Revealing the conformational dynamics in a single-molecule junction by site- and angle resolved dynamic probe method

S. Yoshida1, T. Atsushi1, Y. Sugita1, O. Takeuchi1, H. Shigekawa1.
1University of Tsukuba, Institute of Applied Physics, Tsukuba, Japan.

Single-molecule junctions have been extensively studied because of their high potential for future nanoscale device applications as well as their importance in basic studies for molecular science and technology. Mechanically controlled break junctions (MCBJs) and scanning tunneling microscopy breakjunctions (STM-BJs) have generally been used to analyze the characteristics of single-molecule junctions. However, analyses have been performed assuming the interactive parameters of conformations such as bonding sites and molecular tilt angles, resulting in uncertainties and inconsistencies in the proposed mechanisms. Therefore, direct approach to experimentally visualize the conformational parameters is strongly required.
Here, we present a methodology that enables the analysis of conformational dynamics in single molecule junctions simultaneously with the direct and systematic characterization of molecular bonding sites, tilt angles, and deformation. [1-3] The conductance of a 1,4-benezenedithiol (BDT) single molecular junction 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 can be plotted against x, y, z coordination of STM tip, 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 0.0001 G_0 to 0.1 G_0. In addition to BDT single molecular junction, we have applied the method to 1,4-benzenediamine single molecular junction to clarify the effect of the nitrogen (N) lone-pair in the amine group on the conductance. The detail will be discussed in the presentation.

http://dora.bk.tsukuba.ac.jp/
[1] S. Yoshida et al., ACS nano, **10**, 11211-11218 (2016)
[2] Y. Sugita et al., Sci. Rep. **8**, 5222 (2018)
[3] M. Nakamura et al., Nature comm. **6**, 8465 (2015)