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.


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