Supporting Information:

Structure-Property Relationships in Atomic-Scale Junctions: Histograms and Beyond

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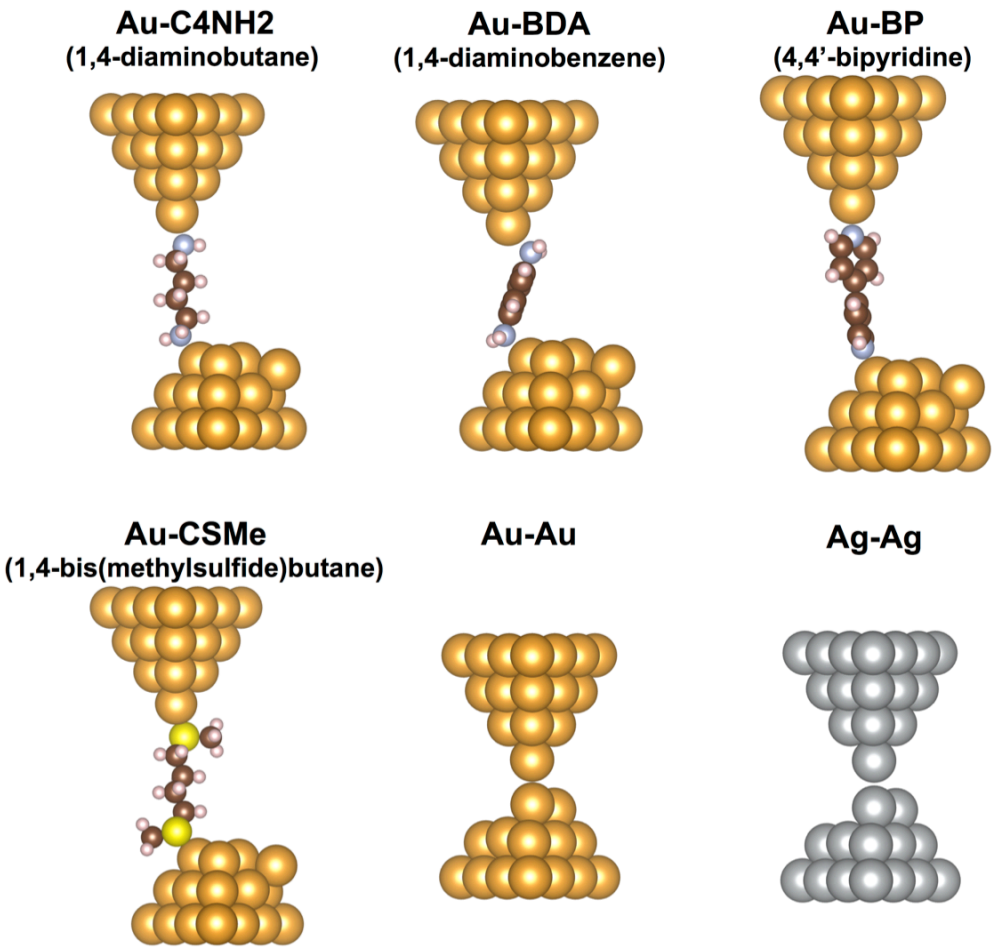

Figure S1: Exemplary structures from the adiabatic trajectory calculated for each of the junctions in Table 1. The single molecule junctions are visualized near the minimum of the trajectory while the metal point contacts are visualized near the point of maximum sustained force. The methodology and prior results for the four single molecule junctions have been previously published.[1,2] The prior calculations were extended and refined for presentation in Figure 7. The structures to simulate the metal point contacts were adapted from the pyramid electrode models by removing two metal atoms from the bottom electrode and aligning the electrodes in a contact geometry that subsequently led to rupture of a single coordinated metal-metal bond. The adiabatic trajectories for the Au-Au and Ag-Ag model junctions in Figure 7 have not been previously published. Visualization with VESTA.[3]

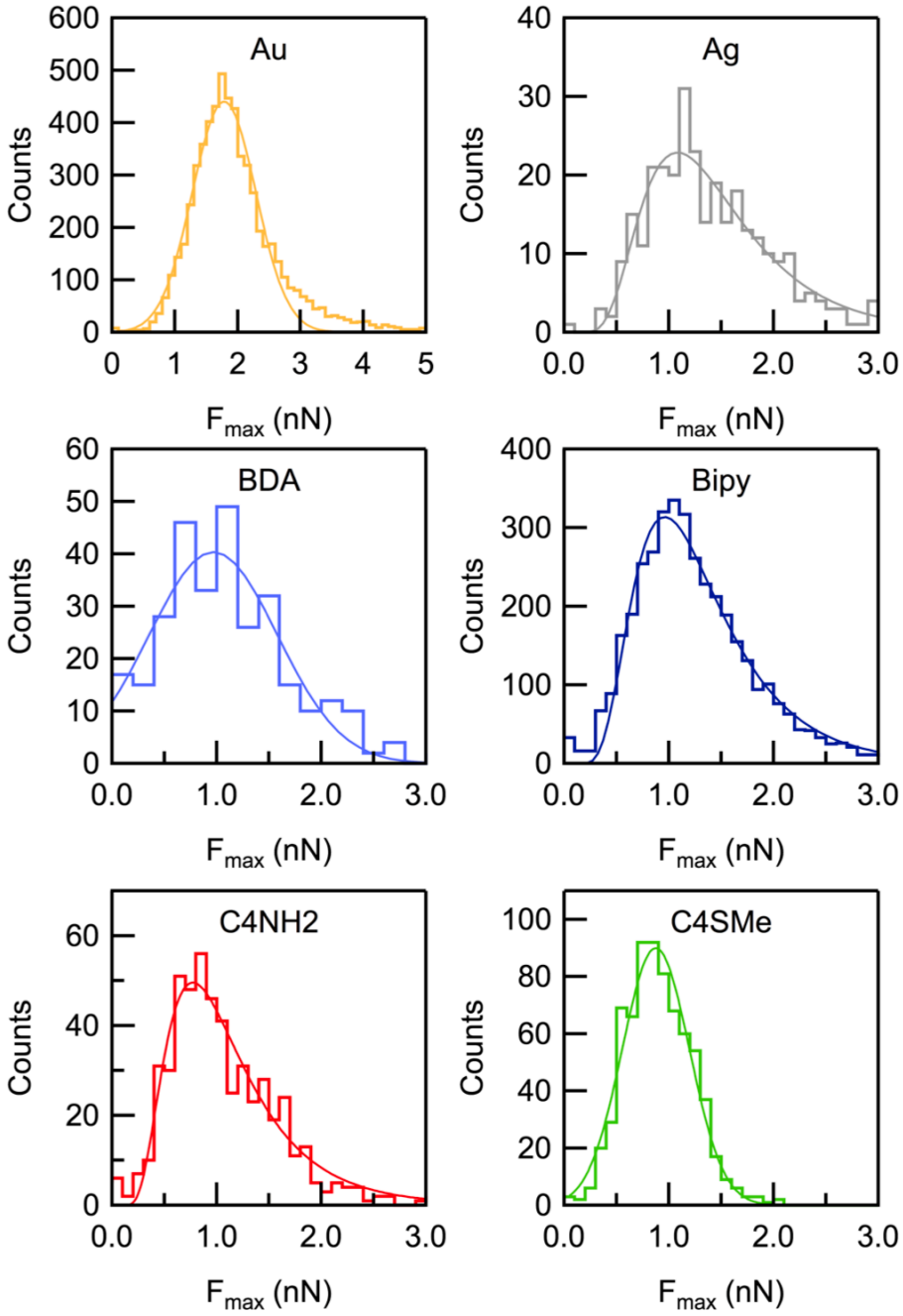

Figure S2: Histograms of fitted values of F_{max} for junctions in Table 1, based on the same data and fits that were previously published.[2] The corresponding histograms of L_{bind} were previously published (Ref. 2, see SI).

References:

(1) Frei, M.; Aradhya, S. V.; Koentopp, M.; Hybertsen, M. S.; Venkataraman, L.: Mechanics and Chemistry: Single Molecule Bond Rupture Forces Correlate with Molecular Backbone Structure. *Nano Lett.* **2011**, *11*, 1518-1523.

(2) Aradhya, S. V.; Nielsen, A.; Hybertsen, M. S.; Venkataraman, L.: Quantitative bond energetics in atomic-scale junctions. *ACS Nano* **2014**, *8*, 7522-30.

(3) Momma, K.; Izumi, F.: VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. *J. Appl. Crystallogr.* **2011**, *44*, 1272-1276.