Supporting Online Material for

Mechanically-controllable single molecule switch based on configuration specific electrical conductivity of metal-molecule-metal junctions

Masateru Taniguchi, Makusu Tsutsui, Kazumichi Yokota and Tomoji Kawai

1. Figure S1: Reproducibility of conductance histograms

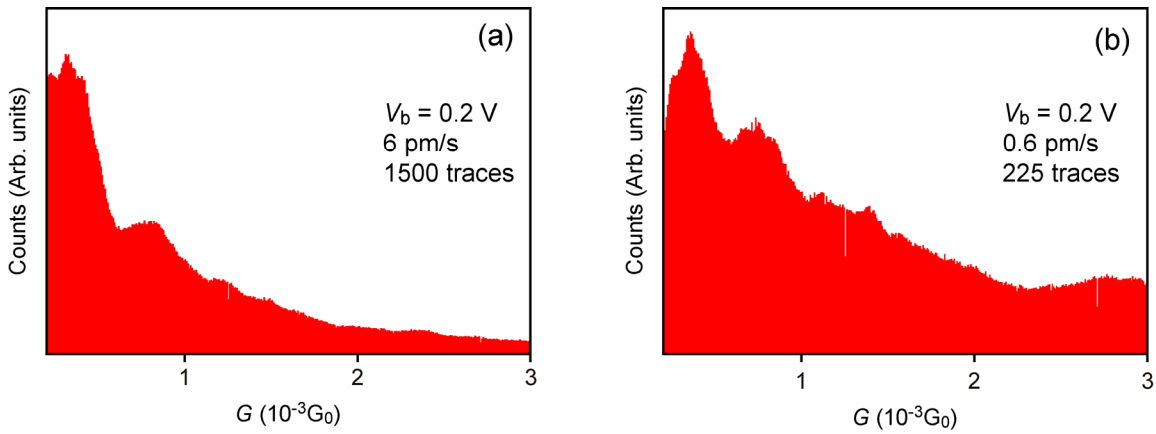

Fig. S1. Conductance histograms of Au-HDT-Au junctions consisting of all the *G-t* curves measured at **(a)** 6 pm/s and **(b)** 0.6 pm/s. These histograms show well-defined peaks at 4×10^{-4} G_0 and 8×10^{-4} G_0 corresponding to one and two HDT molecules binding to top sites of Au electrodes. We also observe a peak at around

1.3×10^{-3} G_0 ascribable to the conductance states of HDT single molecule junctions with hollow-hollow geometries. These results demonstrate the high reproducibility of peak structures in conductance histograms of HDT junctions measured using our nano-MCBJs.

2. Figure S2: *G-t* curve selection criterion

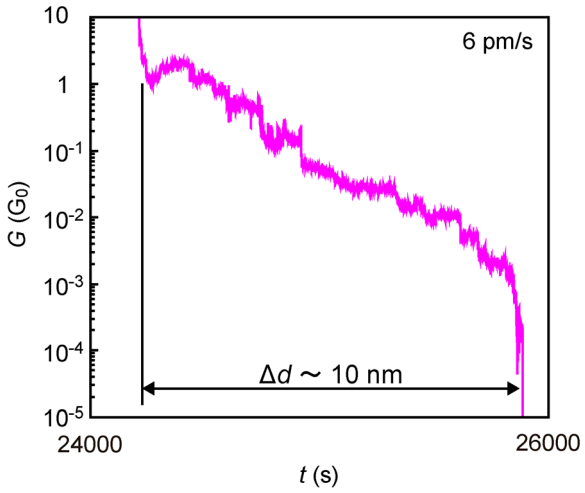

Fig. S2. An example of anomalous *G-t* trace showing considerably long junction holding time after breakdown of Au contacts under a junction stretching speed of 6 pm/s. This would suggest that the molecular junction is sustaining an enormous mechanical strain of $\Delta d \sim 10$ nm. However, it is anticipated that molecular junctions consisting of one or a few HDT molecules cannot be elongated this much considering the relatively small size of HDT molecules, ~ 1 nm. The long junction holding time is rather suggestive of unintentional trapping of a large cluster of HDT molecules or other contaminants between the MCBJ electrodes. About 10 % of consecutively acquired 1500 *G-t* curves exhibited this peculiar characteristic.

Conductance histograms including these traces show significant broadening as we see in Fig. S1. The conductance histograms in Fig. 2 were constructed by excluding the anomalous *G*-*t* curves accompanying $\Delta d > 2$ nm together with other 30 % of the traces wherein no signs of molecular bridging were confirmable.