Supporting Information

Driving a 3rd Generation Molecular Motor with Electrons Across a Surface

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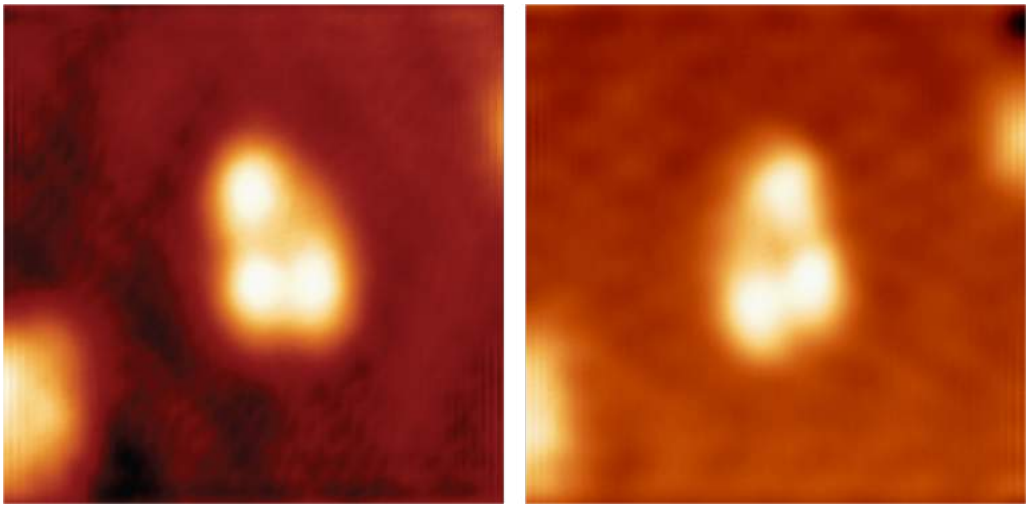

Figure S1. STM images (6 nm × 6 nm, 50 mV, 10 pA) of the *(M)*-**1** (left) and the *(P)*-**1** (right) enantiomer on the Cu(111) surface. Note that both images are from the identical molecule at identical position which has been switched through different conformations (see also Fig. S4). That is, the molecule is at identical position and rotation with respect to its surface position has not occurred.

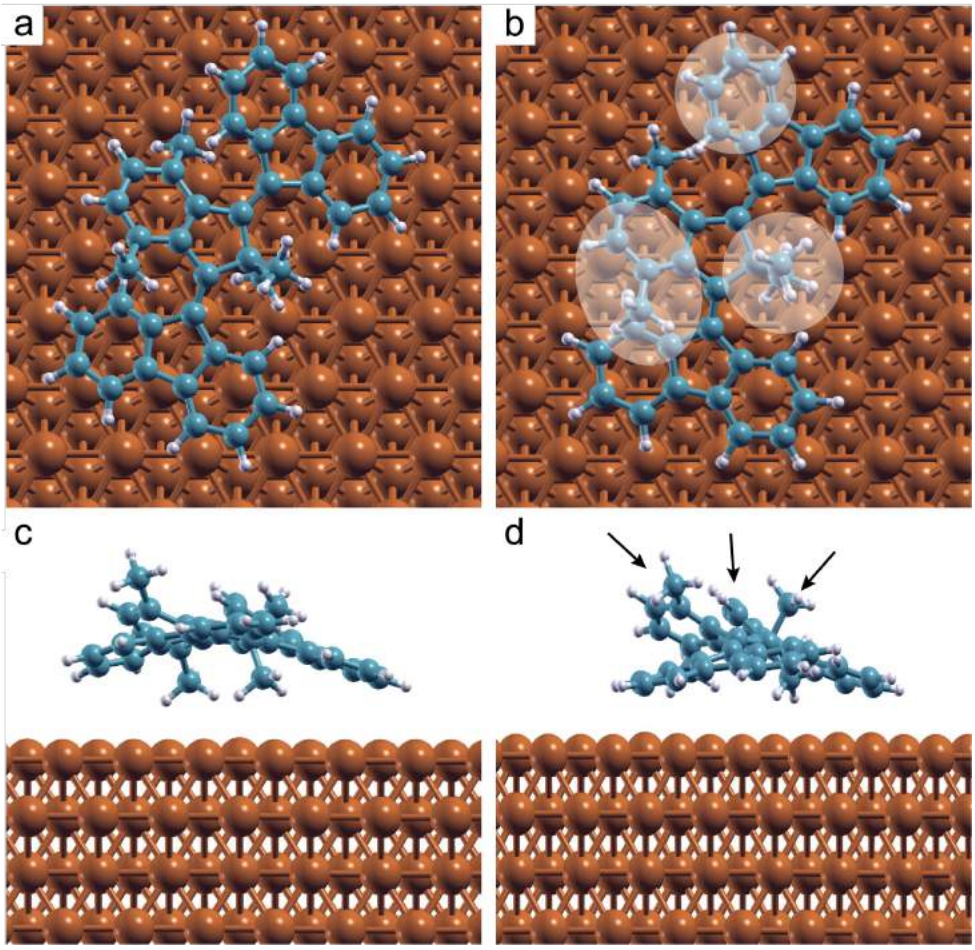

Figure S2. Initial and DFT-relaxed conformation of **1** as calculated on a 4-layer Cu slab. a,c) Top and side view of starting conformation. b,d) Top and side view of final relaxed conformation. The parts of the molecule that contribute according to the contrast calculations most to the constant current STM contrast are indicated as semi-transparent filled ellipses. Three black arrows identify these parts in d) and also identify them as highest parts in the side view (arrows). As the DFT approach used here is a 0 K method, the handedness of the initial **(*P*)-1** conformation leads to the same handedness in the relaxed conformation.

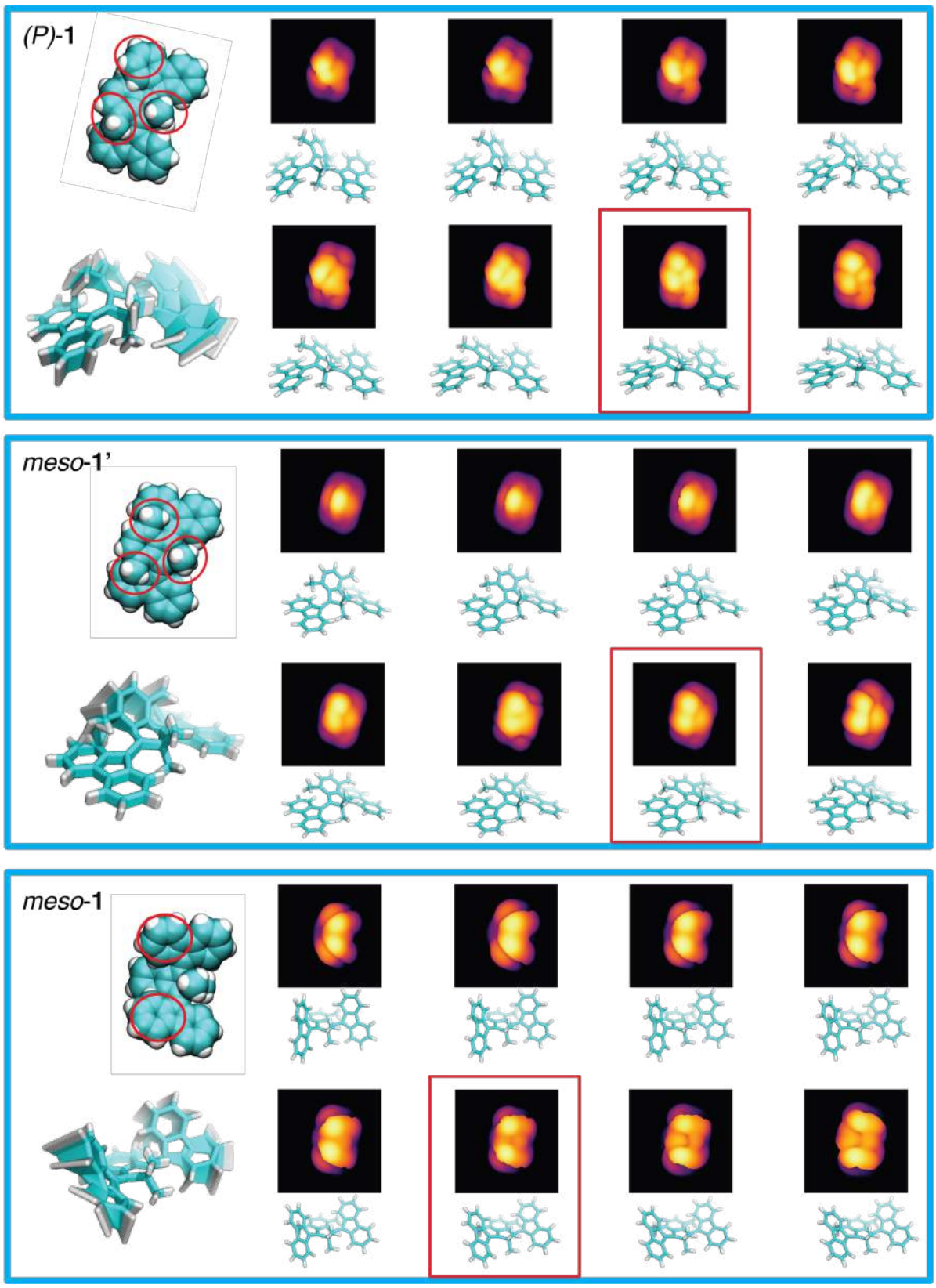
(P)-1
meso-1'
meso-1

Figure S3. Calculated STM contrasts of three conformers (3.0 nm × 3.0 nm, height span from black to white 1.7 nm). The initial conformation in the left upper corner was determined by DFT of the free molecule plus rearrangement of the molecular frame due to surface interactions as calculated by Amber force fields. For achieving good agreement with experimental contrast, stepwise further rearrangement of the molecular frame due to interaction with the tip and surface within the tunnel junction was considered. The constant current STM appearance was calculated for each structure and best agreement (indicated by red boxes) assigned as actual conformation in the tunnel junction. Red ellipses in the shown full-space models indicate the parts of the molecules that dominate the STM contrast. Superpositions of all eight tested structures per conformer are shown in the left lower corners, respectively. Note that no assumption about the STM tip or other corrections have been considered.

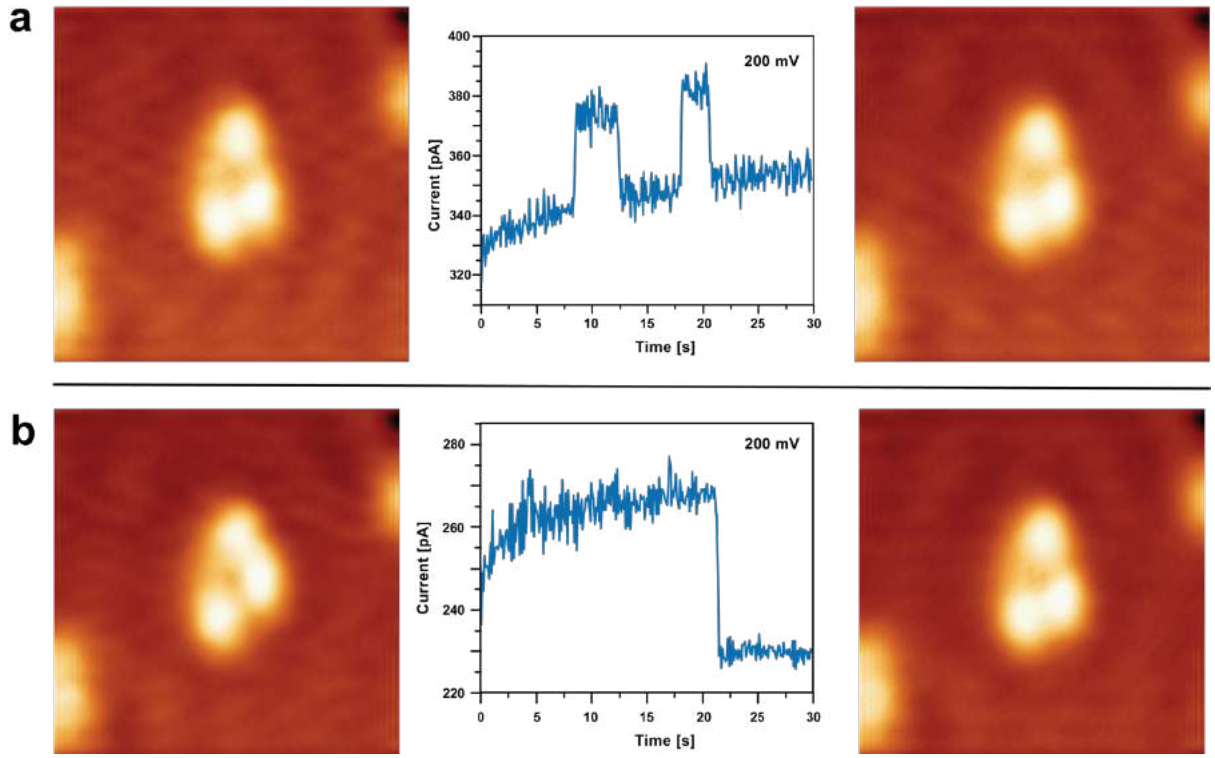

Figure S4. Initial and final STM images (6 nm × 6 nm, 50 mV, 10 pA) and time-current trace of two manipulations. a) The conformation has been switched forth and back twice such that initial state and final state are identical. b) Time-current trace for switching from meso-**1'** to (*P*)-**1**.

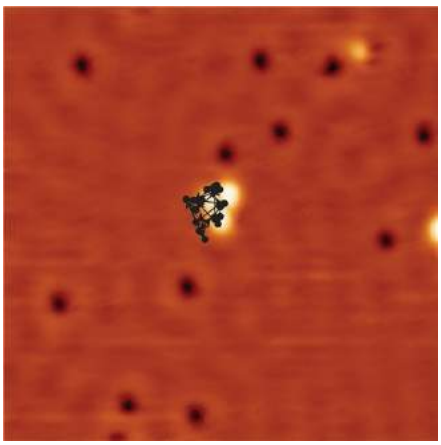

Figure S5. Analysis of position change upon conformational changes shows that no substantial repositioning occurs. The STM image (15 nm × 15 nm, 50 mV, 10 pA) shows a molecule that has been switched 20 times. The center of the molecule after each step is indicated by black dots.

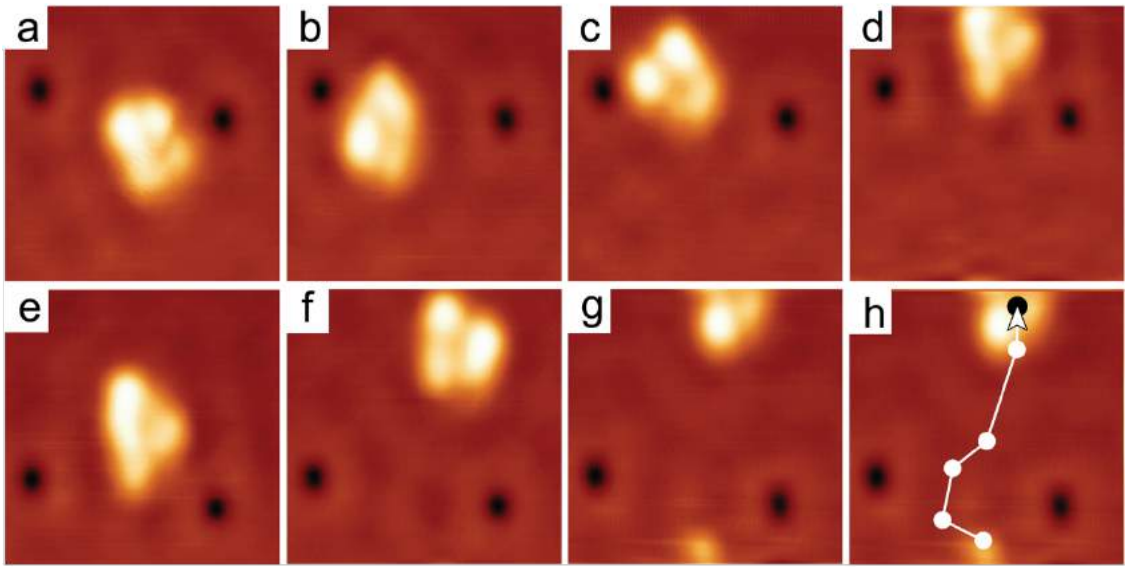

Figure S6. Sequence of STM images (6nm × 6 nm, 50 mV, 10 pA) showing movement of **1** induced by electrons tunneling from occupied states of the adsorbate into unoccupied states of the metal tip. Only re-centering without any manipulation has been performed between frame (d) and (e). Manipulation parameter: –1.0 V, 400 pA. Frames (g) and (h) are identical with the latter summarizing the path.

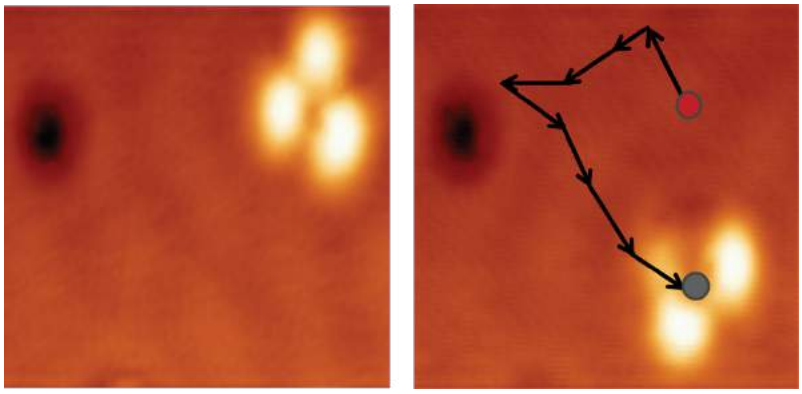

Figure S7. STM images (6 nm × 6 nm, 50 mV, 10 pA) before (left) and after (right) 20 manipulations of **1** at 800 mV bias voltage. The trajectory of movement is indicated by arrows.

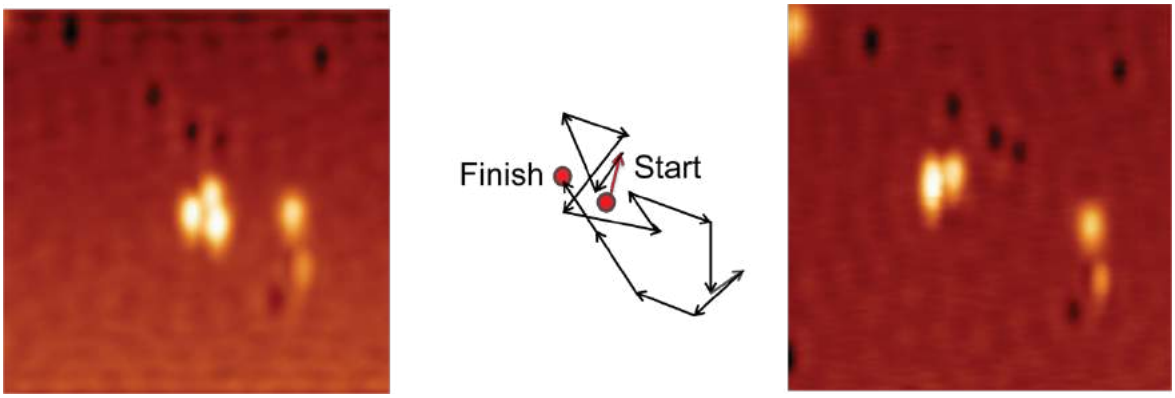

Figure S8. Sequence of STM images (15 nm × 15 nm, 50 mV, 10 pA) showing movement of **1** induced by 20 900 mV pulses. The trajectory of movement is indicated.

Equation S1

Standard deviation derived from the probability for successful events:

$$S = \sqrt{\frac{1}{N-1}\left(1 - \frac{n_S}{N}\right)}$$

n_S : number of successful events

N: number of attempts