Supporting Information for Publication - Signatures of Conformational Dynamics and Electrode-Molecule Interactions in the Conductance Profile During Pulling of Single-Molecule Junctions

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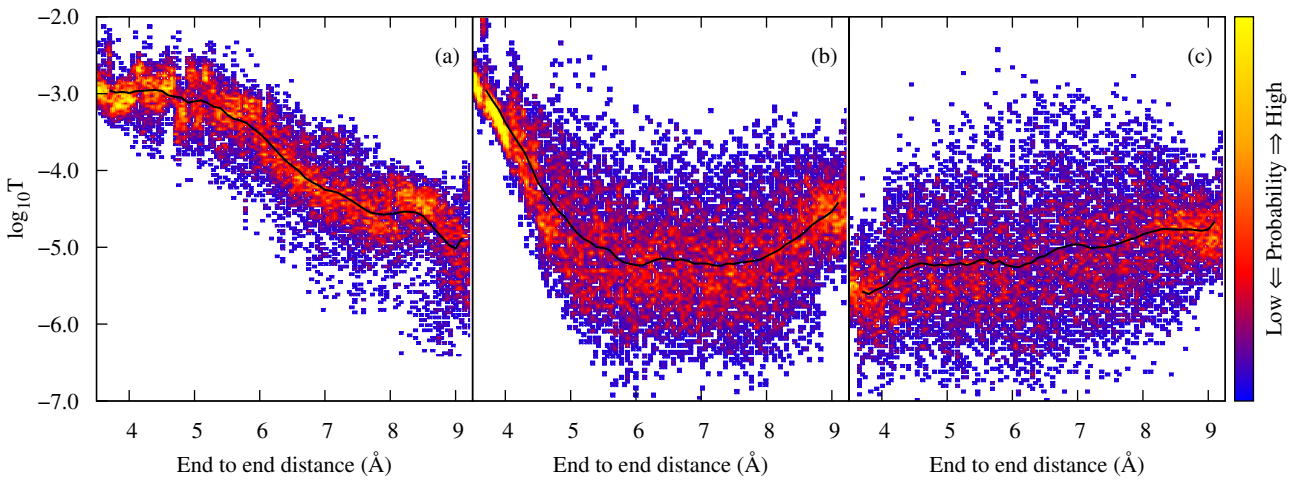

Figure S1: Effect of through-space interactions in the transmission profile during pulling. The plots show the probability density distribution of the transmission as a function of the end-to-end distance (black lines indicate averages) for the Au(111)-S-$(CH_2)_6$-S-Au(111) junction. (a) No intramolecular through-space interactions. (b) No through-space electrode-molecule interactions. (c) Restrictions in (a) and (b) are simultaneously applied. Note that the overall decay of the conductance is lost (in (b)) when the molecule does not have through-space interactions with the gold. Through-space interactions in the molecule play an important role when the molecule is compressed (end-to-end distance less than 6 Å).

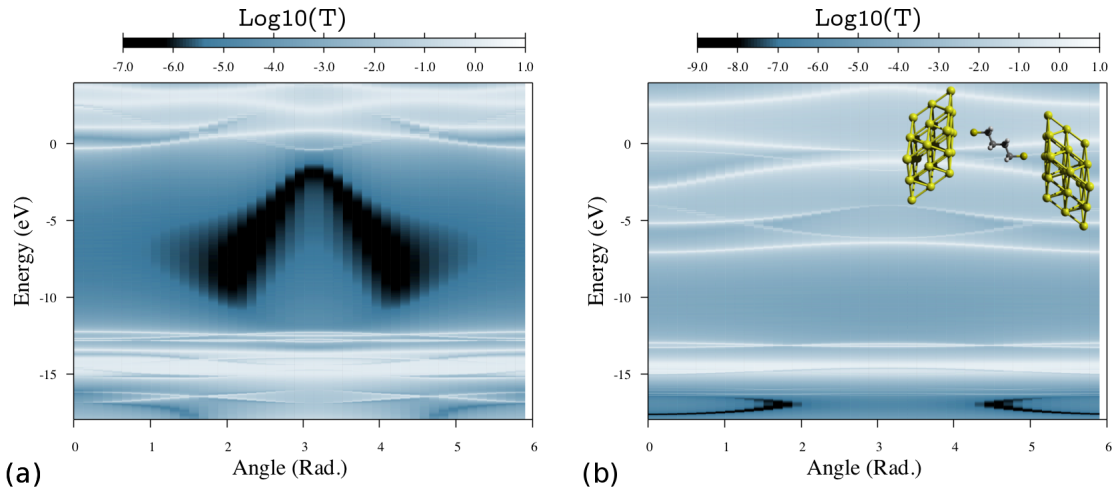

Figure S2: Transmission function $T(E)$ for the Au-S-$(CH_2)_4$-S-Au junction as a function of the carbon dihedral angle for different transmission energies, considering full extended Huckel interactions (a), and restricting intramolecular interactions to only nearest neighbors (b). Note that the interference pattern (dark region in (a)) vanishes when through-space intramolecular interactions are suppressed (b).

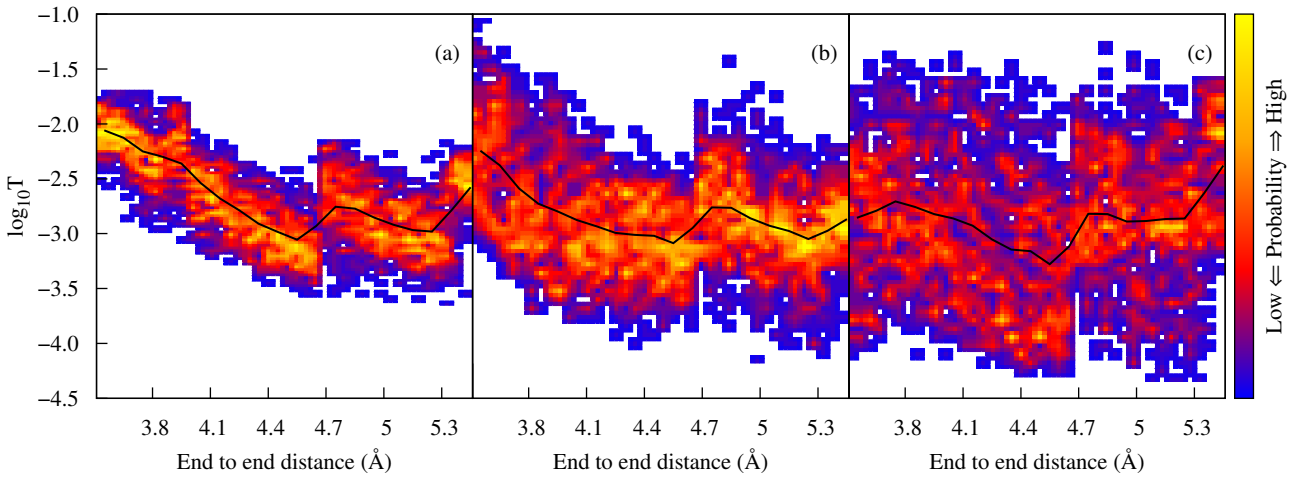

Figure S3: Effect of through-space interactions in the transmission profile during pulling. The plots show the probability density distribution of the transmission as a function of the end-to-end distance (black lines indicate averages) for the Au(111)-S-$(CH_2)_3$-S-Au(111) junction. (a) No intramolecular through-space interactions. (b) No through-space electrode-molecule interactions. (c) Restrictions in (a) and (b) are simultaneously applied. Note that even without considering intramolecular through-space interactions, the kinks in the transmission due to changes in the dihedral angles are still visible.