

Supporting Information

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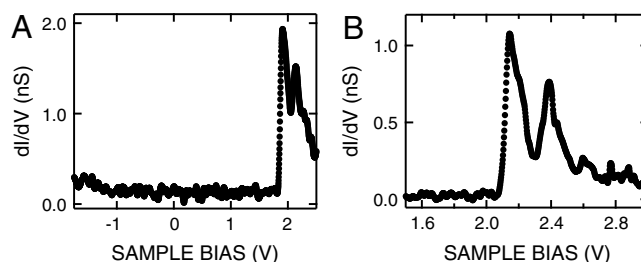


Fig. S1. (A) Differential conductance (dI/dV) versus sample voltage V acquired over an unsubstituted NDI cyclophane. STM feedback was opened at $I = 0.5$ nA, $V = 2.5$ V. A sharp structure at positive voltages, the onset of a broader feature at the negative voltages and a large apparent zero-conductance gap are visible in the spectrum, similarly to the *tert*-butyl-thiol substituted NDI cyclophane case. (B) Detailed view of multiple peaks as in Fig. 2 recorded over an unsubstituted NDI cyclophane. An average peak distance of ≈ 220 mV was found from a linear fit of the peak positions. STM feedback was opened at $I = 0.1$ nA, $V = 3$ V.

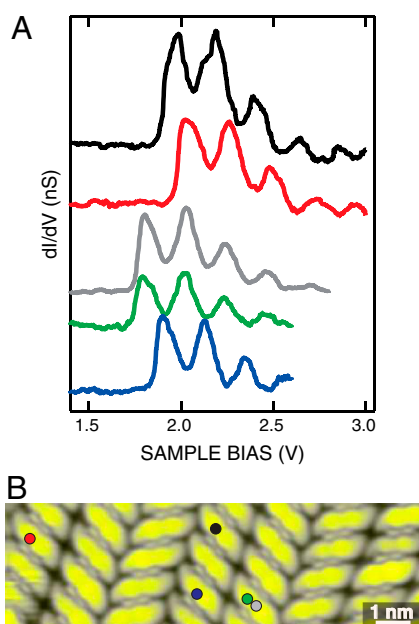


Fig. S2. (A) dI/dV data acquired at $V = 3$ V (black and red spectra from top), $V = 2.8$ V (gray spectrum), $V = 2.6$ V (green and blue spectra) over the molecules marked in B using the same color code. It can be noted that spectra acquired at the same voltage over two different molecules show a different shift of the affinity level peaks (≈ 40 mV in the black and red spectra, at $V = 3$ V, and ≈ 100 mV in the blue and green spectra, at $V = 2.6$ V), whereas spectra acquired over the same molecule at different initial setpoint ($V = 2.8$ V and $V = 2.6$ V) show no apparent shift (gray and green spectra). (B) Constant current STM image of NDI cyclophanes acquired at $V = 2.2$ V, $I = 50$ pA.

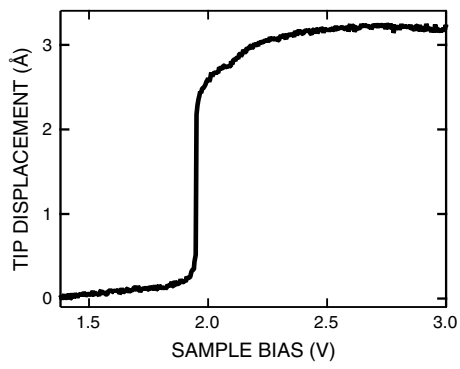


Fig. S3. Typical tip displacement as function of the applied voltage. The sample voltage was swept from $V = 1.4$ V to $V = 3$ V and the tip displacement was recorded, whereas the tunneling current was fixed at $I = 50$ pA, with the feedback kept closed.