

# 3D Dynamic Probe Analysis of 4,4'-Bipyridine

## Single-Molecule Junction

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Single-molecule junctions have been extensively studied because of their high potential for future nanoscale device applications. However, the structure of interactive key factors such as the bonding sites at an electrode and the molecular tilt angles cannot be determined experimentally. To determine these factors, we have developed 3D dynamic probe method that enables the probing of conformational dynamics in single-molecule junctions<sup>1</sup>.

In this study, we have applied the new method to Au/4,4'-bipyridine (BPY)/Au single-molecule junction, which has been considered to have angle-dependent binary conductance states for  $\varphi < 90^\circ$  ( $\varphi$  is tilt angle of BPY molecule from xy-plane)<sup>2</sup>. All measurements were carried out in vacuum ( $< 5.0 \times 10^{-8}$  Pa) at 83 K using a low-temperature scanning tunneling microscopy (LT-STM). Figure 1 schematically shows the 3D dynamic probe method. The current  $I$  was measured while the STM tip, which was moved back and forth in the  $z$ -direction in accordance with a sinusoidal function, was scanned two-dimensionally ( $x$ - and  $y$ -directions). Figure 2a shows volume plot which maps single molecular conductance as a function of the STM tip apex position. As shown in the  $G$ - $z$  curve (Figure 2b), binary conductance states were clearly observed in regions I (High) and II (Low). However, in contrast to the previous model, they were observed for  $\varphi < 90^\circ$  and after reaching  $\varphi \sim 90^\circ$  without angle dependence in both cases. These results suggest that binary conductance switch between high state and low state is triggered by a change of transmission between pyridil N- anchors and Au atoms, which depends on their distance.

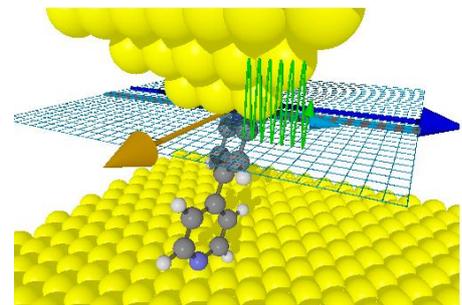


Figure.1 Schematic illustration of the 3D dynamic probe.

[1] M. Nakamura et al, Nature Communications, 6, 8465 (2015)

[2] S. Y. Quek et al, Nature Nanotechnology, 4, 230-234(2009)

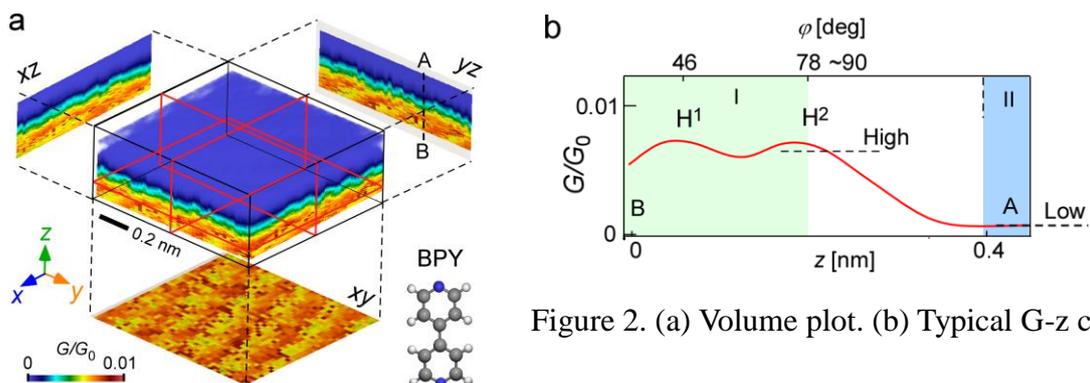


Figure 2. (a) Volume plot. (b) Typical  $G$ - $z$  curve.