THEORY OF QUANTUM TRANSPORT OF NANO-STRUCTURES

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Electron transport of nano-structures including atomic wires or organic molecules bridging over electrodes are recent focus of nano-technologies, because they are considered as basic units of future nano-electronic-devices. Quantum transport properties of such systems would show very attractive features, as predicted by many theoretical works so far. However at the present moment, it is rather difficult to fabricate nano-scale bridge structures well characterized in the level of the atomic scale. Therefore the role of theoretical analyses and prediction is very important at the present stage to give useful guiding principles for the development of novel nano-devices.

At the first part of the talk, various remarkable features of the electron transport revealed theoretically are introduced. One of the theoretical methods is the first-principles recursion transfer matrix method(RTM), which is an extension of the DFT for the open non-equilibrium systems. Recently we succeeded to implement non-local pseudo-potentials to this method, which enabled us to treat any kind of the atoms from the first-principles. As an example of the applied calculations, we show the remarkable effect of the terminal contact structure of the atom wire on the conductance, as well as unexpected bias drop distribution within the bridges. As for the conductance of the molecular bridges, we mainly used the non-equilibrium Green's function method on the basis of TB model parameterized by DFT. The calculation of the quantum conductance has been performed for various molecular bridge systems, and promising candidates of molecular conductors have been searched. They include molecules as tape porphyrin, helical benzothiophene, phenalenyl, fullerene and phenoxy radical. In the case of phenalenyl and fullerene a remarkable strong loop current appears inside the molecule induced by the source-drain current.

In the case of trianglar graphene sheet including several thousands of carbon atoms, we found that large loop currents appear circulating wide area of the triangle carbon layer, when the incident electron energy from a electrode is close to doubly degenerate states. The patterns of the current spatial distribution does not change depending on the positions of the source or drain electrode. Furthermore, almost the same loop current distribution appear when a magnetic field is applied on the isolated triangular graphene sheet, when the incident electron energy is tuned near a magnetically split (originally degenerate) state. Based on these facts, the mechanism of the large loop current is theoretically clarified, and experimental methods for the confirmation of the large loop current are proposed as well as suggestions of possible application to nano-devices. We will also discuss the relation between the source-drain induced large loop current and magnetic field induced persistent current or diamagnetic current. As a closely related topics, we introduce a remarkable persistent current in a certain type of single wall carbon nanotube tori.

In the second part of the talk, the effect of lattice or molecular vibration on the electron transfer processes within a molecule or that between the molecule and the electrodes are discussed. It is clarified when the coupling is of the same order with the electron hopping energy, the effective hopping energy is remarkably reduced which hiders coherent electron transfer between the two sections, either of different intra-molecular sections connected only by the σ(sigma) bond, or that of molecule and the electrode. The issues of the contact resistance of the anchored molecule, decay of the coherence of the quantum state, the guided intra-molecular carrier transfer for the single-molecular electro-luminescence will be discussed from this view point.

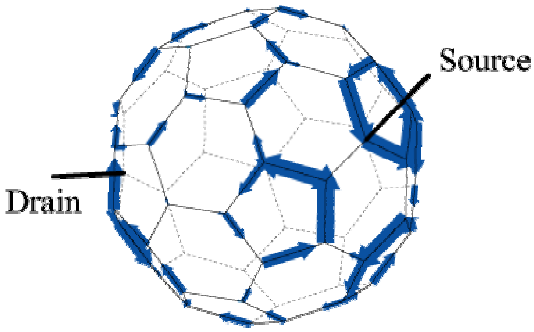

Fig.1 *A large loop current is induced within a C60 molecular bridge near the resonace tunneling condition.*

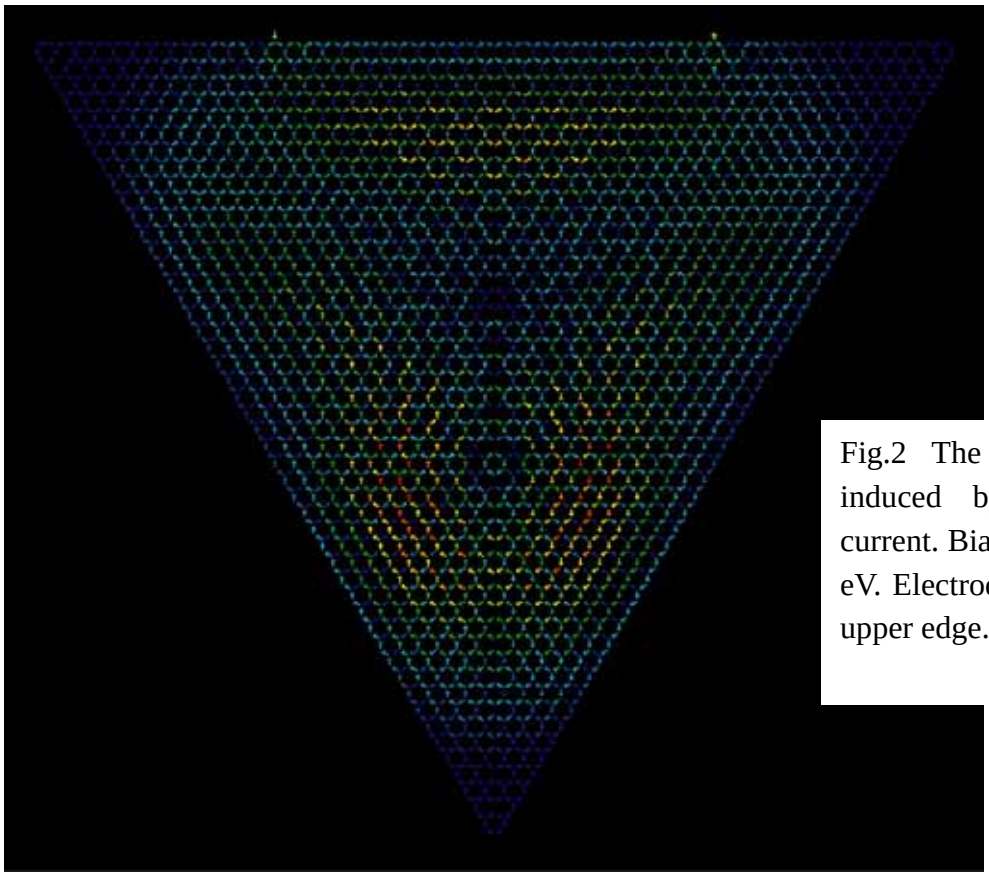

Fig.2 The large loop current induced by the source-drain current. Bias voltage is about 0.9 eV. Electrodes attached on a top upper edge.