

## Mechanically controllable single molecular conductance by changing molecular conformation

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It is essential to study the transport property of single molecule toward the realization of single molecular devices. Until today, most studies have focused on thiol molecules attached on Au electrodes. However, the conductance obtained in this system has been poorly reproducible and temporally unstable due to the weak Au-S bonding. Recently, we have overcome this problem by adopting silicon electrode instead of Au. Rigid Si-C bonding formed between the electrode and the molecule provides robust single molecular junction for long time stable I-V characteristics. Furthermore it also allows us to manipulate the molecular conformation without breaking molecular junction, which will offer an additional way to control transport property of single molecule. In this study, we have investigated the influence of molecular conformation on I-V characteristics of Si based single molecular junction. STM tip and substrate surface made of a same n-type Si (001) wafer were used as electrodes. And we used diethynylbenzene (DEB) molecules, whose triple bonds react covalently with Si electrodes. A single molecular junction was formed by approaching a Si-STM tip toward an isolated DEB molecule adsorbed on H-Si (001) substrate (Fig.1). After the molecular junction was formed, I-V curve measurements were performed. Figure 2 shows I-V curves obtained from a same DEB molecular junction under different electrode separation. I-V curves show semiconducting behavior reflecting semiconducting nature of silicon electrode in addition to the strong rectification property. For positive sample-bias voltages, the conductance increased with a larger electrode separation meanwhile conductance did not change for negative sample-bias voltages. In order to investigate in detail, IV curve measurements were carried out iteratively during modulating electrode separation in triangular waveform. Figure3 indicates current values under positive (+1.8V) and negative sample bias (-1.8V), rectification ratio, and electrode separation. Surprisingly, current value under  $V_s = +1.8V$  switched between high and low conductance state reproducibly around  $d = -0.28nm$  in addition to continuous conductance variation with electrode separation, each of which are assigned to abrupt and gradual conformational change of the molecule. The result clearly demonstrates the mechanical controllability of carrier transport in single molecular junction by changing molecular conformation.

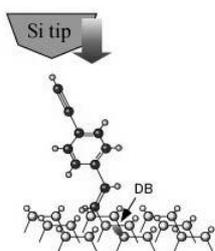


Fig.1 Schematic of measurement

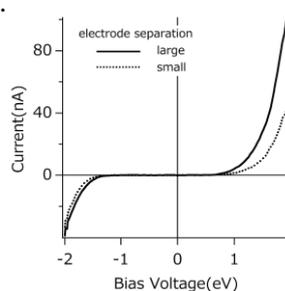


Fig.2 I-V curves under different electrode separation

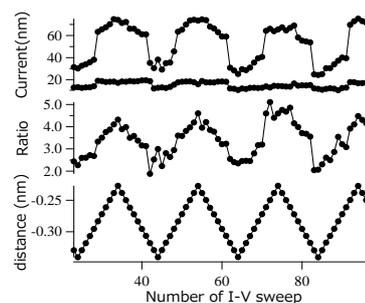


Fig.3 Variation of current (top), rectification ratio (middle) with electrode separation (bottom)