Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Stretch Dependent Electronic Structure and Vibrational Energy of the Bipyridine Single Molecule Junction

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1: Calibration of the displacement ratio of the MCBJ setup

Figure S1 shows the correlation between the conductance of the blank nanogap and relative distance of electrode. In the tunneling mechanism, conductance of the nanogap is represented by

$$G = A_N e^{-BL} \quad (1)$$

The B value for vacuum gap is 2.0 $Å^{-1}$ [1], which almost agrees with our experimental B value of 1.7 $Å^{-1}$, in Fig.S1. This supports the validity of our estimation of the displacement ratio and the stretch length based on the dimension of the experimental setup.

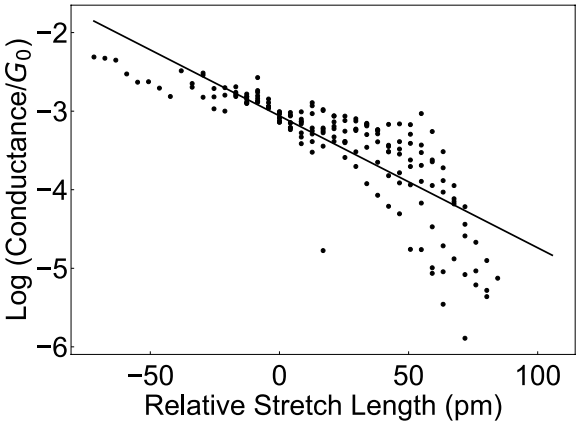

Figure S1. Logarithmic plots of conductance of blank nanogap as a function of stretch length. The plot was obtained from 8 distinct samples. The origin was defined as the point where the conductance was 0.001 G_0, and the stretch length was the relative distance. The line is the fitting result using eq. (1).

References

1 M. Kiguchi and S. Kaneko, *Phys. Chem. Chem. Phys.*, 2013, **15**, 2253-2267.