Charge transport properties of mechanochromic single-molecule junctions

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Single-molecule switches have attracted wide attention in view of their potential application to ultrasmall switches in electronic devices. Transduction of structural and conformational changes into electronic switching is an attractive approach to performing electronic operations using molecular building blocks. In this context, structural isomerization and relevant electronic switching behaviour have been investigated for single-molecule junctions of photochromic molecules using external perturbation of light irradiation [1]. Here, we focus on conformational isomerization and relevant electronic tunability of single-molecule conductance without light irradiation. The structural isomerization of mechanochromic molecules can be induced by internal mechanical perturbation of the junction-stretching and/or compression [2]. In this study, we used Bis{4*H*,8*H*-4-(dicyanomethylene)benzo[1,2-*c*:4,5-*c*']bis[1,2,5]thiadiazole-8-ylidene} (**1**, Fig. 1a) that is known to exhibit a mechanochromic behaviour and has two conformational isomers with a folded or twisted geometry (Fig. 1a) [2]. Figures 1b,c show conductance and *I-V* histograms of the single-molecule junctions of **1** obtained by break junction techniques [3]. The single-molecule junctions of **1** sandwiched by Au electrodes showed two distinct high and low conductance states with the low bias conductance values of ca. 10^{-4} and 10^{-3} G_0. The high conductance state is one order of magnitude more conductive than the low conductance state. The high and low conductance states can be assigned to the twisted and folded conformers of **1**, respectively on the basis of the changes in the electronic states under the conformational isomerization-induced chromism [2]. The conformational isomerization-based conductance modulation would be useful for the development of single-molecule switches.

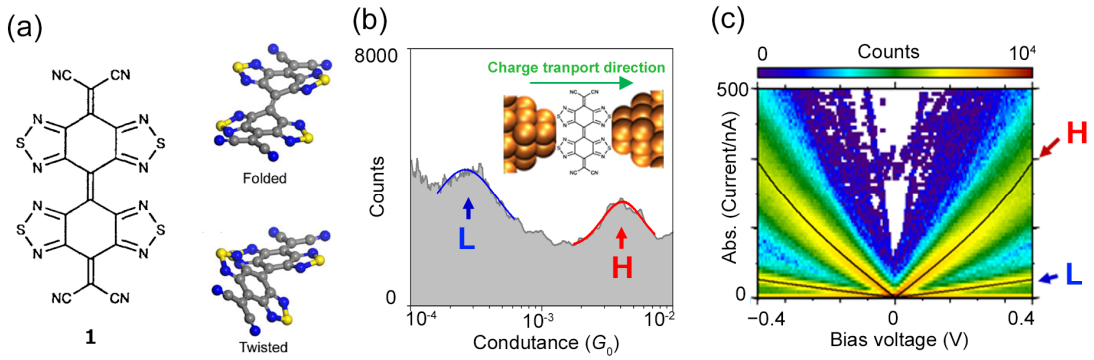

Figure 1 (a) Chemical structure and ball-and-stick models of the folded and twisted conformers of **1**. (b,c) Conductance and *I-V* histograms of the single-molecule junctions of **1**. The arrows in (b) and (c) represent preferential distributions of the high (H) and low (L) conductance states.

References:

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