Supporting Information for:

High-Conductance Conformers in Histograms of Single-Molecule Current-Voltage Characteristics

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NEGF-EH methodology

The electron current flowing through the molecule in contact with the electrodes is computed by integrating the transmission function, according to the Landauer-Büttiker formula:[1,2]

$$\begin{aligned} I &= \frac{2e}{h}\int_{-\infty}^{\infty} T(E)[f_0(E-\mu_L) - f_0(E-\mu_R)]dE, \\ &\approx \frac{2e}{h}\int_{\mu_L}^{\mu_R} T(E)dE, \end{aligned} \tag{1}$$

where e is the electron charge, h is Planck's constant, E is the energy of the channel, and $f_0(E-\mu_{L/R})$ is the room-temperature Fermi-Dirac distribution with $\mu_{L/R}$ being the Fermi energies of the left and right leads, respectively. The transmission function $T(E)$ is defined by the Fisher-Lee formula,[3] $T(E) = Tr[\mathscr{G}_m(E)\Gamma_L(E)\mathscr{G}_m^{\dagger}(E)\Gamma_R(E)]$. Here, $\Gamma_{L/R}(E) = i[\Sigma_{L/R}(E) - \Sigma_{L/R}^{\dagger}(E)]$, with self-energies $\Sigma_L(E) = V_L^{\dagger}\mathscr{G}_L(E)V_L$ and $\Sigma_R(E) = V_R\mathscr{G}_R(E)V_R^{\dagger}$ defined in terms of the Green's functions of the isolated leads, $\mathscr{G}_{L/R}(E) = [(E+i\eta)S_{L/R} - H_{L/R}]^{-1}$. Here, $H_{L/R}$ and $S_{L/R}$ are the Hamiltonians and overlap matrices of the left and right leads, η is a small positive constant, and $V_{L/R}$ defines the molecule-lead coupling interactions. The Green's function of the molecule in contact with the leads, $\mathscr{G}_m(E) = [(E+i\eta)S_m - H_m - \Sigma_L(E) - \Sigma_R(E)]^{-1}$, is defined in terms of the molecular Hamiltonian H_m and overlap matrices S_m, gained from the EH models in the Slater basis set of atomic orbitals.[4]

For computational efficiency, we model the leads as single pseudo-atoms, with self-energies $\Sigma_{L/R}(E) = \gamma^2\mathscr{G}_{L/R}(E)$ and constant diagonal Green's functions $\mathscr{G}_{L/R}(E) = -i/|\beta|$, as recently proposed to mimic semi-infinite one-dimensional nanowires as described by a nearest-neighbor TB Hamiltonian with an intersite coupling constant β.[5] The value of $|\Sigma_{L/R}| = \gamma^2/|\beta|$ is scaled to ensure that the conductance of a reference device at 0 V bias is equal to the unit of quantum conductance (*i.e.*, $G_0 = 2e^2/h = 7.75\times10^{-5}\Omega^{-1}$) when connected to the model leads.[6,7] The reference device consists of a linear chain of gold atoms (Figure S1a) for which $|\Sigma_{L/R}|$ is predicted to be 2.0 eV in order to reach 1.0 G_0 at the EH level (see Figure S2). The system and leads Fermi levels where aligned by shifting the Hamiltonian as $H = H_0 - S_m I E_F$, where I is the identity matrix and E_F is

the Fermi level of the system. Once $|\Sigma_{L/R}|$ is known for a particular metal, the same value can be used to compute the electron transport properties of any molecule in between the pseudo atom contacts (Figure S1 b).

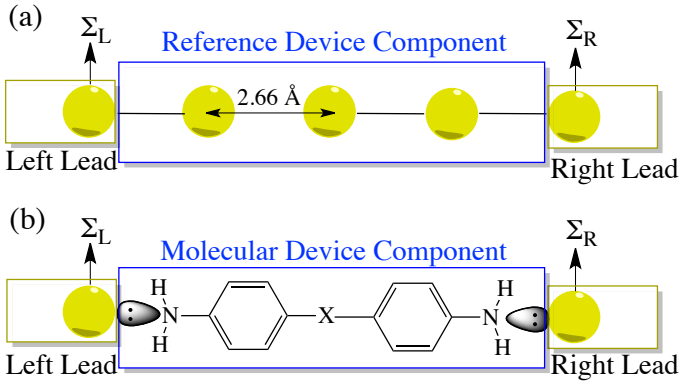


Figure S1: (a) Reference device composed of a linear chain of gold atoms with a Au-Au distance of 2.66 Å.[5] (b) Aniline-linked molecular junction, where X is CH=CH for 4,4'-diaminostilbene.

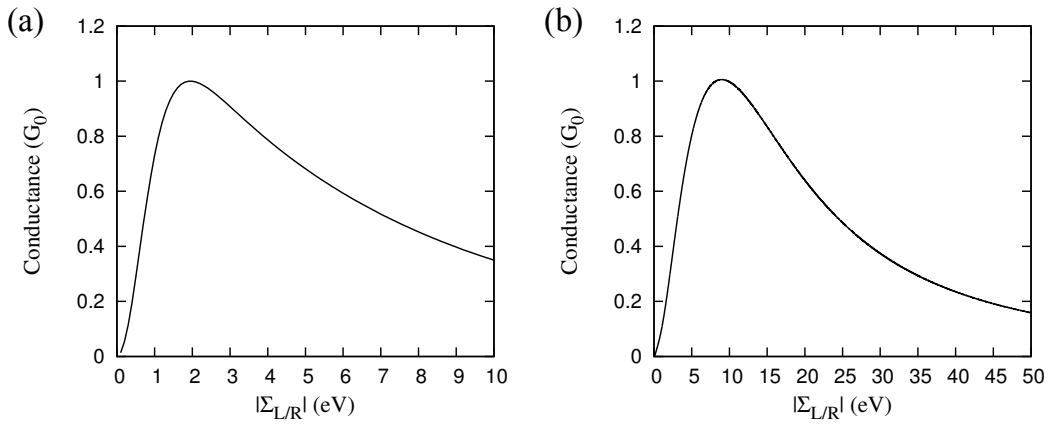


Figure S2: Comparison of molecular conductance at the Fermi level for the benchmark structure of a 5-atom gold chain, as described by EH (a) and DFT (b) Hamiltonians. The value of $|\Sigma_{L/R}|$ which provides 1.0 G_0 at Fermi level is assigned to be $|\Sigma_{L/R}|_{max} = 2.0$ eV and 9.0 eV for EH and DFT, respectively.

We have performed a systematic analysis to test the ability of the NEGF-EH methodology to reproduce experimental results. Our results show that not only trends but also absolute values of conductance are reproduced remarkably well. First, we analyzed linear alkanes with increasing

molecular length, as obtained by adding methylene groups. For molecules where electron transport is governed by superexchange, the molecular conductance (G) has the following expression: $G = A_0 \exp(-\beta N)$, where N is the length of the molecular junction (often reported in number of monomeric units for oligomers) and A_0 is a factor which depends on the contact characteristics.[8–10] One of the most studied and at the same time simplest systems is alkane dithiol spanning two gold nanotips.[11] Even with the difficulty of determining A_0, the conductance decay rate with respect to the elongation of the chain in polymeric systems (adding a CH_2 unit in the case of dithiols) can be accurately determined; for the case of dithiols $\beta \approx 0.94$ per CH_2 unit.[11] Figure S3 shows the ability of the present Σ-fitted EH-NEGF methodology to accurately reproduce experimental values[11] for such systems.

Similarly to previously reported NEGF-DFT calculations for gold nanoclusters leads,[11] our DFT based conductance values based on single pseudo-atoms Au leads overestimate the conductance due to the underestimated HOMO-LUMO gap. This can be seen from the difference between the offset of y-intercept of the linear fit of DFT data (10.6) and that of experimental data (8.8). Moreover, the value of $\beta = 0.97$ per CH_2 using the NEGF-EH conductance is much closer to the reported experimental value of 0.94 per CH_2 than that of the NEGF-DFT method (0.85).[11] Thus, our Σ-fitted NEGF-EH approach can accurately predict the effect of junction length on molecular conductance and was therefore chosen for the calculations shown in the manuscript.

Besides length dependence, molecular conductance also depends on internal dihedral angles in conjugated systems. We perform calculations on one set of molecules with terminal primary amines (**N#**: Table S1). These molecules have a range of internal dihedral angles (ϕ) between the two rings. Previous work showed that for these molecules, conductance increases linearly with $cos^2\phi$,[12] and our EH calculated conductance values show the same dependence on ϕ as reported for the experimental data (Figure S4). In general, our method successfully reproduces the overall trend; however, for molecules with large dihedral angles, the conductance is underestimated. The discrepancy may arise from the DFT structures overestimating the twist angle or the EH method underestimating the coupling between the rings when the dihedral angle is close to 90°. Overall,

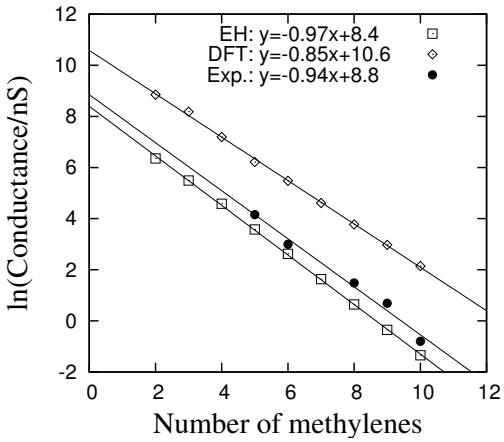


Figure S3: Logarithm of conductance at the Fermi level for a series of linear alkane dithiols of increasing lengths. Calculated values using EH (open squares) and DFT (open diamonds) are compared to experimental values[11] (solid circles). Lines are linear fits with slopes $\beta = 0.97$, 0.85, and 0.94 for EH, DFT, and experimental data, respectively.

our results indicate that the NEGF-EH method provide very satisfactory predictions even when compared to DFT calculations.[12]

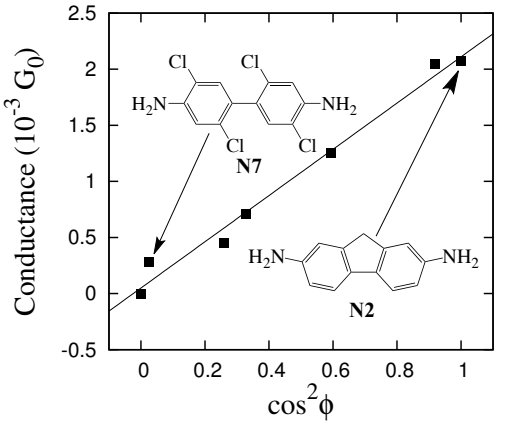
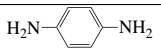
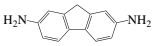
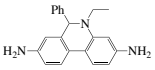
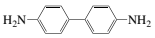
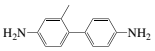
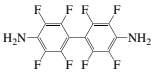
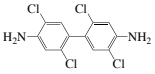
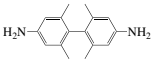


Figure S4: EH conductance of molecules in Table S1 with two phenyl rings. The internal dihedral angle, ϕ, is determined by DFT optimized structures. Line indicates a linear fit for the data set.

Table S1: Conductance values for amine terminated molecules.

	Molecule	Conductance (G_0)		
		Measured[12]	**Ref. Calculated**[12]	**Calculated**
N1		6.40×10^{-3}	6.4×10^{-3}	8.30×10^{-3}
N2		1.54×10^{-3}	2.1×10^{-3}	2.07×10^{-3}
N3		1.37×10^{-3}	2.2×10^{-3}	2.04×10^{-3}
N4		1.16×10^{-3}	1.6×10^{-3}	1.25×10^{-3}
N5		6.50×10^{-4}	1.2×10^{-3}	7.10×10^{-4}
N6		4.90×10^{-4}	7.1×10^{-4}	4.52×10^{-4}
N7		3.70×10^{-4}	5.8×10^{-4}	2.80×10^{-4}
N8		1.80×10^{-4}	3.5×10^{-4}	2.25×10^{-4}
N9		7.60×10^{-5}	6.4×10^{-5}	3.02×10^{-7}

Optimized Molecular Structures

Table S2: DFT optimized structure of anti conformer 4,4'-diaminostilbene binding to one gold atom on each side.

C	-0.455555	0.397517	0.302984
C	-1.863863	0.563836	-0.059938
C	-2.655220	1.473064	0.670585
C	-2.494487	-0.136457	-1.110506
C	-3.833871	0.067322	-1.417152
C	1.863785	-0.563335	0.060140
C	2.655168	-1.472383	-0.670593
C	3.997848	-1.684826	-0.371749
C	4.598696	-0.989684	0.685350
C	3.833767	-0.067127	1.417505
C	2.494387	0.136724	1.110871
H	4.582251	-2.385426	-0.962581
H	4.295528	0.496331	2.224388
H	1.933193	0.854689	1.700254
C	0.455481	-0.396982	-0.302754
C	-3.997909	1.685452	0.371711
C	-4.598784	0.990054	-0.685196
H	-4.295667	-0.496364	-2.223859
H	-1.933319	-0.854567	-1.699738
H	-4.582291	2.386215	0.962378
H	-2.204543	2.026951	1.490164
H	2.204511	-2.026063	-1.490323
N	-5.974640	1.165856	-0.972452
N	5.974537	-1.165600	0.972600
H	-0.142704	0.995690	1.157316
H	0.142620	-0.995113	-1.157110
Au	-7.639415	-0.294594	0.183037
Au	7.639476	0.294294	-0.183162
H	-6.227754	0.958779	-1.932628
H	-6.341782	2.071076	-0.699454
H	6.341593	-2.070884	0.699704
H	6.227680	-0.958442	1.932750

Table S3: DFT optimized structure of syn conformer 4,4'-diaminostilbene binding to one gold atom on each side.

C	0.472276	1.579597	-0.483780
C	1.924519	1.551248	-0.301898
C	2.756659	1.564133	-1.439352
C	2.559072	1.484604	0.956972
C	3.942140	1.424086	1.070196
C	-1.924519	1.551247	0.301898
C	-2.756659	1.564132	1.439352
C	-4.143579	1.504281	1.337633
C	-4.751150	1.433594	0.077679
C	-3.942140	1.424086	-1.070196
C	-2.559071	1.484603	-0.956972
H	-4.754331	1.495049	2.236713
H	-4.401077	1.350402	-2.052919
H	-1.965468	1.466636	-1.865244
C	-0.472276	1.579596	0.483781
C	4.143579	1.504282	-1.337633
C	4.751150	1.433594	-0.077679
H	4.401077	1.350402	2.052919
H	1.965468	1.466637	1.865244
H	4.754331	1.495050	-2.236713
H	2.303333	1.613816	-2.426060
H	-2.303333	1.613815	2.426061
N	6.155751	1.288903	0.037547
N	-6.155750	1.288903	-0.037547
H	0.154698	1.584187	-1.525300
H	-0.154698	1.584183	1.525301
Au	7.030098	-1.051502	0.045436
Au	-7.030098	-1.051502	-0.045437
H	6.538967	1.618580	0.916789
H	6.680456	1.668421	-0.742999
H	-6.538967	1.618581	-0.916789
H	-6.680456	1.668422	0.742998

Table S4: DFT optimized structure of **N1** binding to one gold atom on each side.

C	-0.609578	-1.207552	0.337392
C	0.609458	-1.207945	-0.336182
C	1.227399	-0.000397	-0.686430
C	0.609578	1.207552	-0.337391
C	-0.609458	1.207946	0.336184
C	-1.227399	0.000398	0.686432
H	-1.084859	-2.152366	0.587121
H	1.084607	-2.153062	-0.584999
H	1.084858	2.152366	-0.587119
H	-1.084607	2.153063	0.585001
Au	-4.522330	-0.000062	-0.117702
N	-2.495832	0.000728	1.327522
H	-2.673582	0.831418	1.882393
N	2.495832	-0.000728	-1.327521
H	2.673460	0.829306	-1.883409
Au	4.522331	0.000062	0.117702
H	-2.673461	-0.829305	1.883410
H	2.673581	-0.831417	-1.882393

Table S5: DFT optimized structure of **N2** binding to one gold atom on each side.

C	-2.856269	1.719995	0.996876
C	-1.568488	2.015324	0.547865
C	-0.691543	0.969811	0.243764
C	-1.116443	-0.368959	0.394985
C	-2.396223	-0.666987	0.841537
C	-3.272425	0.387597	1.149498
H	-3.549032	2.526562	1.222670
H	-1.263312	3.052120	0.438813
H	-2.730600	-1.697266	0.939976
C	0.691520	0.969817	-0.243731
C	1.116429	-0.368951	-0.394955
C	1.568456	2.015337	-0.547833
C	2.396211	-0.666969	-0.841510
C	2.856238	1.720018	-0.996849
H	1.263272	3.052130	-0.438779
C	3.272403	0.387623	-1.149474
H	2.730596	-1.697245	-0.939950
H	3.548993	2.526589	-1.222647
C	-0.000005	-1.315586	0.000009
H	0.295452	-1.970512	0.830320
H	-0.295466	-1.970482	-0.830327
Au	-6.247346	-0.292325	-0.278895
Au	6.247361	-0.292329	0.278879
N	-4.606197	0.101039	1.545266
H	-4.709829	-0.772871	2.049815
N	4.606173	0.101075	-1.545251
H	4.709817	-0.772833	-2.049799
H	-5.057663	0.854091	2.053102
H	5.057641	0.854134	-2.053073

Table S6: DFT optimized structure of **N3** binding to one gold atom on each side.

C	3.193035	-1.234384	-1.197260	C	1.944050	2.677928	0.678865
C	2.480029	-0.032099	-1.140632	C	2.327666	4.514047	-1.390282
C	1.137670	-0.009380	-0.755152	H	0.936495	3.301973	-2.507668
C	0.476150	-1.209772	-0.432130	C	2.804988	3.761499	0.856712
C	1.216757	-2.406913	-0.465487	H	1.804668	1.956383	1.478547
C	2.553518	-2.428604	-0.843163	C	2.999801	4.684077	-0.178261
C	0.346359	1.298779	-0.748749	H	2.471894	5.223970	-2.199861
C	-0.936972	-1.160884	-0.039377	H	3.330818	3.882647	1.799531
C	-1.502153	0.089415	0.347664	H	3.672156	5.525783	-0.039511
C	-2.822161	0.102808	0.839579	N	-0.737598	1.257759	0.266707
H	-3.286099	1.026123	1.159291	N	-4.925853	-0.995693	1.372293
C	-3.581770	-1.068141	0.913403	H	-5.288046	-1.885597	1.698507
C	-3.051864	-2.284720	0.474158	N	4.576519	-1.225743	-1.515469
C	-1.740557	-2.307988	0.010546	H	4.919383	-2.099371	-1.900110
H	2.989225	0.895314	-1.382045	C	-1.426947	2.537943	0.508287
H	0.749555	-3.339735	-0.169008	H	-2.434652	2.508527	0.071377
H	3.105601	-3.364709	-0.839323	H	-0.888795	3.316495	-0.032572
H	-3.650596	-3.190569	0.488678	C	-1.485907	2.926750	1.990146
H	-1.332149	-3.253408	-0.330297	H	-0.479218	3.108274	2.377020
H	-0.112647	1.413560	-1.750362	H	-2.071760	3.844868	2.113635
Au	6.148181	-0.929765	0.386792	H	-1.942760	2.145291	2.603924
Au	-6.661917	-0.333806	-0.228249	H	-5.077102	-0.282525	2.078304
C	1.259528	2.501988	-0.533361	H	4.861246	-0.447483	-2.100356
C	1.461514	3.427989	-1.563381				

Table S7: DFT optimized structure of **N4** binding to one gold atom on each side.

C	2.853599	1.715209	-0.398846
C	1.519963	1.697039	0.003912
C	0.706336	0.568161	-0.200289
C	1.289467	-0.547489	-0.828896
C	2.621689	-0.540690	-1.233405
C	3.415186	0.595728	-1.026643
H	3.464707	2.593962	-0.208682
H	1.112770	2.567481	0.509795
H	0.685748	-1.428646	-1.024568
H	3.047605	-1.419276	-1.711074
C	-0.711895	0.549646	0.234345
C	-1.283741	-0.603299	0.803011
C	-1.536642	1.679737	0.089870
C	-2.615907	-0.630741	1.207333
H	-0.671248	-1.487436	0.952494
C	-2.870077	1.663750	0.493085
H	-1.138225	2.579381	-0.369797
C	-3.420135	0.507262	1.061097
H	-3.032665	-1.537247	1.638775
H	-3.490063	2.544877	0.348473
Au	6.406568	-0.354289	0.243137
Au	-6.403318	-0.334094	-0.264625
N	4.786147	0.585786	-1.392053
H	5.182927	1.508215	-1.536149
N	-4.791629	0.465820	1.426113
H	-4.996611	-0.187691	2.174610
H	-5.187682	1.375022	1.640591
H	4.997383	-0.013515	-2.182778

Table S8: DFT optimized structure of **N5** binding to one gold atom on each side.

C	-2.516962	-0.883874	1.262470
C	-1.196311	-0.714401	0.856626
C	-0.711532	0.516165	0.378914
C	-1.607924	1.611028	0.305480
C	-2.933794	1.430001	0.715857
C	-3.397248	0.201027	1.198080
H	-2.859503	-1.850794	1.621615
H	-0.512616	-1.555652	0.925304
H	-3.631532	2.259739	0.626215
C	0.710396	0.601834	-0.058033
C	1.591645	1.574404	0.445896
C	1.229570	-0.330797	-0.973801
C	2.926125	1.623964	0.048798
H	1.236009	2.292354	1.178157
C	2.562579	-0.291183	-1.379001
C	3.420550	0.695673	-0.877355
H	3.590109	2.373801	0.471219
H	2.935734	-1.026257	-2.087728
Au	-6.330244	-0.435140	-0.328342
Au	6.438211	-0.486114	0.163963
C	-1.201482	2.964127	-0.239034
H	-0.714108	3.582057	0.524694
H	-0.500541	2.870439	-1.073075
H	-2.079214	3.514562	-0.589713
H	0.573401	-1.090055	-1.389634
N	-4.766320	0.043425	1.540899
H	-5.200964	0.883652	1.906810
N	4.787952	0.721203	-1.256790
H	5.205426	1.645375	-1.228287
H	4.973483	0.282532	-2.152575
H	-4.950133	-0.742878	2.154807

Table S9: DFT optimized structure of **N6** binding to one gold atom on each side.

C	-2.574535	-0.443122	1.397867
C	-1.243592	-0.439987	1.004597
C	-0.709796	0.584088	0.211159
C	-1.588799	1.611612	-0.156060
C	-2.918458	1.615001	0.241055
C	-3.446808	0.586631	1.028977
C	0.709681	0.583966	-0.210912
C	1.588724	1.611609	0.155762
C	1.243404	-0.440526	-1.003917
C	2.918403	1.614809	-0.241390
C	2.574300	-0.443826	-1.397240
C	3.446650	0.586082	-1.028867
Au	-6.375820	-0.603193	-0.337198
Au	6.375961	-0.602980	0.337030
N	-4.801139	0.550109	1.366063
H	-5.255257	1.456282	1.387472
N	4.800952	0.549181	-1.366054
H	5.016327	-0.017663	-2.178500
F	-3.734674	2.626255	-0.126567
F	-1.150986	2.621173	-0.927301
F	-0.453235	-1.443336	1.420034
F	-3.050576	-1.439074	2.176215
F	0.453001	-1.444046	-1.418808
F	3.050342	-1.440126	-2.175186
F	3.734624	2.626172	0.125832
F	1.151002	2.621550	0.926580
H	-5.016751	-0.016356	2.178707
H	5.255304	1.455223	-1.387882

Table S10: DFT optimized structure of **N7** binding to one gold atom on each side.

C	2.628821	0.030711	-1.459005
C	1.278889	-0.057517	-1.129912
C	0.730137	0.665232	-0.056222
C	1.601991	1.490937	0.668888
C	2.949509	1.589354	0.344194
C	3.490401	0.859044	-0.728075
C	-0.702267	0.566464	0.343090
C	-1.618912	1.620624	0.186741
C	-1.183544	-0.615488	0.925653
C	-2.947548	1.503163	0.584919
C	-2.508649	-0.742396	1.325307
C	-3.417935	0.317057	1.163956
Au	6.294373	-0.908573	0.056238
Au	-6.346642	-0.329717	-0.430231
N	4.862734	0.895313	-1.026740
H	5.344202	1.723056	-0.690656
N	-4.776826	0.184072	1.497863
H	-4.979959	-0.584153	2.128950
H	1.216661	2.069662	1.500945
H	3.018305	-0.555128	-2.284947
H	-3.632510	2.327931	0.419016
H	-0.506491	-1.450054	1.070693
Cl	3.986291	2.653247	1.279703
Cl	0.267743	-1.093371	-2.120721
Cl	-1.125378	3.132575	-0.556085
Cl	-3.046426	-2.243400	2.060869
H	-5.223339	1.042947	1.797335
H	5.087814	0.697998	-1.994968

Table S11: DFT optimized structure of **N8** binding to one gold atom on each side.

C	4.890678	0.558568	-1.574591
C	3.532561	0.282188	-1.436826
C	2.833168	0.601385	-0.258669
C	3.557473	1.215635	0.779445
C	4.915400	1.497168	0.652167
C	5.593772	1.174016	-0.530611
H	5.405764	0.297184	-2.495488
H	3.002155	-0.169859	-2.269534
H	3.058071	1.452288	1.714165
H	5.455483	1.947784	1.480919
C	1.388622	0.297010	-0.113748
C	0.520869	1.175667	0.559567
C	0.834658	-0.882676	-0.642984
C	-0.835900	0.889545	0.695590
H	0.904652	2.113748	0.950374
C	-0.521978	-1.169052	-0.506427
H	1.479863	-1.604019	-1.136182
C	-1.390058	-0.289986	0.166078
H	-1.480984	1.611322	1.188259
H	-0.905409	-2.107361	-0.896967
Au	8.511428	-0.381931	0.161950
N	6.989421	1.405449	-0.642587
H	7.325579	2.180976	-0.081806
C	-2.835143	-0.593052	0.308358
C	-3.555549	-1.215609	-0.727699
C	-3.539618	-0.263673	1.480628
C	-4.914107	-1.494967	-0.604242
H	-3.052563	-1.460063	-1.658445
C	-4.898749	-0.537536	1.614465
H	-3.012755	0.194396	2.312279
C	-5.597829	-1.160841	0.572508
H	-5.451050	-1.951341	-1.431844
H	-5.417338	-0.268742	2.531285
N	-6.994139	-1.389646	0.678337
H	-7.331725	-1.454325	1.632728
Au	-8.508992	0.372904	-0.202770
H	-7.325915	-2.179307	0.135035
H	7.317153	1.497088	-1.598292

Table S12: DFT optimized structure of **N9** binding to one gold atom on each side.

C	-2.984736	1.807472	0.199712
C	-1.622050	1.829915	0.516874
C	-0.731035	0.975848	-0.169518
C	-1.224932	0.110224	-1.171904
C	-2.591258	0.108154	-1.470688
C	-3.473799	0.953268	-0.792101
H	-3.671568	2.454903	0.740145
H	-2.974155	-0.571770	-2.228058
C	0.731141	0.975798	0.169449
C	1.622315	1.829315	-0.517456
C	1.224883	0.110684	1.172327
C	2.984979	1.806855	-0.200255
C	2.591213	0.108592	1.471150
C	3.473883	0.953196	0.792120
H	3.671948	2.453790	-0.741105
H	2.973979	-0.570947	2.228934
Au	-6.201766	-0.794387	0.168380
Au	6.201693	-0.794395	-0.168383
C	-0.299190	-0.821379	-1.922887
H	0.473614	-0.270166	-2.470126
H	0.227562	-1.499877	-1.243194
H	-0.854153	-1.428956	-2.642909
C	0.298926	-0.820013	1.924179
H	-0.470703	-0.267746	2.474893
H	-0.231734	-1.495706	1.244799
H	0.854404	-1.430386	2.641435
C	-1.127542	2.769971	1.594511
H	-0.638633	2.226300	2.410398
H	-0.387333	3.477904	1.204802
H	-1.953656	3.345733	2.020712
C	1.127970	2.768706	-1.595742
H	0.639451	2.224502	-2.411514
H	0.387459	3.476667	-1.206661
H	1.954104	3.344417	-2.021970
N	-4.867300	0.894742	-1.065076
H	-5.087052	0.618279	-2.016132
N	4.867377	0.894698	1.065161
H	5.087068	0.618041	2.016175
H	-5.370370	1.741514	-0.821970
H	5.370384	1.741583	0.822314

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