# Electron transport properties of $C_{60}$ single electron transistor

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**Abstract**

We investigate theoretically the electron transport in the $C_{60}$ single electron transistors, based on the shuttle mechanism where charges are carried by the motion of $C_{60}$ molecule. The gate voltage affects directly the electron tunneling and indirectly the motion of $C_{60}$ by shifting the center of vibrations. The latter effect stops the molecular movement at a large gate voltage, leading to the conduction gap that widens in proportion to the gate voltage.

*Key words:* single electron transistor ; $C_{60}$ ; shuttle mechanism ; conduction gap

Electric transport properties of single electron transistor (SET) using a $C_{60}$ molecule have been recently reported by Park *et al.*[1], in which the $C_{60}$ molecule was adsorbed onto the substrate or an electrode by van der Waals interaction. The transport properties show not only Coulomb staircase structure but also gate voltage dependence which is unpredictable from the orthodox theory. That is, the zero conductance source-drain voltage region, termed *conduction gap*, widens in proportion to the gate voltage. This gate voltage dependence is considered to stem from the shuttle mechanism[2,3] for electron transport, in which the center of mass motion of the molecule carries charges between the electrodes. However, the gate voltage dependence of the current in the $C_{60}$ SET has not been elucidated from the theoretical viewpoint. In this work, we investigate theoretically the transport properties of $C_{60}$ SET, postulating that the electron transport in the $C_{60}$ SET is attributed to the shuttle mechanism.

We treat the center of mass motion of molecule classically because of the large mass of the molecule, and limit the motion to the longitudinal displacement of the molecule relevant to electron transport. Then we have the equation of motion of the molecule, in the harmonic approximation for the confining potential,

$$M_0\ddot{u} = -M_0\omega^2(u - x_0) - \gamma M_0\dot{u} + en(t)\mathcal{E}, \qquad (1)$$

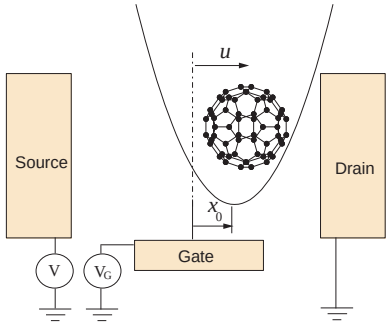


Fig. 1. Model of a $C_{60}$ molecule single electron transistor. The molecule is moveable, whose displacement $u$ and the bottom $x_0$ of the harmonic confining potential are measured from the midpoint between the electrodes. $x_0$ at the zero voltages is an adsorbed position $d$ of the molecule, but varies with respect to the gate voltage. The molecule vibration is driven by Coulomb force reflecting the change in the number of loaded electrons.

where $M_0$ is the mass of molecule, and $\omega$ the natural angular frequency of molecule vibrations. The displacement $u$ and the bottom $x_0$ of the harmonic confining potential are measured from the midpoint between the electrodes. The offset of the potential $x_0$ coincides with an adsorbed position $d$ at the zero voltages. The electric field is given by $\mathcal{E} = \frac{V}{L}$, where $L$ is the distance between the electrodes, and $\gamma$ represents the rate of energy dissipation of the molecule motion through coupling to

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loss processes such as phonon emission into the substrate. The number of electrons $n(t)$ on the molecule changes owing to electron tunneling, and the probability that the molecule has $n$ electrons obeys a master equation. We derived the transport properties, evaluating the mechanical vibration energy of the molecule pumped by the applied source-drain voltage based on the master equation.

The resultant response of the current for variation of the source-drain and gate voltages as follows: in the vicinity of the left electrode, the molecule has $N_e$ electrons after a series of electron tunneling from the electrode. On the other hand, the molecule has $N_h$ holes near the right electrode as a consequence of electron tunneling to the right electrode. The molecule keeps the number of electrons on the molecule while traveling between the electrodes. Then the current per cycle, $J = 2\pi I/\omega e$, is given by the sum of $N_e$ and $N_h$: $J = N_e + N_h$, where $N_e$ and $N_h$ are functions of the voltages, given by

$$\begin{aligned} N_e &= \left\lfloor \left(\frac{1}{2} - \frac{d}{L}\right) U - U_G + \frac{1}{2} \right\rfloor, \\ N_h &= \left\lfloor \left(\frac{1}{2} + \frac{d}{L}\right) U + U_G + \frac{1}{2} \right\rfloor, \end{aligned} \tag{2}$$

where we assumed the electrical neutrality of the molecule at the adsorbed position at the zero voltages. $\lfloor x \rfloor$ generates the nearest integer smaller than $x$. $U$ and $U_G$ are $U = VC/e$ and $U_G = V_G C/e$, and $C$ is the capacitance of the molecule. $N_e$ discretely decreases in steps of unity with increasing $U_G$, while $N_h$ discretely increases in steps of unity and cancels out the decrease of $N_e$. In general, the steps in $N_h$ occur at different gate voltages from those in $N_e$. The current $J$ then exhibits a periodic response with respect to changes in $U_G$.

On the other hand, the increasing imbalance between $N_e$ and $N_h$ produced by the gate voltage significantly influences the electron tunneling as well as the molecule vibrations.[4] The quantity $\frac{e}{2}(N_e - N_h)$ represents the molecule charge averaged over one cycle. The averaged charge is, in general, finite and the relevant electrostatic force moves the mechanical equilibrium position of the molecule from the adsorbed position. The shift in $x_0$ varies nonlinearly with respect to the gate voltage, and substantially increases when either $N_e$ or $N_h$ becomes negative. The shift in $x_0$ leads to a suppression in the number of the tunnel events between the molecule and the electrode from which the molecule recedes because of the exponential decrease in the tunneling rate. The substantial increase in $x_0$ results in an extreme suppression of the tunneling events, which stops the molecule vibrations. The resultant current decreases by the factor of $10^{-5}$ in comparison with the shuttle current.

Figure 2 shows the shuttle current per cycle $J$ in the source drain voltage-the gate voltage plane. Each

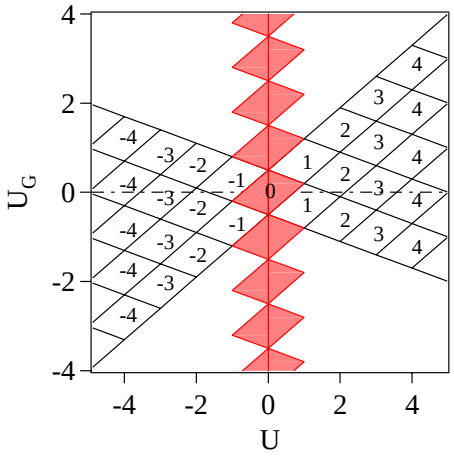


Fig. 2. The diagram of the current $J$ in the ($U$,$U_G$) plane for $d/L = -0.2$ at $T = 0$ K. The numbers in the rhombi denote $J$. The electron tunneling is prohibited in the shaded voltage region containing the center region. The current is not owing to the shuttle mechanism outside the butterfly region, but due to the usual tunnelling, whose magnitude decreases by the factor of $10^{-5}$ in comparison with the shuttle current.

number in the rhombi denotes the sum of $N_e$ and $N_h$. Because both $N_e$ and $N_h$ must be non-negative, the diagram results in a butterfly-shape. As readily understood from Eq. (2), the butterfly-shape shears, depending on the adsorbed position $d$. Considering that it will actually be difficult in practice to put molecules precisely on target, the equilibrium position may obey some distribution function, leading to a sample-dependent butterfly-shape of the voltage regions for the shuttle current. Such variously sheared butterfly-shaped voltage regions are reported in the experimental work on the $C_{60}$ SET[1] together with a conduction gap which widens in proportion to the gate voltage. The experiment also indicated that the number of excess electrons on the $C_{60}$ molecule at the critical voltage of the conduction gap is 0 or 1. This is all consistent with the findings of the present work. We therefore conclude that the effect of vibration region shift induced by the gate voltage is essential for describing the transport properties of Coulomb Blockade devices due to the shuttle mechanism.

## References


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