Supporting information

The regulation effect of coordination number on conductance of single-molecule junctions

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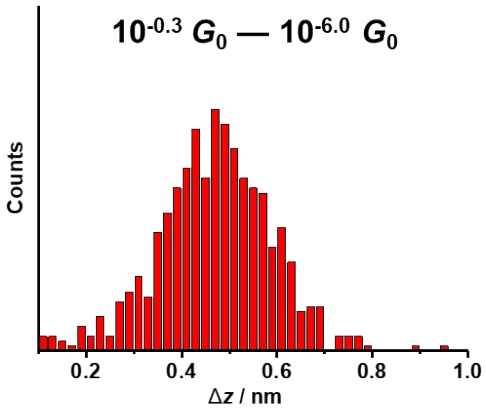

Fig. S1. Relative stretching displacement histograms for N2.

To analyze the step length distribution for each group, we statistically analyze displacements in all conductance-displacement curves from $10^{-0.3}$ to $10^{-6.0}$ G_0. As shown in Fig. S1, the step stretching displacement (Δz) distributions are centered at 0.5 nm. Typically, by adding the snapback distance (0.5 nm) of breaking Au-Au contacts with the Δz, the most probable absolute displacement for molecular junctions is about 1 nm, which is in good agreement with the molecular length of N2.

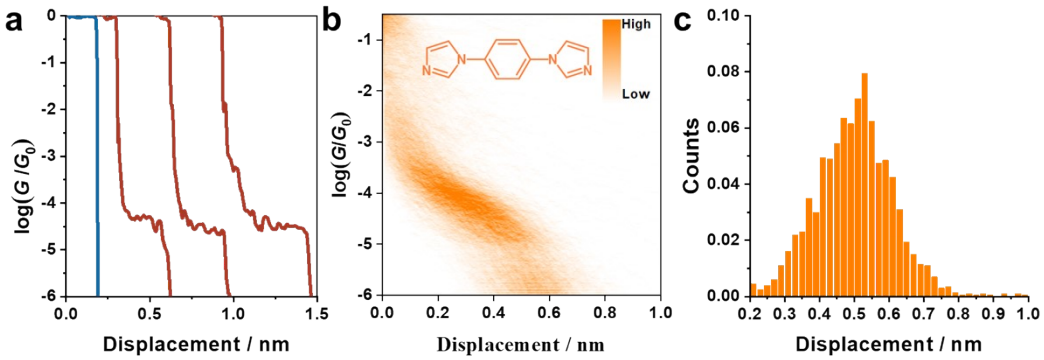

Fig. S2 (a) Typical conductance-distance traces of single molecular junction, (b) two-dimensional (2D) conductance histograms as function of relative displacement for **N1**. (c) Relative stretching displacement histograms of **N1.**

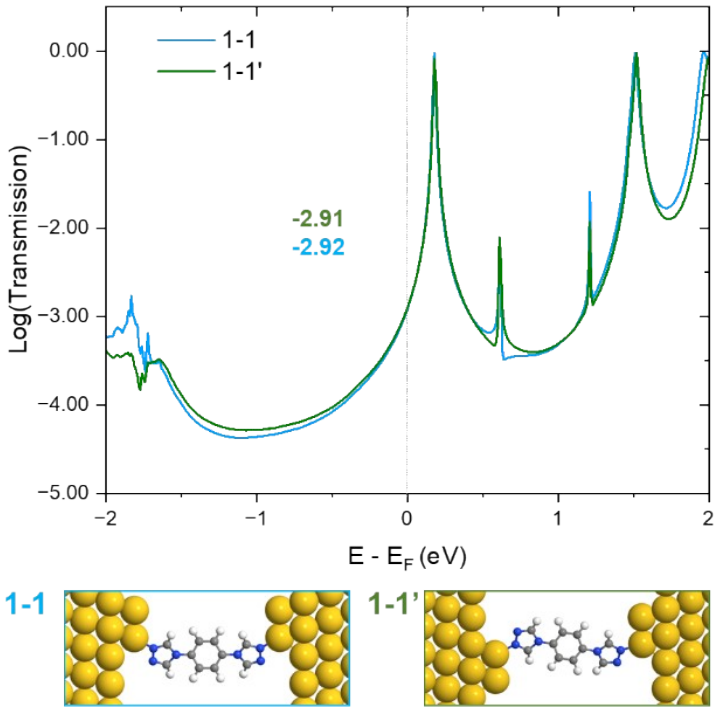

Fig. S3 Calculated transmission spectra for two different 1-1 modes of N2 molecule.

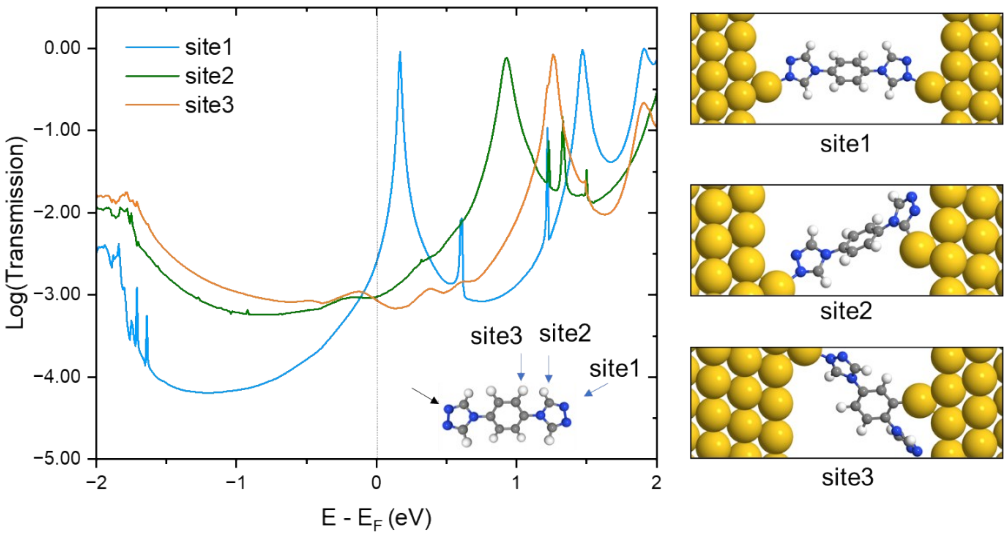

Fig. S4 Calculated transmission spectra for **N2** molecule binding to Au electrodes by various sites.

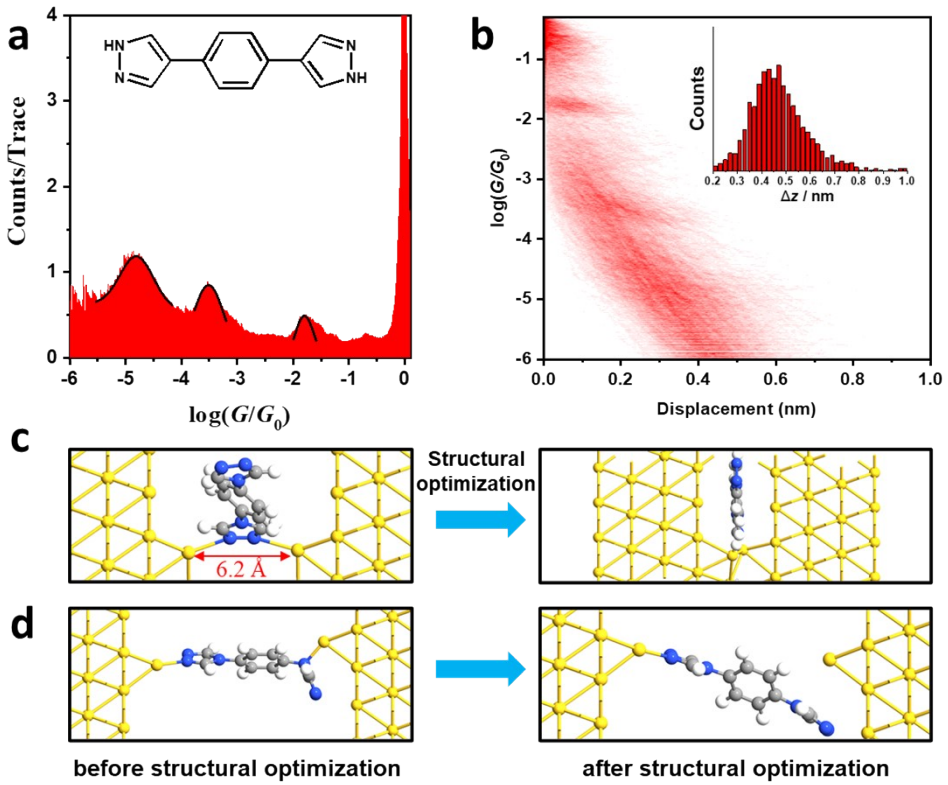

Fig. S5. (a) 1D conductance histograms and (b) 2D conductance histograms as function of relative displacement for 1,4-bis (1H-pyrazol-4-yl) benzene. Structural evolution while structural optimization for (c) electrodes binding to two N atoms of N2 in the same triazole ring as the initial configuration and (d) one of the electrodes being bound to the internal nitrogen.

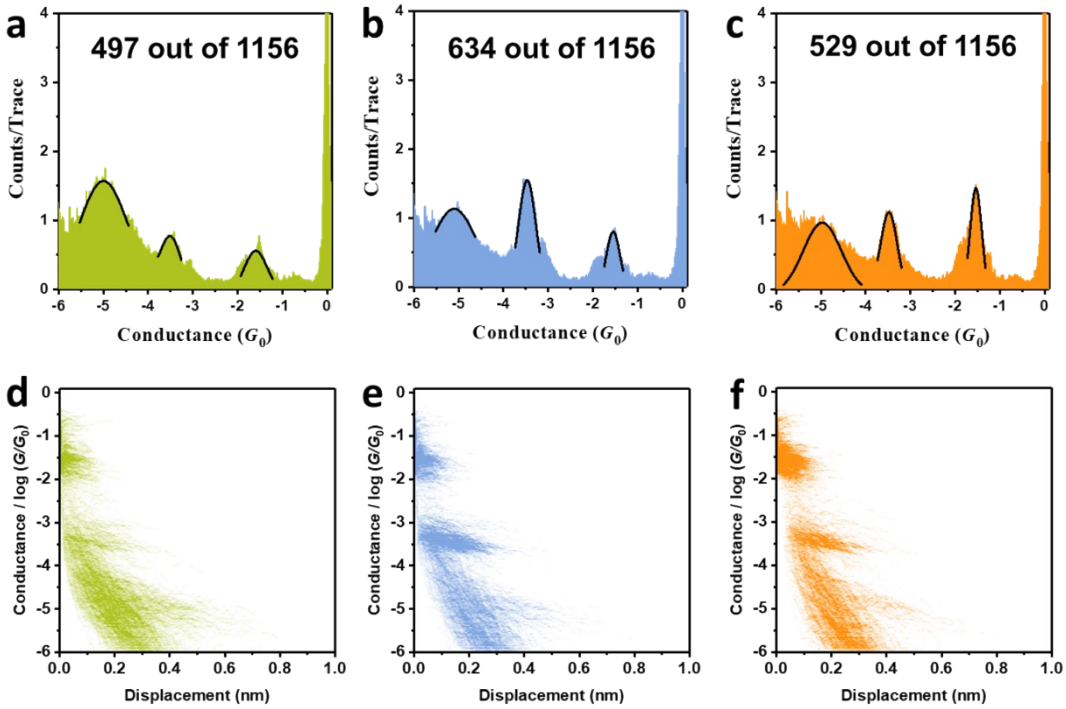

Fig. S6. 1D (a-c) and 2D (d-f) conductance histograms from the selected conductance-distance trances displayed the LC, MC, and HC steps, respectively.

All conductance-distance traces displayed the corresponding HC, MC, and LC steps have been selected, respectively (Taking HC as example, if there is HC step appearing in the trace, the conductance-distance trace is selected regardless of whether steps appear in the MC and LC). It is found that 497, 634 and 529 out of 1156 traces occurred LC, MC and HC steps, respectively. Corresponding 1D and 2D conductance histograms were shown in Fig. S1. Three conductance peaks assigned to HC, MC and LC can be clearly observed in each group, indicating that these steps appear simultaneously in most conductance-distance traces. This further supports that a 2-2 or 2-1 configuration of the molecular junction is firstly formed when the tip is driven into the SAM of N2 with both two N binding to the Au substrate.