Three dimensional conformational dynamics in single molecular junction studied by Scanning Tunneling Microscopy

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With the development of various techniques to fabricate single molecular junctions, tremendous effort has been devoted to elucidate the transport properties of single molecules. A single molecular conductance is known to be strongly affected by the change of their conformational change, however experimental efforts has been yet insufficient to understand the molecular conformation effect due to the lack of an appropriate measurement method.

In this study, we report a new methodology for realizing a three dimensional (3D) dynamic probe of single-molecule conductance which enables elaborate 3D analysis of molecular conformation effect using scanning tunneling microscopy (STM).[1] Fig. 1 shows the schematic of the experimental set-up. The conductance of a 1,4-benezenedithiol (BDT) single molecular between a Au tip and Au(111) surface was measured with a fixed bias voltage V_s applied between the STM tip and the substrate, while the STM tip, which was moved back and forth in the *z* direction in accordance with a sine function, was scanned two dimensionally (*x* and *y* directions). Molecular conductance was plotted against *x*, *y*, *z* coordination of STM tip and shown in fig.2, from which we can analyze key parameter of molecular conformation such as adsorption-site, tilt-angle, and molecular deformation. Such conformational changes alter the conductance of BDT junction significantly, which leads to quite broad conductance variation ranging from $0.0001G_0$ to $0.1G_0$. The detail will be discussed in the presentation.

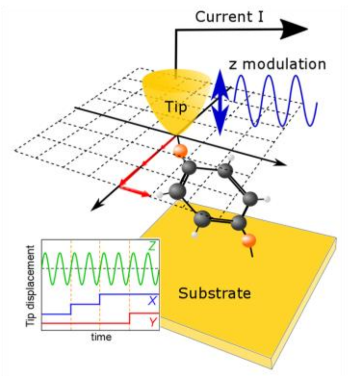

Fig. 1 Schematics of measurement setup and tip control scheme

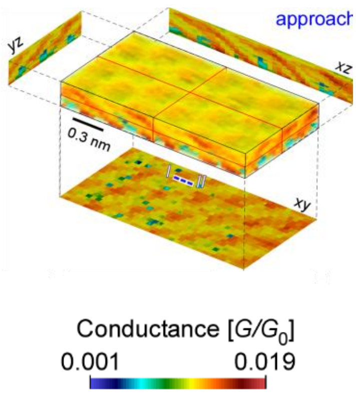

Fig. 2 3D conductance map of BDT single molecular junction.

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