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SUPPLEMENTARY INFORMATION

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Supplementary Information for

Atomic-scale engineering of electrodes for single-molecule contacts

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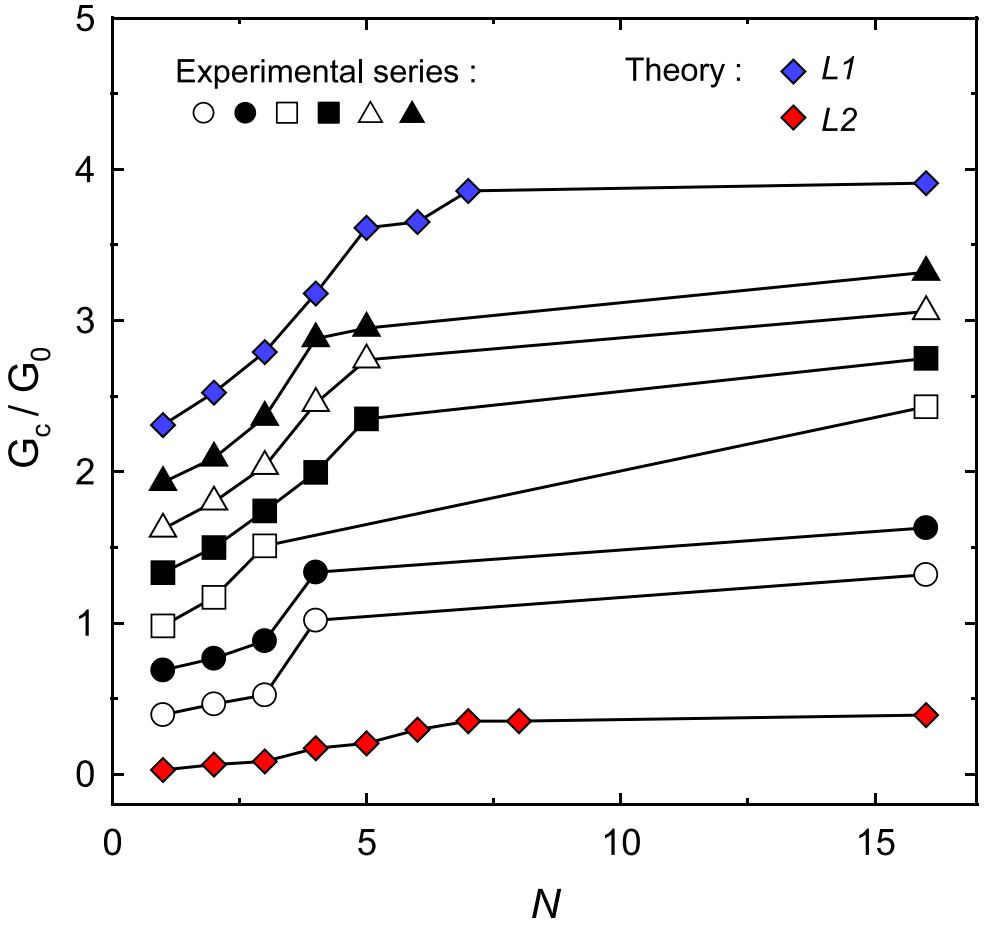

FIG. S1. Contact conductance $G_c(N)$ vs cluster size corresponding to the experimental and theoretical data sets of Fig. 3a. The experimental series comprises data from six different molecular tips and the theoretical series shows results for two electrode separations $L_1 = 17.2$ Å and $L_2 = 18.0$ Å (measured between the second-topmost layers) around the point of contact. For clarity the curves have been offset in units of 0.3 G_0 with respect to the L_2 data. Whereas Fig. 3a reports on the generic behavior of $G_c(N)$ across the different series (by normalization of the data), this figure emphazises that we also obtain a very good agreement, on an absolute scale, between each of the experimental series as well as between experiment and theory.

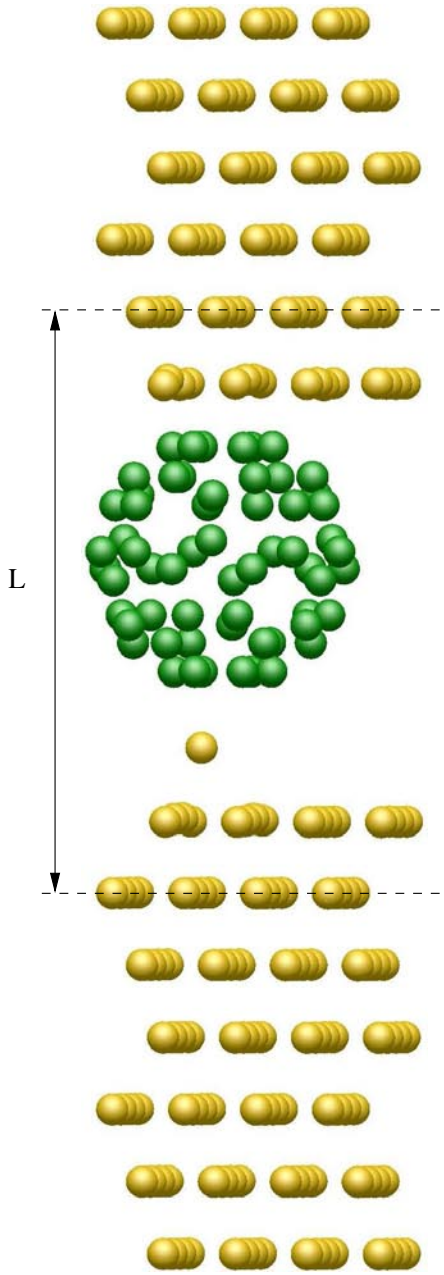

FIG. S2. Example of the supercell setup used in the electronic structure calculations. One C_{60} molecule is adsorbed with a hexagon on an hcp hollow-site on a 4×4 representation of a slab containing 13 Cu(111) layers. Cu_N clusters are positioned on the reverse side of the film. The electrode separation L is measured between the second-topmost layers of the electrodes.

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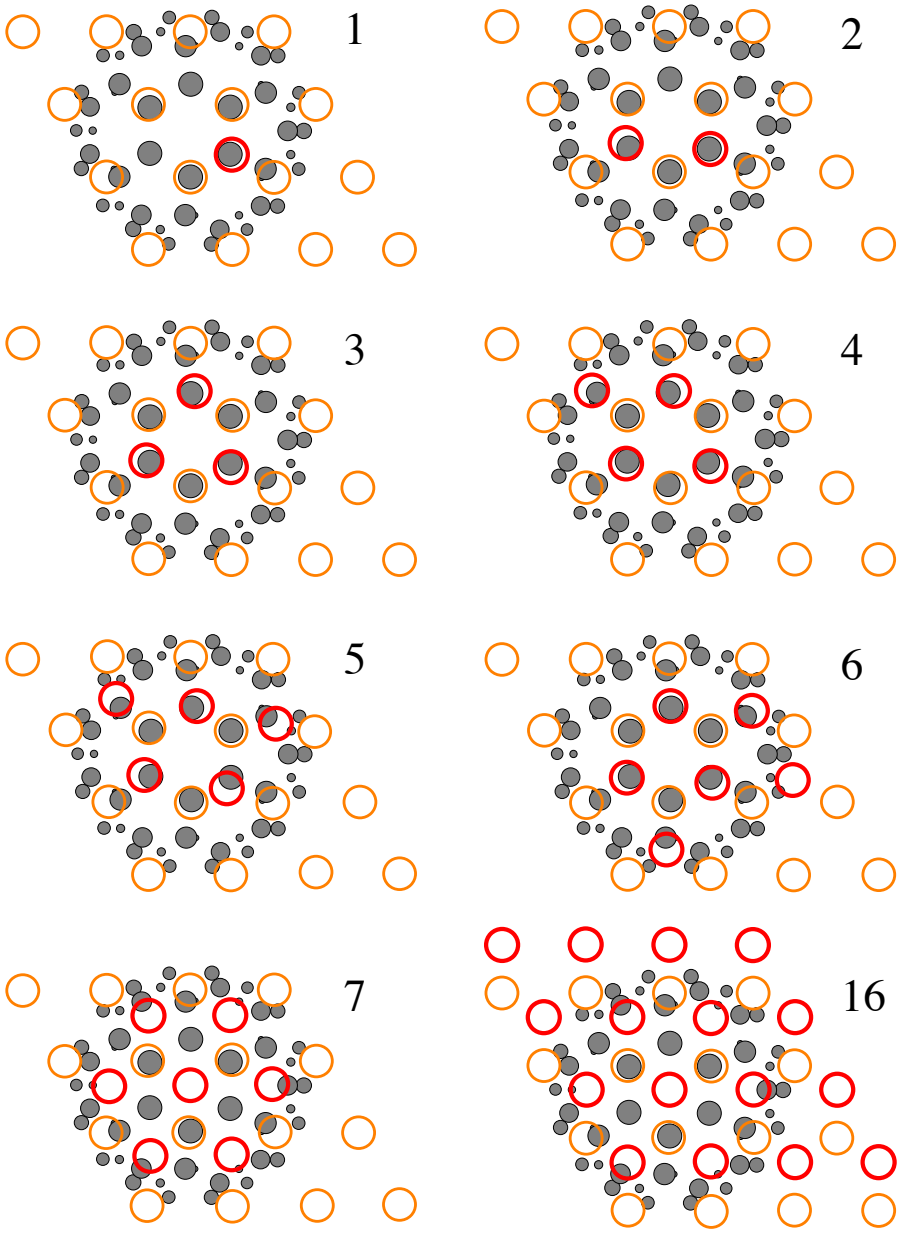

FIG. S3. Projection of the atomic positions of the contact, optimized at separation $L_1 = 17.2$ Å, onto a plane parallel to the Cu(111) substrate. Orange circles represent Cu atoms of the substrate, red circles the positions of the Cu atoms of the clusters, and gray disks the C atoms. Increasing gray disk diameters represent increasing distances of the C atoms from the Cu surface.

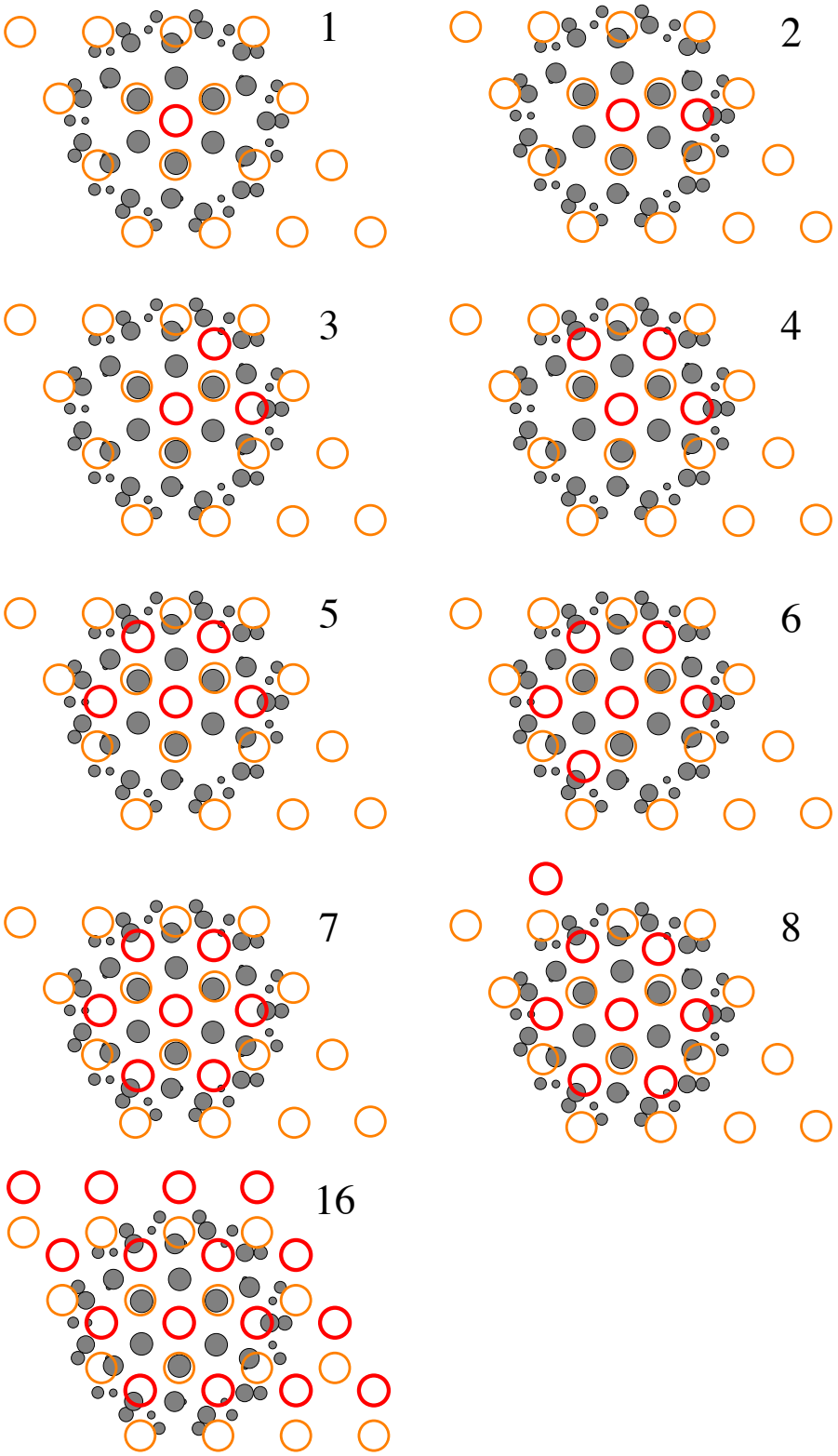

FIG. S4. Projection of the atomic positions of the contact, optimized at separation $L_2 = 18.0$ Å, onto a plane parallel to the Cu(111) substrate. Orange circles represent Cu atoms of the substrate, red circles the positions of the Cu atoms of the clusters, and gray disks the C atoms. Increasing gray disk diameters represent increasing distances of the C atoms from the Cu surface.

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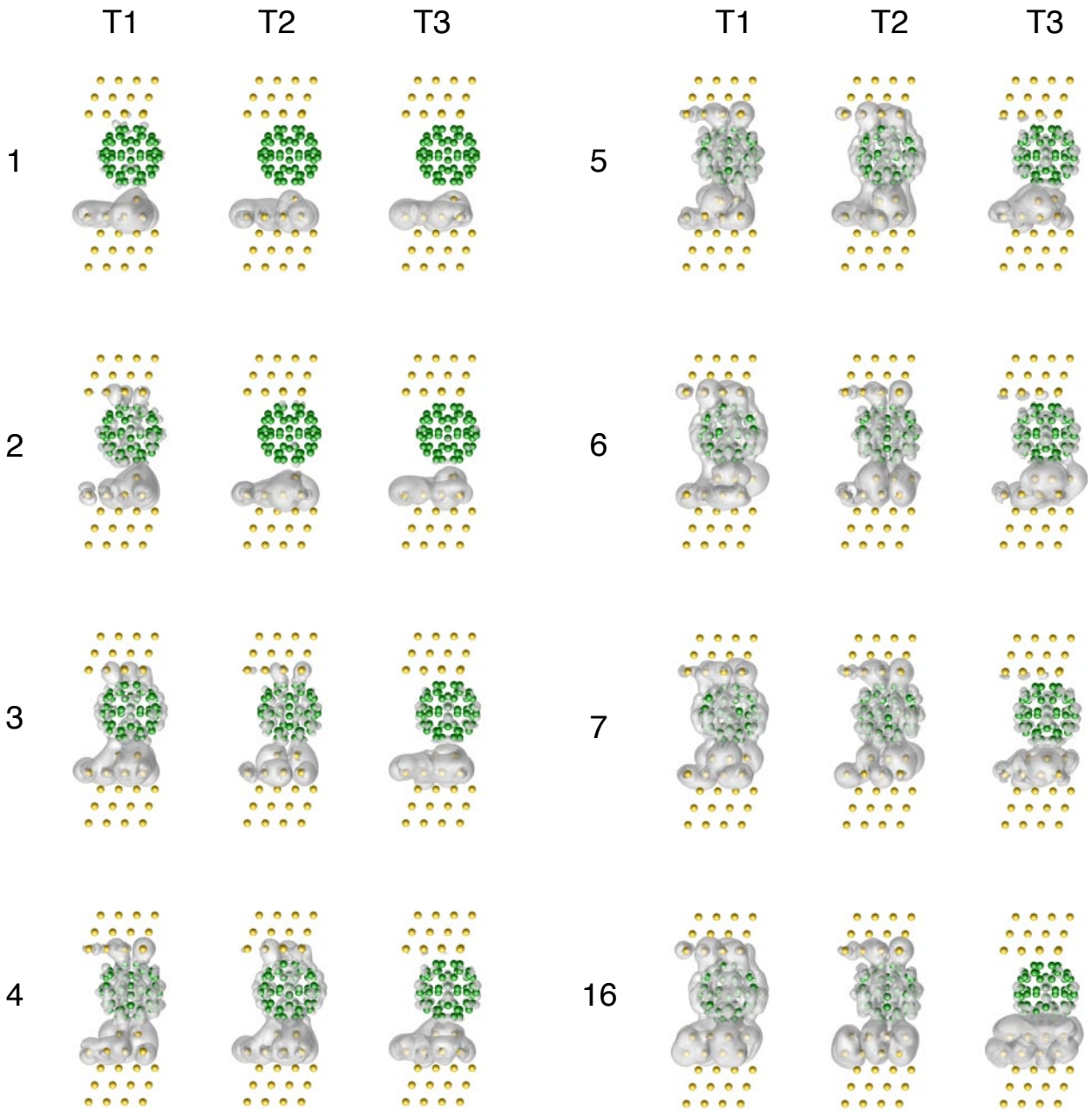

FIG. S5. Visualization of the eigenchannel scattering states at the Fermi energy for different number of contacting atoms. The calculated isosurfaces represent the electron density in the junction at the center of the Brillouin zone for electron waves incoming from below. The data was calculated for clusters with $N = 1 \ldots 7, 16$ adatoms at an electrode separation $L_1 = 17.2$ Å (measured between the second-topmost layers). The first, second, and third column show the electron density from the three most transmitting eigenchannels T_1, T_2, T_3, respectively. The scattering states are only calculated in the region of space defined by the topmost Cu surface layers.