Electronic Supplementary Information (ESI)

Electron tunneling through molecule-electrode contacts of single alkane molecular junctions: experimental determination and a practical barrier model

Kun Wang and Bingqian Xu*

Single Molecule Study Laboratory, Faculty of Engineering and Nanoscale Science and Engineering Center, University of Georgia, Athens, Georgia 30602, USA

* Email: bxu@engr.uga.edu

SI-1 Example conductance traces

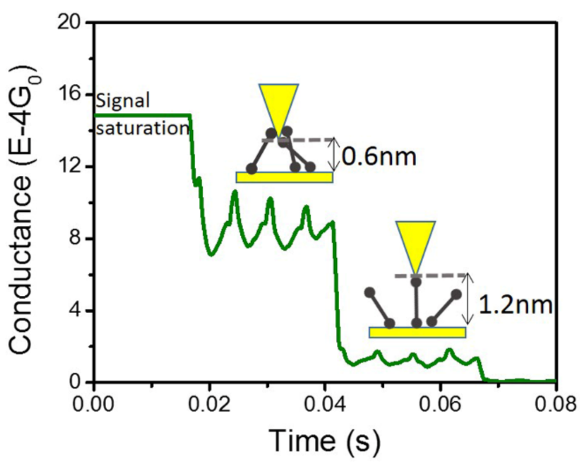

Fig. S1 Example case of a full-scale modulated conductance trace.

Note that as shown in Fig. S1, , the single-molecule plateaus of C8DT and C8DA in our measurements mostly appeared under the junction separation of ~ 1.2nm which was created by twice the abrupt stretching of 0.6nm. For this case, the distance between the electrodes is about the C8 molecular length. Thus, the molecule should stand still nearly perpendicular to the substrate. This setup greatly diminished the influence of the conductance change caused by molecular angle tilt when the mechanical modulation was applied.

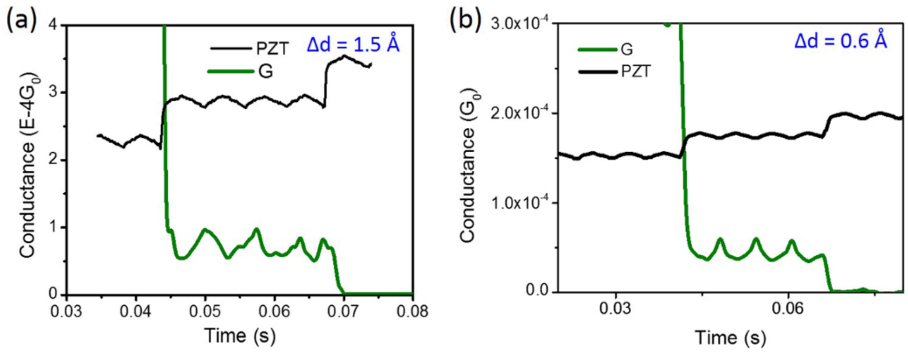

Fig. S2 Typical modulated C8DT conductance traces and corresponding PZT signals for Δd=1.5Å (a) and Δd=0.6Å (b).

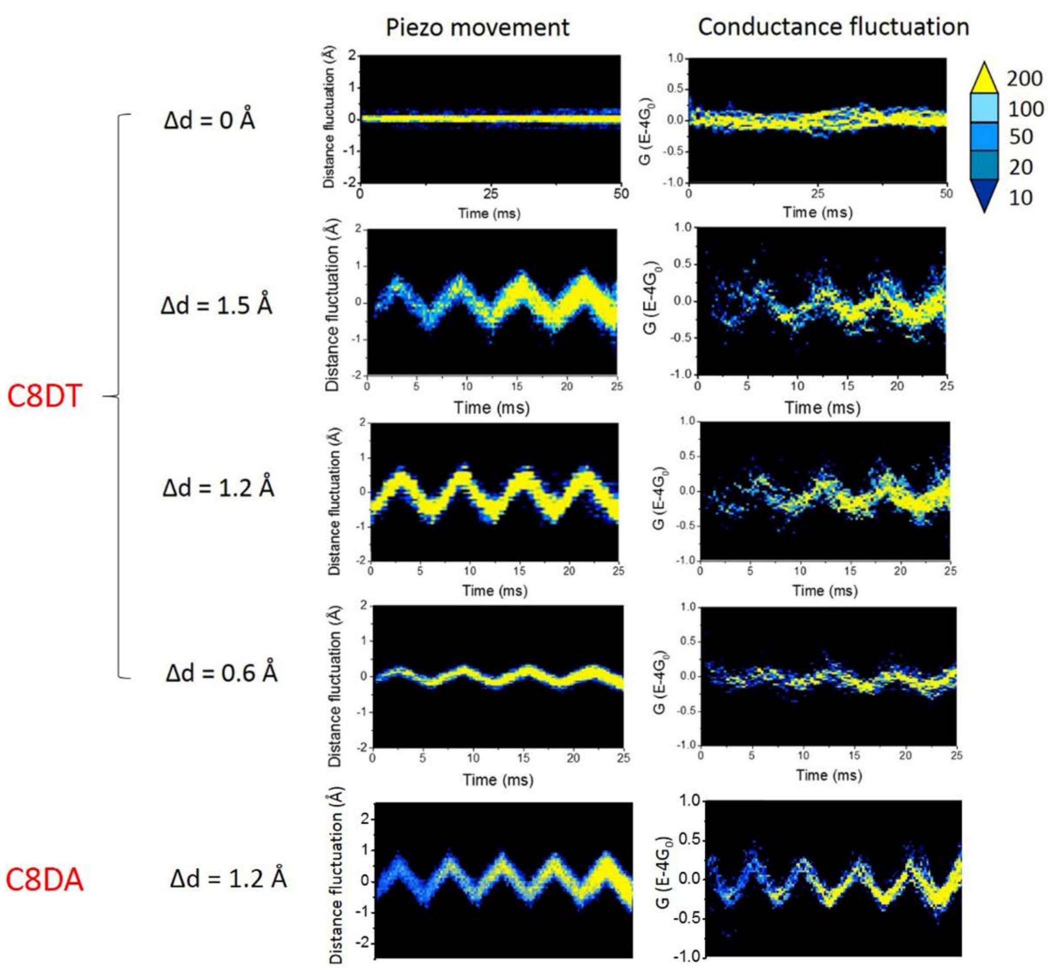

Fig. S3 Two-dimensional (2D) illustration of the overlay of piezo signal and conductance signal of around 70~80 conductance plateaus for C8DT and C8DA at each modulation amplitude with regular conductance fluctuation.

Note that in Fig. S3, the conductance plateaus for each modulation amplitude has been offset to zero by deducting a value of 6.5E-5G_0 for C8DT and 4E-5G_0 for C8DA which is the average value of all the conductance plateaus under the TRI modulation. By doing so, we aims to show the change in degree of conductance fluctuation that corresponds to different modulation amplitudes. It can be clearly seen that the degree of conductance fluctuation increases with the increase of modulation amplitude. We emphasize that the regular conductance fluctuation only occurred when the TRI mechanical modulation was applied. This proves that this regular conductance change was predominantly caused by the junction separation regulation instead of other factors like thermal vibration or mechanical noise. We also notice that the noise level for modulated conductance plateaus (~1E-5G_0) is smaller than that of non-modulated plateaus (~2E-5G_0).

SI-2. Conductance switching examples and switching probability distribution under different modulation amplitudes

Using stretch-hold mode STM break junction technique, four single-molecule conductance sets have been observed.[1] Under the TRI modulations, we observed evident conductance switching among the different conductance sets (Figure S4a and S4b), and that the switching probability increased with the increase of modulation amplitude (Figure S4c).

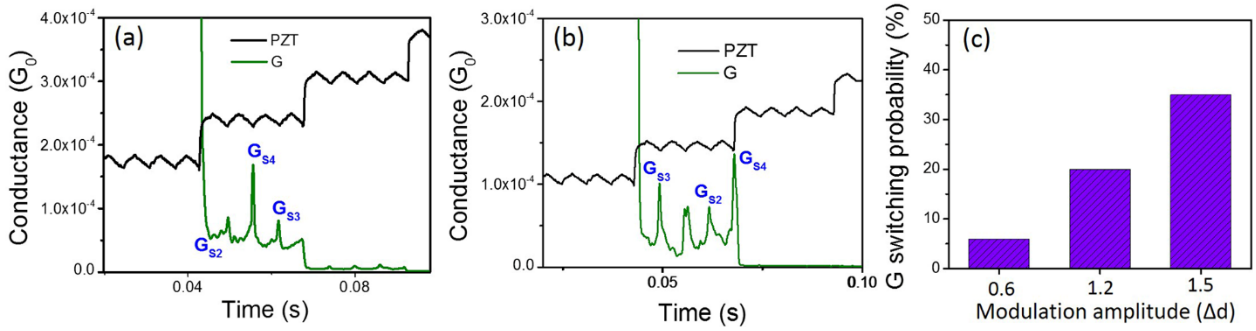

Fig. S4. Example conductance traces containing conductance switching events among different single-molecule conductance sets (a and b) under $\Delta d = 1.5$Å and the switching probability under three modulation amplitudes (c).

SI-3 Two-dimensional (2D) β_C vs Δd and Φ_C vs Δd plots

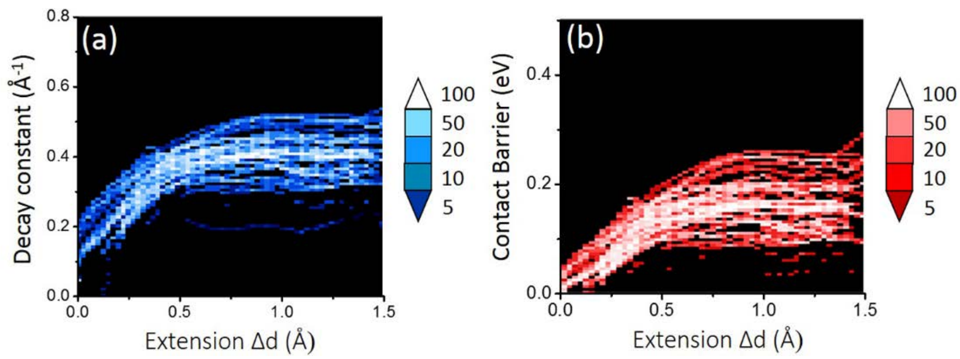

Fig. S5 C8DT two-dimensional (2D) contact decay constant β_C vs extension Δd (a) and contact tunneling barrier Φ_C vs extension Δd (b) plot of around 100 conductance decrease regions.

SI-4. Linear fitting of the contact barrier data

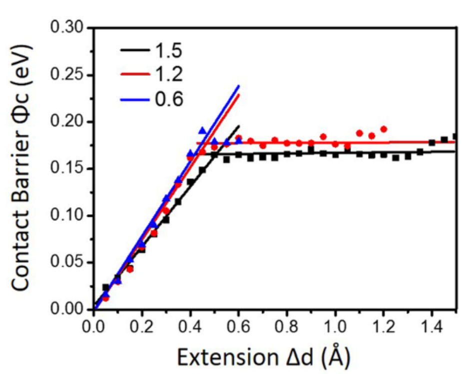

Fig. S6. The linear fitting of the contact barrier data shown in Fig. 2a in the main text.

SI-5. Distribution of experimental G_{mol} and distribution of conductance decrease

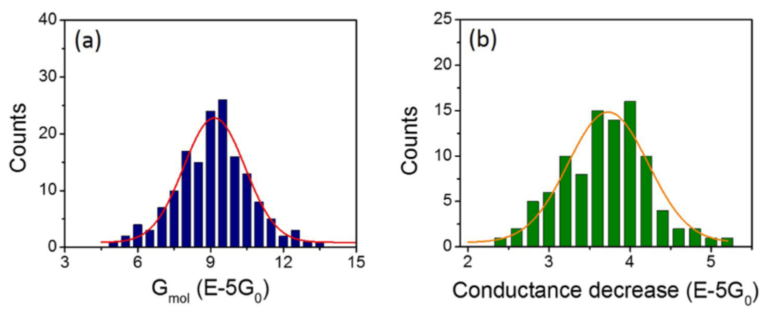

Fig. S7. (a) $\mathrm{G_{mol}}$ histogram of 158 conductance decrease events which contain no conductance switching under $\Delta d = 1.5$Å. (b) The distribution of conductance decrease of 68 experimental curves initiated from experimental G_{mol} within range of $9(\pm1) \times 10^{-5} G_0$.

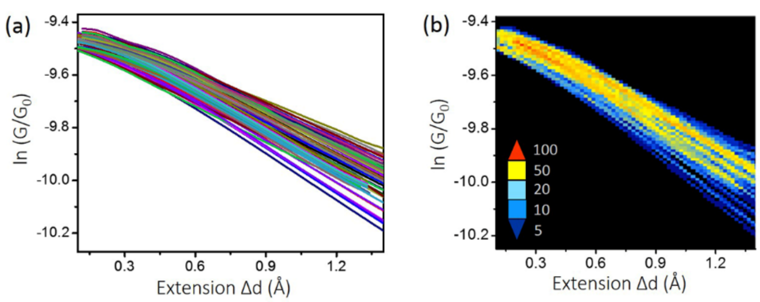

Fig. S8 The raw experimental data of lnG vs Δd plot (a) and the 2D illustration of lnG vs Δd plot (b) over 68 conductance decrease curves that have a $\mathrm{G_{mol}}$ of $9(\pm1)$E-5$\mathrm{G_0}$.

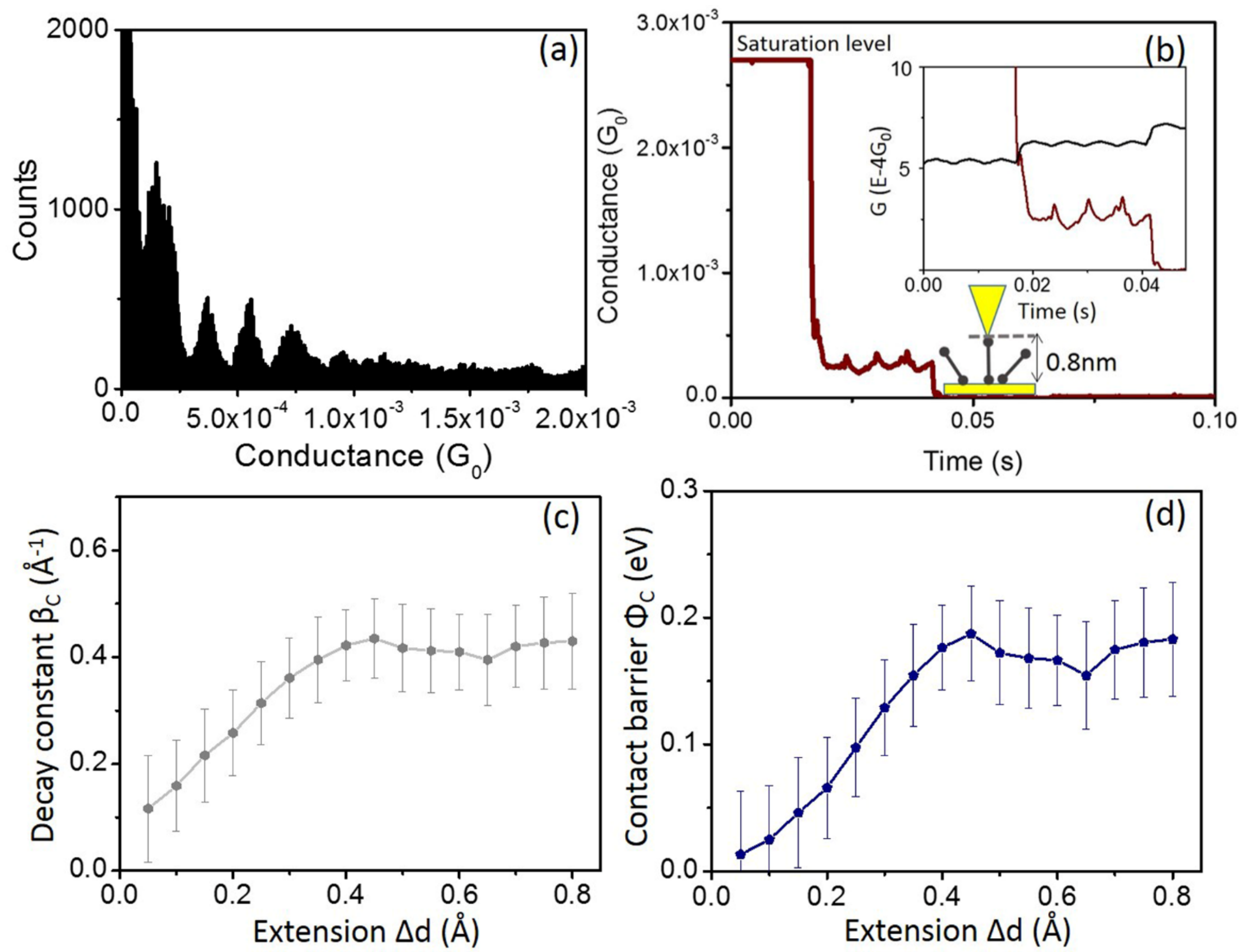

Fig. S9 (a) Stretch-hold mode conductance histogram of C6DT measured under 0.3V. Note that only the conductance plateaus within the first peak range (1.5~2.5E-4G_0) of the histogram were used for further statistical analysis. (b) Typical full-scale modulated C6DT conductance trace. The inset shows a magnified view of the conductance plateau region. Note that the conductance plateau appeared after one abrupt stretching of 0.8nm. (c) and (d) show the C6DT contact decay constant β_C vs extension distance Δd plot and contact barrier height $\emptyset_C$ vs extension distance Δd plot, respectively, based on around 100 conductance decrease events,

References

1. J. Zhou, F. Chen and B. Xu, *J. Am. Chem. Soc.*, 2009, **131**, 10439-10446.