# The effects of molecular conformation on 1,4-Benzenediamine single molecular conductance

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Single-molecule junctions have been extensively studied because of their high potential for future nanoscale device applications. A single molecular conductance is known to be strongly affected by the change of their conformational change. To clarify the effect, We have recently developed 3D dynamic probe system that enables to directly visualize the conformational dynamics in single-molecule junctions.

In this study, we have applied the 3D dynamic probe system to Au/1,4-Benzenediamine/Au single-molecule junction. Figure 1 schematically shows the 3D dynamic probe system. The current $I$ was measured while the STM tip was moved back and forth in the $z$-direction in accordance with sinusoidal function and scanned two-dimensionally ($x$- and $y$-directions). Figure 2 shows the volume plots in the form of conductance maps as a function of the STM tip apex position which consist of the conductance [$G/G_0$] data obtained while the STM tip was retracted from Au surface and the cross section corresponding to the frames indicated by the blue lines in the volume plots is shown together. A clear periodicity of Au(111) atomic structure observed in the $xy$ cross section indicates high repeatability of site dependent conductance change. Figure 3 is G-z curve and schematic illustrations of the high- and low-conductance states models. As shown in G-z curve, conductance switching to higher state was observed during tip retraction. Our analysis and calculations revealed this change was caused by the conformational change of the end group on Au(111) surface. These results clearly reveal the influence of interactive conformational factors, such as the bonding sites and the bonding conformation, on a single molecular conductance.
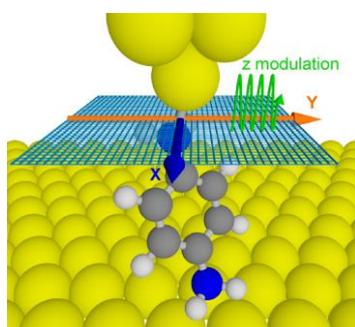


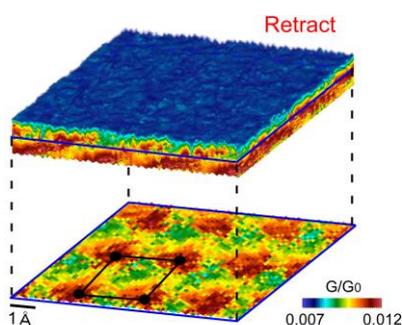Fig 1. Schematic illustration of the 3D dynamic probe system.
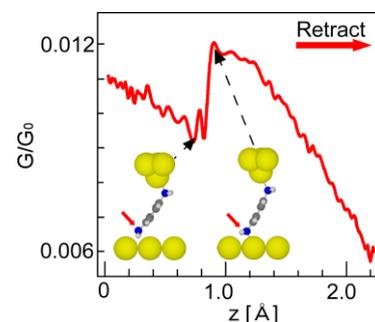
Fig 2. 3D volume plots and xy cross-section

Fig 3. G-z curve and the high- and low-conductance state models

[1] M. Nakamura et al, Nature Communications, 6, 8465 (2015)
[2] S. Yoshida et al, ACSnano, 2016, 10 (12), pp 11211–11218