electronic states of single molecules and the contact effect at the electrodes for the transport properties.

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