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Thermoelectric Effect of Thiophene-based Tripodal Molecular Junctions

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There has been considerable interest in the studies on single molecular junctions [1]. It is important to establish strong binding between the anchoring groups of the bridging molecule and the metal electrodes. Tripodal structure anchoring molecule is interesting since it satisfy the following conditions; (i) form robust junction with the metal electrodes, (ii) maintain sufficient electron density of states close to the Fermi level to pass an electron or hole through the molecule and (iii) control well-ordered molecular orientation. It is expected that the conduction path can be tuned by changing the anchoring group of the molecule.

Previously, pyridine-based tripodal anchor molecule was synthesized and the conduction channel has been predicted to be through the lowest unoccupied molecular orbital (MO) channel [2]. In this work, the anchoring group of the pyridine-based molecule was changed into thiophene (Fig. 1: 3Th-Ph-3Th) and its effect on the conductance channel was investigated.

In our experiment, the conductance and thermoelectric voltage of 3Th-Ph-3Th molecular junctions using Au electrodes were measured with a home build scanning tunneling microscope (STM) [3]. Temperature difference between the tip and the substrate were controlled by the substrate's temperature with a Peltier device. Si diode temperature sensors were used to monitor the temperatures of the tip and substrate. The STM tip was brought close to the substrate until the threshold current value was reached. This value chosen was larger than the current for a single molecular junction determined by break junction measurements. Then, the voltage difference between the tip and the substrate was measured during the retraction of the tip.

Figure 2(a) shows the conductance histogram obtained for 3Th-Ph-3Th molecule. The peak that appeared at 2×10^{-5} G_0 ($G_0 = 2e^2/h$) in the histogram is attributed to the conductance of 3Th-Ph-3Th. Figure 2 shows the thermoelectric voltage as a function of ΔT for Au-3Th-Ph-3Th–Au. Positive S (~+22.4 μV/K) was observed, which indicates that the charge transport is through the highest occupied MO level for the thiophene-based tripodal molecule. This result demonstrated the ability of the tripod anchor to control charge transport channel of molecular junctions.

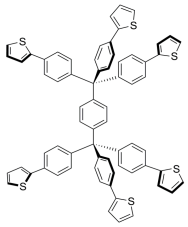

Figure 1: Structure of 3Th-Ph-3Th molecule.

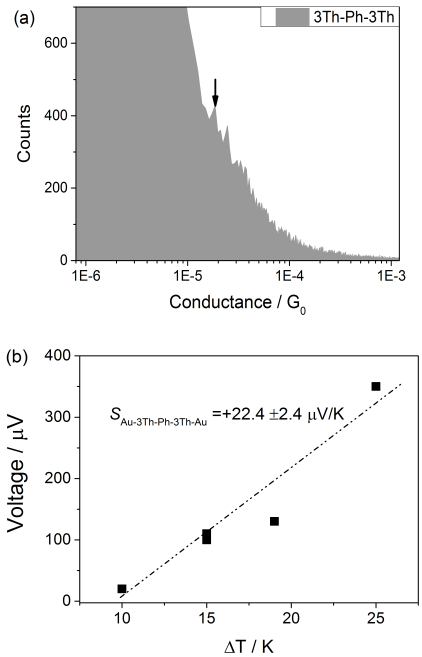

Figure 2: (a) Conductance histogram and (b) thermoelectric voltage as a function of ΔT for 3Th-Ph-3Th molecular junctions.

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