Conformational Effect in Single Molecular Junction for Short-Distance Electrodes studied by Molecular Dynamics Simulation and Dynamic Probe Method

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A methodology using scanning tunneling microscopy (STM) for realizing a three-dimensional (3D) dynamic probe of single-molecule conductance was reported, in which conformational effects of 1,4-benzenedithiol (BDT) and 1,4-benzene diamine (BDA) were analyzed [1,2]. For further understanding, we carried out experiments and simulations under short-distance electrode conditions. Figures 1a and 1b show the conductance curves of BDA obtained by simulations and experiments for two different initial conditions. Details will be discussed at the conference.

[1] S. Yoshida *et al.*, *ACS Nano* 2016, 10, 11211-11218.

[2] Y. Sugita *et al.*, *Scientific Reports* 2018, 8, 5222.

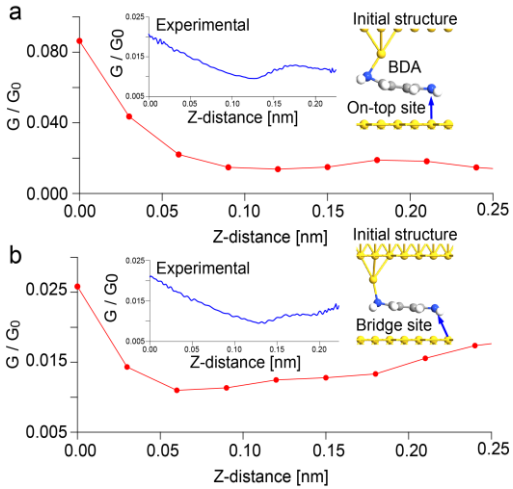

Fig. 1 Conductance curves of BDA for (a) on-top and (b) bridge sites, respectively.