Supporting Information

Quantum Interference Enhances Rectification Behavior of Molecular Devices

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Scheme of Extended Molecule

Figure S1 shows the setup used for the transport calculations in TranSIESTA. The Au (111) electrodes consist of two sub-layers (with three and seven Au atoms) repeated using periodic boundary conditions along the transport direction (Z axis). Each lead terminates in a seven atom face. The molecular structures from DFT geometry optimizations were connected to the electrodes by removing the hydrogen atoms of the thiol groups and fixing the Au–S bond distance to 2.32 Å.

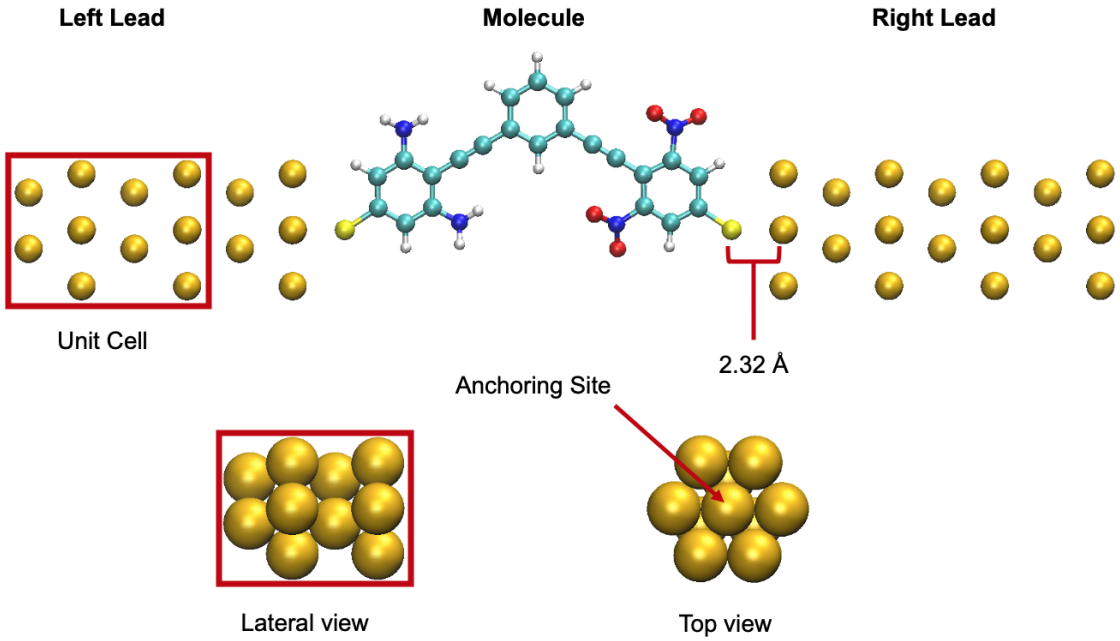

Figure S1: Schematic of the lead–molecule–lead system exemplified for structure **BenzDA**. The repeatable units of the leads are indicated by boxes.

Molecular Orbitals of Six-Membered Ring Structures

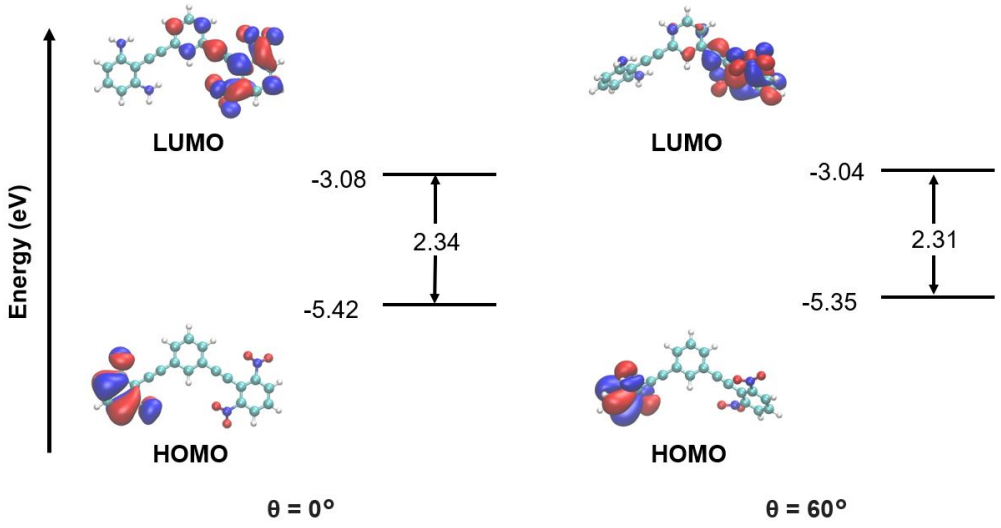

Figure S2: HOMO and LUMO isosurfaces and energies of meta-benzene core at 0 and 60° torsion angles between subsequent aromatic rings.

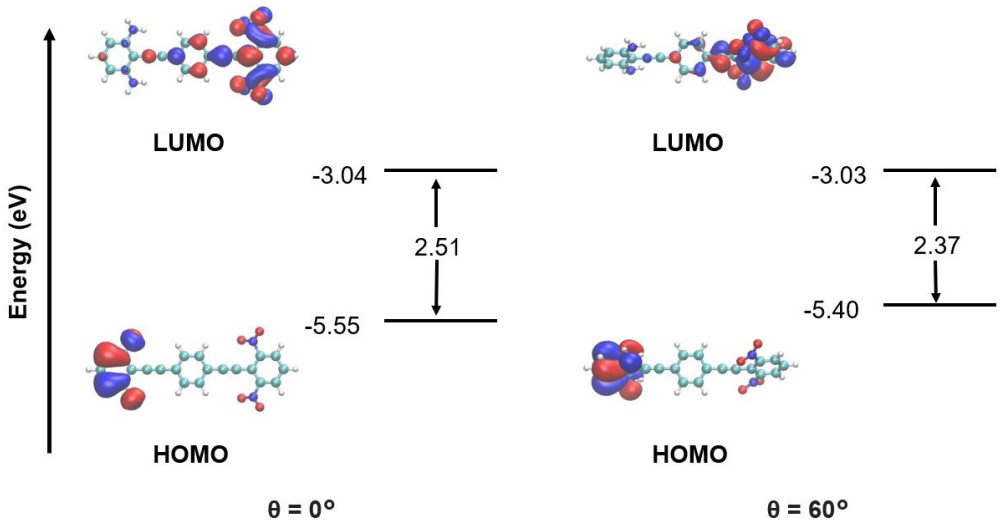

Figure S3: HOMO and LUMO isosurfaces and energies of para-benzene core at 0 and 60° torsion angles between subsequent aromatic rings.

Transmission coefficients within the WBL approximation

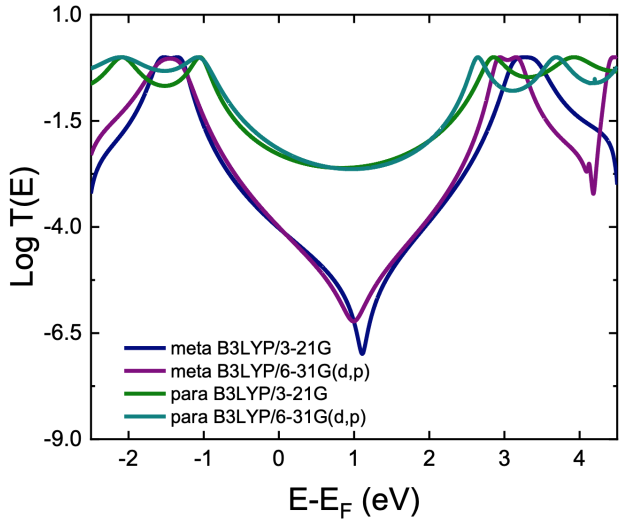

Figure S4: Transmission coefficients T(E) of structures with the benzene core with no substituent groups. Insets show the meta- and para- substitution

Transmission coefficients from TranSIESTA calculation

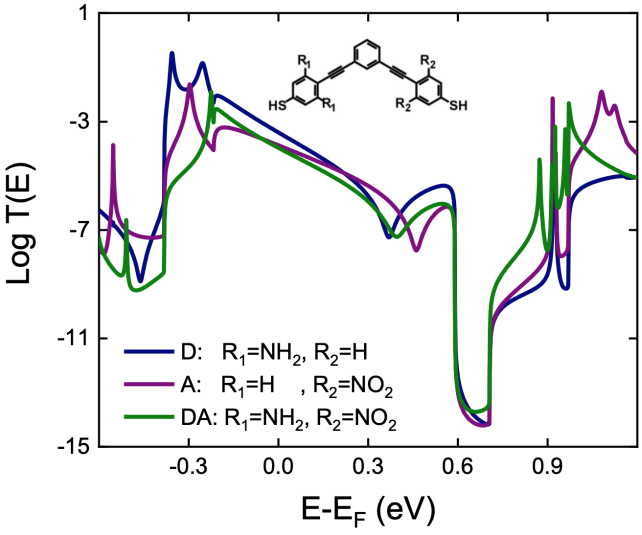

Figure S5: Transmission coefficients T(E) at zero bias of structures with the benzene core when donor, acceptor and both groups are present calculated in TranSIESTA.

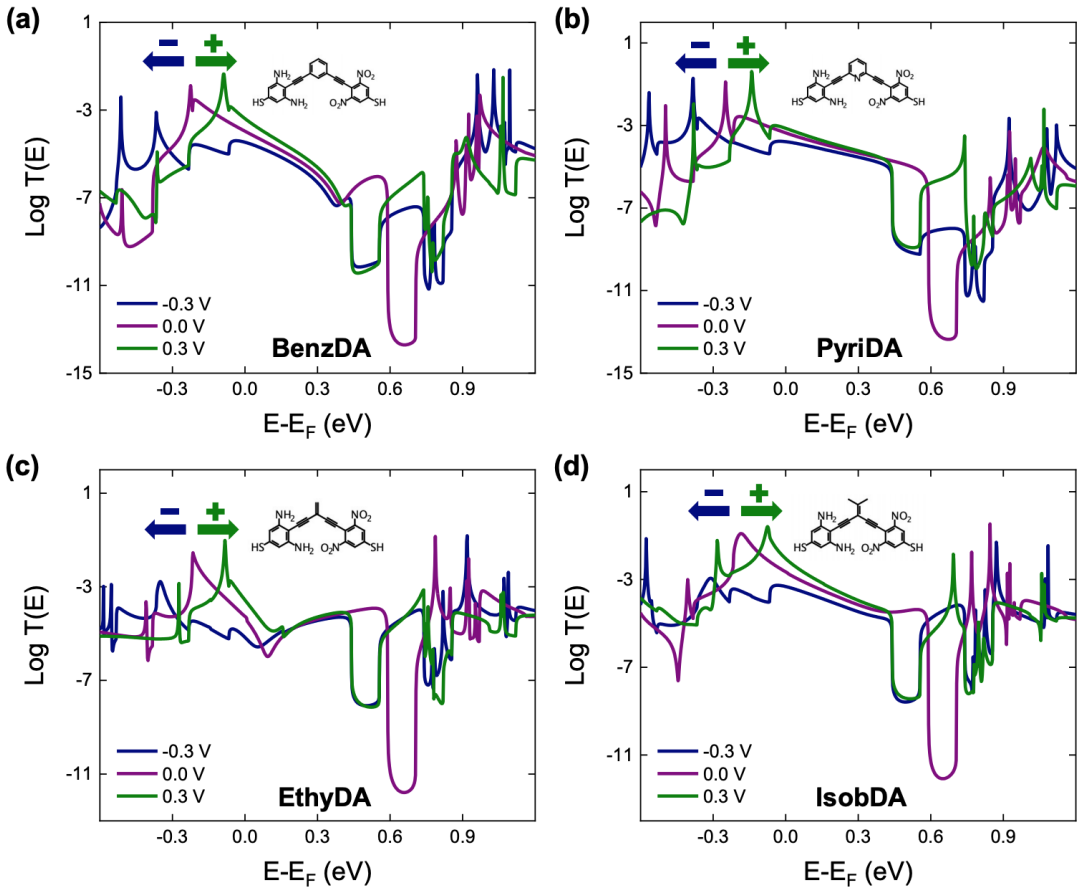

Figure S6: Transmission coefficients T(E) of (a) **BenzDA**, (b) **PyriDA**, (c) **EthyDA** and (d) **IsobDA** at different bias.

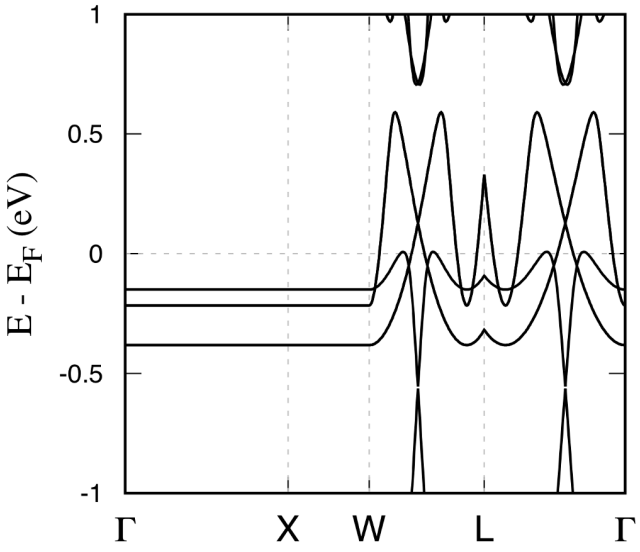

Figure S7: Band structure of gold electrodes calculated in TranSIESTA.

Additional I-V Curves

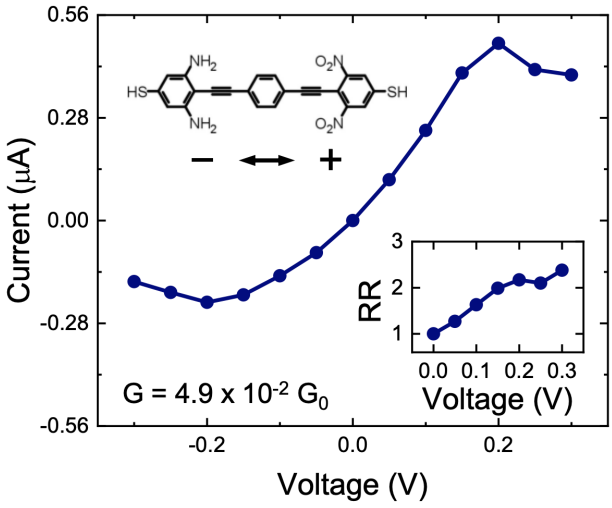

Figure S8: I-V curve and RRs of parabenzene.

Transport Calculations with DZ Basis Set

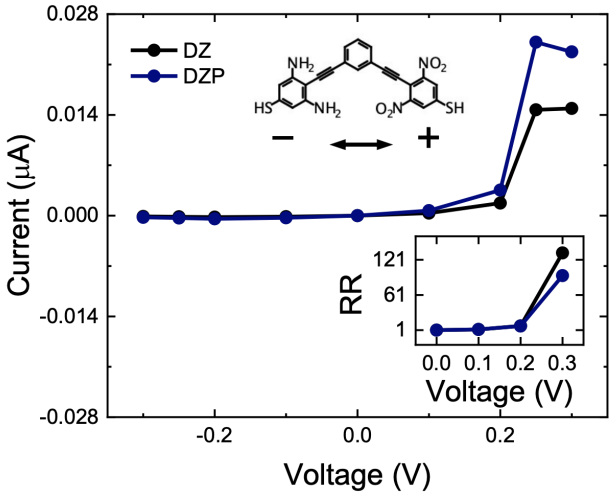

Figure S9: Comparison of transport calculations with DZ and DZP basis sets for **BenzDA**.

Table S1: Calculated Values of Conductance (G) and RRs for selected D-B-A systems with the DZ basis set.

System	**G(G0)**	**RR(0.2 V)**	**RR(0.3V)**
2,5-ThioDA	3.2×10^{-2}	2.08	5.17
2,4-ThioDA	1.8×10^{-3}	7.22	55.21
BenzDA	5.4×10^{-5}	8.35	132.63
PyriDA	1.7×10^{-4}	4.23	113.93
EthyDA	4.1×10^{-5}	19.05	378.40
IsobDA	1.4×10^{-3}	23.97	107.53

Coordinates of Extended Molecules

Table S2: Coordinates of **2,5-ThioD**.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000
Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800
Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200
Au	0.000000	0.000000	-7.031200
Au	-2.498500	1.442500	-7.031200
Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600
Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600

Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000
S	0.000000	0.000000	0.000000
H	2.607660	0.510900	1.299490
C	0.545440	-0.018870	1.698940
C	1.865330	0.274560	2.055640
H	-1.431500	-0.568620	2.380710
C	-0.414050	-0.322560	2.669270
H	4.125450	1.011470	3.105000
C	2.241950	0.261050	3.405260
N	3.555970	0.504930	3.766600
C	-0.058280	-0.336310	4.024340
C	1.280390	-0.040460	4.410560
H	3.723270	0.748740	4.732990
H	-1.963230	-0.597370	4.742210
N	-0.988080	-0.682050	4.986110
C	1.647660	-0.032040	5.776600
H	-0.769060	-0.459530	5.946530
C	1.975170	-0.015040	6.955970
H	4.505320	0.001570	8.266260
C	2.336030	-0.002920	8.313520
C	3.606960	0.010250	8.871630

S	1.111730	0.005710	9.574800
C	3.604650	0.025670	10.284020
C	2.334150	0.021370	10.840110
H	4.500400	0.033580	10.893360
C	1.972560	0.022450	12.196730
C	1.645340	0.023490	13.372550
H	-0.848270	-0.115440	14.365880
C	1.274810	0.021580	14.744980
C	-0.080570	-0.056970	15.130490
H	3.300120	0.157970	15.484210
C	2.252130	0.096680	15.759250
C	-0.441390	-0.060460	16.472980
H	-1.491530	-0.120650	16.743740
C	1.890490	0.091700	17.102600
C	0.539820	0.013830	17.474770
H	2.666150	0.149030	17.860670
S	0.000000	0.000000	19.174100
Au	0.000000	-2.885000	21.494100
Au	-2.498500	-1.442500	21.494100
Au	2.498500	-1.442500	21.494100
Au	0.000000	0.000000	21.494100
Au	-2.498500	1.442500	21.494100
Au	2.498500	1.442500	21.494100
Au	0.000000	2.885000	21.494100
Au	-0.832800	-1.442500	23.849700
Au	1.665600	0.000000	23.849700
Au	-0.832800	1.442500	23.849700

Au	0.000000	-2.885000	26.205300
Au	-2.498500	-1.442500	26.205300
Au	2.498500	-1.442500	26.205300
Au	0.000000	0.000000	26.205300
Au	-2.498500	1.442500	26.205300
Au	2.498500	1.442500	26.205300
Au	0.000000	2.885000	26.205300
Au	-0.832800	-1.442500	28.560900
Au	1.665600	0.000000	28.560900
Au	-0.832800	1.442500	28.560900
Au	0.000000	-2.885000	30.916500
Au	-2.498500	-1.442500	30.916500
Au	2.498500	-1.442500	30.916500
Au	0.000000	0.000000	30.916500
Au	-2.498500	1.442500	30.916500
Au	2.498500	1.442500	30.916500
Au	0.000000	2.885000	30.916500
Au	-0.832800	-1.442500	33.272100
Au	1.665600	0.000000	33.272100
Au	-0.832800	1.442500	33.272100
Au	0.000000	-2.885000	35.627700
Au	-2.498500	-1.442500	35.627700
Au	2.498500	-1.442500	35.627700
Au	0.000000	0.000000	35.627700
Au	-2.498500	1.442500	35.627700
Au	2.498500	1.442500	35.627700
Au	0.000000	2.885000	35.627700

Table S3: Coordinates of **2,5-ThioA** connected to Au electrodes.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000
Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800
Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200
Au	0.000000	0.000000	-7.031200
Au	-2.498500	1.442500	-7.031200
Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600
Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600

Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000
S	0.000000	0.000000	0.000000
H	2.656250	-0.034280	1.338600
C	0.521850	0.010950	1.702820
C	1.871330	-0.010410	2.088690
H	-1.521770	0.058710	2.411490
C	-0.473250	0.041550	2.693980
C	2.218480	-0.001000	3.435280
H	3.264950	-0.017320	3.722030
C	-0.127270	0.050530	4.039730
C	1.226710	0.029440	4.437790
H	-0.904350	0.074280	4.796610
C	1.580950	0.038910	5.813570
C	1.889170	0.047420	6.994370
H	4.401060	-0.009620	8.317910
C	2.229890	0.057680	8.355680
C	3.502050	0.027500	8.920700
S	0.993600	0.116600	9.595360
C	3.488800	0.049470	10.327220
C	2.206970	0.097690	10.867510
H	4.374410	0.033500	10.950990

C	1.851310	0.135200	12.216110
O	-1.095570	0.775560	13.195190
C	1.536600	0.181440	13.394750
N	-1.279480	0.242380	14.286010
O	3.983100	0.699250	14.471320
O	-2.352200	-0.235590	14.664310
C	1.197010	0.197210	14.759870
C	-0.147230	0.183510	15.230620
N	3.608300	0.134700	15.495340
C	2.165430	0.131510	15.800960
O	4.355570	-0.417490	16.308290
C	-0.489170	0.109510	16.573930
H	-1.541280	0.092880	16.833070
C	1.840750	0.056560	17.150120
C	0.504230	0.058920	17.557980
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S	0.000000	0.000000	19.261310
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Au	-2.498500	-1.442500	21.581310
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Au	2.498500	1.442500	21.581310
Au	0.000000	2.885000	21.581310
Au	-0.832800	-1.442500	23.936910
Au	1.665600	0.000000	23.936910
Au	-0.832800	1.442500	23.936910

Au	0.000000	-2.885000	26.292510
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Au	2.498500	-1.442500	26.292510
Au	0.000000	0.000000	26.292510
Au	-2.498500	1.442500	26.292510
Au	2.498500	1.442500	26.292510
Au	0.000000	2.885000	26.292510
Au	-0.832800	-1.442500	28.648110
Au	1.665600	0.000000	28.648110
Au	-0.832800	1.442500	28.648110
Au	0.000000	-2.885000	31.003710
Au	-2.498500	-1.442500	31.003710
Au	2.498500	-1.442500	31.003710
Au	0.000000	0.000000	31.003710
Au	-2.498500	1.442500	31.003710
Au	2.498500	1.442500	31.003710
Au	0.000000	2.885000	31.003710
Au	-0.832800	-1.442500	33.359310
Au	1.665600	0.000000	33.359310
Au	-0.832800	1.442500	33.359310
Au	0.000000	-2.885000	35.714910
Au	-2.498500	-1.442500	35.714910
Au	2.498500	-1.442500	35.714910
Au	0.000000	0.000000	35.714910
Au	-2.498500	1.442500	35.714910
Au	2.498500	1.442500	35.714910
Au	0.000000	2.885000	35.714910

Table S4: Coordinates of **2,5-ThioDA** connected to Au electrodes.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000
Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800
Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200
Au	0.000000	0.000000	-7.031200
Au	-2.498500	1.442500	-7.031200
Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600
Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600

Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000
S	0.000000	0.000000	0.000000
S	1.026040	0.026080	9.563830
O	-1.124440	-0.188070	13.124960
O	4.017320	0.477600	14.466240
O	-2.302250	0.796340	14.675300
O	4.315210	-0.728560	16.260520
N	3.578970	0.186330	3.768590
N	-1.090110	-0.294410	4.997730
N	-1.269210	0.265940	14.257230
N	3.605740	-0.102400	15.467510
C	0.532000	-0.008470	1.701030
C	1.879510	0.114450	2.055820
C	-0.464530	-0.129900	2.674560
C	2.247280	0.112040	3.407290
C	-0.120010	-0.130280	4.031990
C	1.248170	-0.005630	4.417260
C	1.606580	0.014180	5.781440
C	1.923000	0.042360	6.964640
C	2.264570	0.064360	8.323910
C	3.535580	0.120810	8.893620

C	3.518050	0.136460	10.299500
C	2.236890	0.091250	10.841520
C	1.876060	0.087830	12.187170
C	1.548000	0.088870	13.363850
C	1.201760	0.076360	14.726310
C	-0.140120	0.158960	15.199190
C	2.164880	-0.030980	15.770110
C	-0.481730	0.149610	16.545260
C	1.837250	-0.079800	17.119290
C	0.504300	0.016560	17.528180
H	2.649530	0.206230	1.296160
H	-1.505650	-0.240110	2.386850
H	4.223480	0.558970	3.087620
H	3.784930	0.435360	4.725600
H	-2.048140	-0.114970	4.738860
H	-0.852410	-0.065430	5.951760
H	4.438250	0.147580	8.295750
H	4.402510	0.178590	10.923860
H	-1.529760	0.237650	16.806240
H	2.645350	-0.188380	17.832530
S	0.000000	0.000000	19.233200
Au	0.000000	-2.885000	21.553200
Au	-2.498500	-1.442500	21.553200
Au	2.498500	-1.442500	21.553200
Au	0.000000	0.000000	21.553200
Au	-2.498500	1.442500	21.553200
Au	2.498500	1.442500	21.553200

Au	0.000000	2.885000	21.553200
Au	-0.832800	-1.442500	23.908800
Au	1.665600	0.000000	23.908800
Au	-0.832800	1.442500	23.908800
Au	0.000000	-2.885000	26.264400
Au	-2.498500	-1.442500	26.264400
Au	2.498500	-1.442500	26.264400
Au	0.000000	0.000000	26.264400
Au	-2.498500	1.442500	26.264400
Au	2.498500	1.442500	26.264400
Au	0.000000	2.885000	26.264400
Au	-0.832800	-1.442500	28.620000
Au	1.665600	0.000000	28.620000
Au	-0.832800	1.442500	28.620000
Au	0.000000	-2.885000	30.975600
Au	-2.498500	-1.442500	30.975600
Au	2.498500	-1.442500	30.975600
Au	0.000000	0.000000	30.975600
Au	-2.498500	1.442500	30.975600
Au	2.498500	1.442500	30.975600
Au	0.000000	2.885000	30.975600
Au	-0.832800	-1.442500	33.331200
Au	1.665600	0.000000	33.331200
Au	-0.832800	1.442500	33.331200
Au	0.000000	-2.885000	35.686800
Au	-2.498500	-1.442500	35.686800
Au	2.498500	-1.442500	35.686800

Au	0.000000	0.000000	35.686800
Au	-2.498500	1.442500	35.686800
Au	2.498500	1.442500	35.686800
Au	0.000000	2.885000	35.686800

Table S5: Coordinates of **2,4-ThioD** connected to Au electrodes.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000
Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800
Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200
Au	0.000000	0.000000	-7.031200
Au	-2.498500	1.442500	-7.031200

Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600
Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600
Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000
S	0.000000	0.000000	0.000000
H	2.064440	1.687900	1.281370
C	0.674130	0.068910	1.652120
C	1.676750	0.976790	2.004430
H	-0.625280	-1.532220	2.303880
C	0.167000	-0.843650	2.581800
H	3.689250	2.331510	2.956760
C	2.182050	0.983580	3.312820
N	3.132280	1.916750	3.688630
C	0.669530	-0.858930	3.890040
C	1.689520	0.055950	4.270630
H	-0.323310	-2.552630	4.479600
H	3.627340	1.743970	4.552370
N	0.147270	-1.731250	4.829480
C	2.218580	0.033730	5.587900

H	0.700700	-1.887210	5.660790
C	2.684180	0.005350	6.716650
H	5.369020	-0.064510	7.688490
C	3.187380	-0.015170	8.047970
C	4.532690	-0.042400	8.373170
H	1.274330	0.020780	9.180080
C	2.356070	-0.006130	9.217420
S	4.798240	-0.049490	10.077140
C	3.066330	-0.026450	10.399440
C	2.575290	-0.021380	11.718280
C	2.164970	-0.018690	12.866430
H	-0.410680	0.051270	13.628710
C	1.671760	-0.014100	14.200930
C	0.285550	0.024230	14.460550
H	3.625200	-0.077220	15.120970
C	2.555160	-0.047480	15.299260
C	-0.195780	0.029180	15.764740
H	-1.267390	0.060720	15.938700
C	2.073020	-0.043760	16.604380
C	0.692450	-0.004640	16.851810
H	2.778060	-0.071360	17.430000
S	0.000000	0.000000	18.494680
Au	0.000000	-2.885000	20.814680
Au	-2.498500	-1.442500	20.814680
Au	2.498500	-1.442500	20.814680
Au	0.000000	0.000000	20.814680
Au	-2.498500	1.442500	20.814680

Au	2.498500	1.442500	20.814680
Au	0.000000	2.885000	20.814680
Au	-0.832800	-1.442500	23.170280
Au	1.665600	0.000000	23.170280
Au	-0.832800	1.442500	23.170280
Au	0.000000	-2.885000	25.525880
Au	-2.498500	-1.442500	25.525880
Au	2.498500	-1.442500	25.525880
Au	0.000000	0.000000	25.525880
Au	-2.498500	1.442500	25.525880
Au	2.498500	1.442500	25.525880
Au	0.000000	2.885000	25.525880
Au	-0.832800	-1.442500	27.881480
Au	1.665600	0.000000	27.881480
Au	-0.832800	1.442500	27.881480
Au	0.000000	-2.885000	30.237080
Au	-2.498500	-1.442500	30.237080
Au	2.498500	-1.442500	30.237080
Au	0.000000	0.000000	30.237080
Au	-2.498500	1.442500	30.237080
Au	2.498500	1.442500	30.237080
Au	0.000000	2.885000	30.237080
Au	-0.832800	-1.442500	32.592680
Au	1.665600	0.000000	32.592680
Au	-0.832800	1.442500	32.592680
Au	0.000000	-2.885000	34.948280
Au	-2.498500	-1.442500	34.948280

Au	2.498500	-1.442500	34.948280
Au	0.000000	0.000000	34.948280
Au	-2.498500	1.442500	34.948280
Au	2.498500	1.442500	34.948280
Au	0.000000	2.885000	34.948280

Table S6: Coordinates of **2,4-ThioA** connected to Au electrodes.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000
Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800
Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200
Au	0.000000	0.000000	-7.031200

Au	-2.498500	1.442500	-7.031200
Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600
Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600
Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000
S	0.000000	0.000000	0.000000
H	2.660840	-0.056510	1.028700
C	0.599140	0.016460	1.678980
C	1.988220	-0.020910	1.880700
H	-1.329360	0.091660	2.660830
C	-0.251870	0.062750	2.793580
C	2.513650	-0.012030	3.167950
H	3.588880	-0.041060	3.311260
C	0.274420	0.072440	4.081590
C	1.667140	0.034970	4.294890
H	-0.393970	0.109080	4.935730
C	2.204480	0.044670	5.614090
C	2.666400	0.053210	6.740650
H	5.364950	0.001780	7.658120

C	3.190940	0.063720	8.060550
C	4.545530	0.034870	8.362950
H	1.305370	0.133490	9.236500
C	2.387690	0.104540	9.242940
S	4.854290	0.058420	10.053590
C	3.129610	0.106630	10.409450
C	2.658690	0.146240	11.726570
O	-0.354990	0.870520	12.396400
C	2.261540	0.193420	12.878310
N	-0.630450	0.229890	13.406680
O	-1.695200	-0.360850	13.601410
C	1.762770	0.207570	14.196130
O	4.554500	0.663000	14.219690
C	0.371040	0.179430	14.490570
N	4.061500	0.166930	15.228720
C	2.590620	0.152400	15.350260
C	-0.142010	0.096460	15.776740
H	-1.218350	0.060320	15.899040
O	4.707750	-0.308870	16.166430
C	2.095500	0.079630	16.647690
C	0.718260	0.061190	16.880660
H	2.811450	0.037370	17.459250
S	0.000000	0.000000	18.504800
Au	0.000000	-2.885000	20.824800
Au	-2.498500	-1.442500	20.824800
Au	2.498500	-1.442500	20.824800
Au	0.000000	0.000000	20.824800

Au	-2.498500	1.442500	20.824800
Au	2.498500	1.442500	20.824800
Au	0.000000	2.885000	20.824800
Au	-0.832800	-1.442500	23.180400
Au	1.665600	0.000000	23.180400
Au	-0.832800	1.442500	23.180400
Au	0.000000	-2.885000	25.536000
Au	-2.498500	-1.442500	25.536000
Au	2.498500	-1.442500	25.536000
Au	0.000000	0.000000	25.536000
Au	-2.498500	1.442500	25.536000
Au	2.498500	1.442500	25.536000
Au	0.000000	2.885000	25.536000
Au	-0.832800	-1.442500	27.891600
Au	1.665600	0.000000	27.891600
Au	-0.832800	1.442500	27.891600
Au	0.000000	-2.885000	30.247200
Au	-2.498500	-1.442500	30.247200
Au	2.498500	-1.442500	30.247200
Au	0.000000	0.000000	30.247200
Au	-2.498500	1.442500	30.247200
Au	2.498500	1.442500	30.247200
Au	0.000000	2.885000	30.247200
Au	-0.832800	-1.442500	32.602800
Au	1.665600	0.000000	32.602800
Au	-0.832800	1.442500	32.602800
Au	0.000000	-2.885000	34.958400

Au	-2.498500	-1.442500	34.958400
Au	2.498500	-1.442500	34.958400
Au	0.000000	0.000000	34.958400
Au	-2.498500	1.442500	34.958400
Au	2.498500	1.442500	34.958400
Au	0.000000	2.885000	34.958400

Table S7: Coordinates of **2,4-ThioDA** connected to Au electrodes.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000
Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800
Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200

Au	0.000000	0.000000	-7.031200
Au	-2.498500	1.442500	-7.031200
Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600
Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600
Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000
S	0.000000	0.000000	0.000000
H	2.503960	1.129050	1.098240
C	0.731800	0.001250	1.627920
C	1.953210	0.629730	1.889480
H	-0.919630	-1.143060	2.426840
C	0.017530	-0.639610	2.644110
H	4.030520	1.895930	2.797140
C	2.479440	0.615950	3.188480
N	3.710040	1.196160	3.450300
C	0.525490	-0.658850	3.950250
C	1.766990	-0.025950	4.238470
H	3.910510	1.410350	4.417620
H	-1.134000	-1.503640	4.813540

N	-0.149330	-1.332440	4.950690
C	2.284370	-0.026850	5.558720
H	0.119730	-1.136120	5.904180
C	2.731740	-0.022290	6.695160
H	5.426940	-0.156900	7.618260
C	3.254700	-0.027870	8.017070
C	4.608130	-0.090380	8.321510
H	1.372450	0.093870	9.195970
C	2.453550	0.033210	9.200190
S	4.917210	-0.066640	10.012960
C	3.194510	0.016930	10.367510
C	2.721170	0.070920	11.683150
O	-0.296120	0.797470	12.317380
C	2.318200	0.129770	12.832380
N	-0.577760	0.164570	13.330960
O	-1.640480	-0.431690	13.519930
C	1.807230	0.158470	14.145180
O	4.597280	0.611870	14.187580
C	0.412460	0.130940	14.425600
N	4.095230	0.135730	15.201770
C	2.623190	0.119330	15.308380
C	-0.113810	0.062780	15.707230
H	-1.191290	0.025720	15.818970
O	4.733240	-0.318350	16.155760
C	2.114600	0.061670	16.601420
C	0.735070	0.043380	16.820390
H	2.822200	0.031040	17.420770

S	0.000000	0.000000	18.437510
Au	0.000000	-2.885000	20.757510
Au	-2.498500	-1.442500	20.757510
Au	2.498500	-1.442500	20.757510
Au	0.000000	0.000000	20.757510
Au	-2.498500	1.442500	20.757510
Au	2.498500	1.442500	20.757510
Au	0.000000	2.885000	20.757510
Au	-0.832800	-1.442500	23.113110
Au	1.665600	0.000000	23.113110
Au	-0.832800	1.442500	23.113110
Au	0.000000	-2.885000	25.468710
Au	-2.498500	-1.442500	25.468710
Au	2.498500	-1.442500	25.468710
Au	0.000000	0.000000	25.468710
Au	-2.498500	1.442500	25.468710
Au	2.498500	1.442500	25.468710
Au	0.000000	2.885000	25.468710
Au	-0.832800	-1.442500	27.824310
Au	1.665600	0.000000	27.824310
Au	-0.832800	1.442500	27.824310
Au	0.000000	-2.885000	30.179910
Au	-2.498500	-1.442500	30.179910
Au	2.498500	-1.442500	30.179910
Au	0.000000	0.000000	30.179910
Au	-2.498500	1.442500	30.179910
Au	2.498500	1.442500	30.179910

Au	0.000000	2.885000	30.179910
Au	-0.832800	-1.442500	32.535510
Au	1.665600	0.000000	32.535510
Au	-0.832800	1.442500	32.535510
Au	0.000000	-2.885000	34.891110
Au	-2.498500	-1.442500	34.891110
Au	2.498500	-1.442500	34.891110
Au	0.000000	0.000000	34.891110
Au	-2.498500	1.442500	34.891110
Au	2.498500	1.442500	34.891110
Au	0.000000	2.885000	34.891110

Table S8: Coordinates of **BenzDA** connected to Au electrodes.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000
Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800

Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200
Au	0.000000	0.000000	-7.031200
Au	-2.498500	1.442500	-7.031200
Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600
Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600
Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000
S	0.000000	0.000000	0.000000
H	2.907980	0.154840	0.508290
C	2.377420	0.096130	1.453430
C	0.984150	0.003030	1.490240
H	4.910150	0.545010	1.802490
N	4.486900	0.149190	2.628510
C	3.105030	0.105000	2.650090
C	0.294660	-0.079800	2.701810

H	-0.787210	-0.167810	2.716600
H	4.930470	0.426430	3.492980
C	2.423420	0.031690	3.896410
C	1.003080	-0.069450	3.909820
C	3.148780	0.067990	5.111360
N	0.338790	-0.197990	5.111600
H	-0.637960	0.052780	5.123300
H	0.851120	0.066800	5.940620
C	3.770130	0.111560	6.161560
H	6.438190	0.131950	6.454840
C	4.491030	0.146440	7.387830
C	5.903200	0.156770	7.398460
H	7.691150	0.201990	8.586850
C	6.605620	0.194000	8.600530
C	3.809700	0.172050	8.617040
H	2.725920	0.166310	8.638920
C	5.930100	0.219920	9.817240
C	4.520330	0.208100	9.828780
H	6.468820	0.251430	10.757830
C	3.811790	0.237190	11.059320
O	0.698500	0.754110	11.140660
C	3.197500	0.275880	12.107700
N	0.248990	0.176340	12.124540
O	-0.842530	-0.392360	12.171570
C	2.471110	0.269860	13.317100
C	1.053620	0.178580	13.363710
O	5.197770	0.862530	13.835270

H	-0.748050	0.003160	14.475410
C	0.330010	0.085160	14.543350
C	3.087850	0.253770	14.595550
N	4.556360	0.333450	14.736040
O	5.042040	-0.124170	15.772290
C	0.985980	0.090320	15.778120
C	2.379740	0.166070	15.787640
H	2.947310	0.152050	16.709550
S	0.000000	0.000000	17.254780
Au	0.000000	-2.885000	19.574780
Au	-2.498500	-1.442500	19.574780
Au	2.498500	-1.442500	19.574780
Au	0.000000	0.000000	19.574780
Au	-2.498500	1.442500	19.574780
Au	2.498500	1.442500	19.574780
Au	0.000000	2.885000	19.574780
Au	-0.832800	-1.442500	21.930380
Au	1.665600	0.000000	21.930380
Au	-0.832800	1.442500	21.930380
Au	0.000000	-2.885000	24.285980
Au	-2.498500	-1.442500	24.285980
Au	2.498500	-1.442500	24.285980
Au	0.000000	0.000000	24.285980
Au	-2.498500	1.442500	24.285980
Au	2.498500	1.442500	24.285980
Au	0.000000	2.885000	24.285980
Au	-0.832800	-1.442500	26.641580

Au	1.665600	0.000000	26.641580
Au	-0.832800	1.442500	26.641580
Au	0.000000	-2.885000	28.997180
Au	-2.498500	-1.442500	28.997180
Au	2.498500	-1.442500	28.997180
Au	0.000000	0.000000	28.997180
Au	-2.498500	1.442500	28.997180
Au	2.498500	1.442500	28.997180
Au	0.000000	2.885000	28.997180
Au	-0.832800	-1.442500	31.352780
Au	1.665600	0.000000	31.352780
Au	-0.832800	1.442500	31.352780
Au	0.000000	-2.885000	33.708380
Au	-2.498500	-1.442500	33.708380
Au	2.498500	-1.442500	33.708380
Au	0.000000	0.000000	33.708380
Au	-2.498500	1.442500	33.708380
Au	2.498500	1.442500	33.708380
Au	0.000000	2.885000	33.708380

Table S9: Coordinates of **PyriDA** connected to Au electrodes.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000

Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800
Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200
Au	0.000000	0.000000	-7.031200
Au	-2.498500	1.442500	-7.031200
Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600
Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600
Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000

S	0.000000	0.000000	0.000000
O	1.051840	1.522760	10.573040
O	-0.488340	0.104430	11.198460
O	5.428970	0.773880	13.402290
O	5.097060	-0.564180	15.094080
N	4.761040	0.290860	2.079490
N	0.928510	0.057510	5.039620
N	4.319050	0.361260	8.100070
N	0.568860	0.717280	11.360260
N	4.702770	0.133150	14.156320
C	2.531870	0.128080	1.160700
C	1.147720	0.082470	1.363550
C	3.393040	0.183410	2.263860
C	0.601940	0.075620	2.649630
C	2.861110	0.175190	3.582970
C	1.446880	0.114210	3.768850
C	3.704480	0.233690	4.713930
C	4.358950	0.289510	5.743840
C	5.067470	0.362830	6.978200
C	6.478580	0.436860	7.010780
C	7.119080	0.507990	8.242430
C	4.956040	0.433780	9.283620
C	6.355820	0.505950	9.409650
C	4.139860	0.438290	10.458490
C	3.486530	0.460780	11.482690
C	1.285640	0.484370	12.632250
C	2.702200	0.426530	12.658820

C	0.486620	0.335600	13.755630
C	3.242230	0.218140	13.952790
C	1.071280	0.142170	15.013960
C	2.465000	0.075160	15.096650
H	2.948500	0.130960	0.158300
H	5.127750	-0.009850	1.188620
H	-0.473750	0.038710	2.792240
H	5.345730	0.059550	2.870480
H	-0.052830	0.245670	5.170380
H	1.529620	0.275190	5.822050
H	7.039980	0.438980	6.082890
H	8.202110	0.565230	8.295430
H	6.810310	0.560850	10.392390
H	-0.590020	0.370430	13.633390
H	2.972430	-0.091380	16.039080
S	0.000000	0.000000	16.423350
Au	0.000000	-2.885000	18.743350
Au	-2.498500	-1.442500	18.743350
Au	2.498500	-1.442500	18.743350
Au	0.000000	0.000000	18.743350
Au	-2.498500	1.442500	18.743350
Au	2.498500	1.442500	18.743350
Au	0.000000	2.885000	18.743350
Au	-0.832800	-1.442500	21.098950
Au	1.665600	0.000000	21.098950
Au	-0.832800	1.442500	21.098950
Au	0.000000	-2.885000	23.454550

Au	-2.498500	-1.442500	23.454550
Au	2.498500	-1.442500	23.454550
Au	0.000000	0.000000	23.454550
Au	-2.498500	1.442500	23.454550
Au	2.498500	1.442500	23.454550
Au	0.000000	2.885000	23.454550
Au	-0.832800	-1.442500	25.810150
Au	1.665600	0.000000	25.810150
Au	-0.832800	1.442500	25.810150
Au	0.000000	-2.885000	28.165750
Au	-2.498500	-1.442500	28.165750
Au	2.498500	-1.442500	28.165750
Au	0.000000	0.000000	28.165750
Au	-2.498500	1.442500	28.165750
Au	2.498500	1.442500	28.165750
Au	0.000000	2.885000	28.165750
Au	-0.832800	-1.442500	30.521350
Au	1.665600	0.000000	30.521350
Au	-0.832800	1.442500	30.521350
Au	0.000000	-2.885000	32.876950
Au	-2.498500	-1.442500	32.876950
Au	2.498500	-1.442500	32.876950
Au	0.000000	0.000000	32.876950
Au	-2.498500	1.442500	32.876950
Au	2.498500	1.442500	32.876950
Au	0.000000	2.885000	32.876950

Table S10: Coordinates of **EthyDA** connected to Au electrodes.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000
Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800
Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200
Au	0.000000	0.000000	-7.031200
Au	-2.498500	1.442500	-7.031200
Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600
Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600

Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000
S	0.000000	0.000000	0.000000
O	1.026900	-0.843690	8.169390
O	-0.522780	0.390560	9.080860
O	5.303950	-1.253150	11.185160
O	5.152240	0.038800	12.938760
N	4.659700	-0.345640	2.286270
N	0.704040	0.008240	5.073710
N	0.541050	-0.229630	9.117610
N	4.673360	-0.546280	11.964380
C	2.472770	-0.206690	1.271820
C	1.086590	-0.077150	1.413220
C	3.283150	-0.270320	2.412440
C	0.489380	-0.017270	2.674240
C	2.697230	-0.215240	3.708680
C	1.281120	-0.087070	3.831350
C	3.507830	-0.289470	4.864020
C	4.207350	-0.355190	5.863440
C	4.954380	-0.418830	7.077600
C	6.311130	-0.481370	7.136690
C	4.180600	-0.418050	8.280760

C	3.481620	-0.431700	9.275520
C	1.265310	-0.255000	10.403030
C	2.678400	-0.399770	10.436910
C	0.478090	-0.121380	11.539370
C	3.218840	-0.401770	11.748500
C	1.063020	-0.140500	12.810440
C	2.452710	-0.268940	12.899610
H	2.932180	-0.249530	0.289150
H	5.020670	-0.694380	1.410790
H	-0.586490	0.093500	2.770400
H	5.175230	-0.647130	3.101310
H	-0.293760	-0.115110	5.147700
H	1.225540	-0.270250	5.893060
H	6.907240	-0.483110	6.231320
H	6.819090	-0.532810	8.092360
H	-0.591570	-0.001900	11.413040
H	2.964620	-0.267700	13.854490
S	0.000000	0.000000	14.226390
Au	0.000000	-2.885000	16.546390
Au	-2.498500	-1.442500	16.546390
Au	2.498500	-1.442500	16.546390
Au	0.000000	0.000000	16.546390
Au	-2.498500	1.442500	16.546390
Au	2.498500	1.442500	16.546390
Au	0.000000	2.885000	16.546390
Au	-0.832800	-1.442500	18.901990
Au	1.665600	0.000000	18.901990

Au	-0.832800	1.442500	18.901990
Au	0.000000	-2.885000	21.257590
Au	-2.498500	-1.442500	21.257590
Au	2.498500	-1.442500	21.257590
Au	0.000000	0.000000	21.257590
Au	-2.498500	1.442500	21.257590
Au	2.498500	1.442500	21.257590
Au	0.000000	2.885000	21.257590
Au	-0.832800	-1.442500	23.613190
Au	1.665600	0.000000	23.613190
Au	-0.832800	1.442500	23.613190
Au	0.000000	-2.885000	25.968790
Au	-2.498500	-1.442500	25.968790
Au	2.498500	-1.442500	25.968790
Au	0.000000	0.000000	25.968790
Au	-2.498500	1.442500	25.968790
Au	2.498500	1.442500	25.968790
Au	0.000000	2.885000	25.968790
Au	-0.832800	-1.442500	28.324390
Au	1.665600	0.000000	28.324390
Au	-0.832800	1.442500	28.324390
Au	0.000000	-2.885000	30.679990
Au	-2.498500	-1.442500	30.679990
Au	2.498500	-1.442500	30.679990
Au	0.000000	0.000000	30.679990
Au	-2.498500	1.442500	30.679990
Au	2.498500	1.442500	30.679990

Au	0.000000	2.885000	30.679990

Table S11: Coordinates of **IsobDA** connected to Au electrodes.

Atom	**X**	**Y**	**Z**
Au	-0.832800	-1.442500	-14.098000
Au	1.665600	0.000000	-14.098000
Au	-0.832800	1.442500	-14.098000
Au	0.000000	-2.885000	-11.742400
Au	-2.498500	-1.442500	-11.742400
Au	2.498500	-1.442500	-11.742400
Au	0.000000	0.000000	-11.742400
Au	-2.498500	1.442500	-11.742400
Au	2.498500	1.442500	-11.742400
Au	0.000000	2.885000	-11.742400
Au	-0.832800	-1.442500	-9.386800
Au	1.665600	0.000000	-9.386800
Au	-0.832800	1.442500	-9.386800
Au	0.000000	-2.885000	-7.031200
Au	-2.498500	-1.442500	-7.031200
Au	2.498500	-1.442500	-7.031200
Au	0.000000	0.000000	-7.031200
Au	-2.498500	1.442500	-7.031200
Au	2.498500	1.442500	-7.031200
Au	0.000000	2.885000	-7.031200
Au	-0.832800	-1.442500	-4.675600

Au	1.665600	0.000000	-4.675600
Au	-0.832800	1.442500	-4.675600
Au	0.000000	-2.885000	-2.320000
Au	-2.498500	-1.442500	-2.320000
Au	2.498500	-1.442500	-2.320000
Au	0.000000	0.000000	-2.320000
Au	-2.498500	1.442500	-2.320000
Au	2.498500	1.442500	-2.320000
Au	0.000000	2.885000	-2.320000
S	0.000000	0.000000	0.000000
O	1.371870	-0.816150	8.076720
O	-0.233050	0.471490	8.804770
O	5.559040	0.616080	11.190030
O	5.184390	-0.409350	13.078160
N	4.558200	0.923690	2.340700
N	0.927020	-0.972670	4.945830
N	0.833830	-0.129030	8.942900
N	4.815690	0.077010	12.006020
C	2.417310	0.490200	1.303360
C	1.108150	0.005720	1.400800
C	3.241930	0.489800	2.435260
C	0.602470	-0.468040	2.612260
C	2.749790	0.011030	3.680600
C	1.410070	-0.468340	3.761610
C	3.584320	0.017810	4.826080
C	7.255120	0.062860	5.639630
C	4.319440	0.024000	5.801540

C	6.508150	0.089370	6.940590
C	5.134700	0.052850	6.977900
C	7.345410	0.169050	8.181970
C	4.419690	0.043220	8.211610
C	3.746760	0.017600	9.227330
C	1.490250	-0.045320	10.259630
C	2.909230	-0.004340	10.362010
C	0.632390	-0.020420	11.349550
C	3.373960	0.023000	11.704220
C	1.146620	-0.009590	12.651600
C	2.533830	-0.001540	12.813180
H	2.804320	0.867240	0.361620
H	4.769310	1.535050	1.564910
H	-0.409170	-0.857920	2.672850
H	4.991860	1.207580	3.209070
H	6.618120	-0.212940	4.797260
H	-0.072860	-1.058760	5.045100
H	7.696310	1.048900	5.433890
H	8.091930	-0.644130	5.694260
H	1.414360	-0.771380	5.808390
H	8.011490	1.041200	8.132720
H	7.998190	-0.711610	8.254520
H	6.753830	0.240010	9.094380
H	-0.435880	-0.023540	11.165610
H	2.992300	-0.004030	13.794490
S	0.000000	0.000000	14.009620
Au	0.000000	-2.885000	16.329620

Au	-2.498500	-1.442500	16.329620
Au	2.498500	-1.442500	16.329620
Au	0.000000	0.000000	16.329620
Au	-2.498500	1.442500	16.329620
Au	2.498500	1.442500	16.329620
Au	0.000000	2.885000	16.329620
Au	-0.832800	-1.442500	18.685220
Au	1.665600	0.000000	18.685220
Au	-0.832800	1.442500	18.685220
Au	0.000000	-2.885000	21.040820
Au	-2.498500	-1.442500	21.040820
Au	2.498500	-1.442500	21.040820
Au	0.000000	0.000000	21.040820
Au	-2.498500	1.442500	21.040820
Au	2.498500	1.442500	21.040820
Au	0.000000	2.885000	21.040820
Au	-0.832800	-1.442500	23.396420
Au	1.665600	0.000000	23.396420
Au	-0.832800	1.442500	23.396420
Au	0.000000	-2.885000	25.752020
Au	-2.498500	-1.442500	25.752020
Au	2.498500	-1.442500	25.752020
Au	0.000000	0.000000	25.752020
Au	-2.498500	1.442500	25.752020
Au	2.498500	1.442500	25.752020
Au	0.000000	2.885000	25.752020
Au	-0.832800	-1.442500	28.107620

Au	1.665600	0.000000	28.107620
Au	-0.832800	1.442500	28.107620
Au	0.000000	-2.885000	30.463220
Au	-2.498500	-1.442500	30.463220
Au	2.498500	-1.442500	30.463220
Au	0.000000	0.000000	30.463220
Au	-2.498500	1.442500	30.463220
Au	2.498500	1.442500	30.463220
Au	0.000000	2.885000	30.463220

Sample TranSIESTA Input File for Electrode

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SystemName  Elec_ABC_Au

SystemLabel Elec_ABC_Au


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# SPECIES AND BASIS


# Number of species

NumberOfSpecies 1

%block ChemicalSpeciesLabel

  1  79 Au

%endblock ChemicalSpeciesLabel

PAO.EnergyShift 0.01 eV

PAO.BasisType split

PAO.SplitNorm 0.15

%block    PAO.BasisSizes

  Au        DZ

%endblock PAO.BasisSizes


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# K-points


%block kgrid_Monkhorst_Pack

1   0   0   0.0

0   1   0   0.0
```

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0   0   50  0.0
%endblock kgrid_Monkhorst_Pack

=================================================
=================================================
# UNIT CELL AND ATOMIC POSITIONS

# UNIT CELL
LatticeConstant       1.00 Ang
%block LatticeVectors
30.00000000   0.00000000000   0.0000000000
0.000000000   30.0000000000   0.0000000000
0.000000000   0.00000000000   9.4224001000
%endblock LatticeVectors

# Atomic coordinates
NumberOfAtoms 20
AtomicCoordinatesFormat ScaledCartesian
%block AtomicCoordinatesAndAtomicSpecies
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     1.6656000      0.0000000    -14.0980000      1  Au      2
    -0.8328000      1.4425000    -14.0980000      1  Au      3
     0.0000000     -2.8850000    -11.7424000      1  Au      4
    -2.4985000     -1.4425000    -11.7424000      1  Au      5
     2.4985000     -1.4425000    -11.7424000      1  Au      6
     0.0000000      0.0000000    -11.7424000      1  Au      7
    -2.4985000      1.4425000    -11.7424000      1  Au      8
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     2.4985000      1.4425000    -11.7424000      1  Au      9
     0.0000000      2.8850000    -11.7424000      1  Au     10
    -0.8328000     -1.4425000     -9.3868000      1  Au     11
     1.6656000      0.0000000     -9.3868000      1  Au     12
    -0.8328000      1.4425000     -9.3868000      1  Au     13
     0.0000000     -2.8850000     -7.0312000      1  Au     14
    -2.4985000     -1.4425000     -7.0312000      1  Au     15
     2.4985000     -1.4425000     -7.0312000      1  Au     16
     0.0000000      0.0000000     -7.0312000      1  Au     17
    -2.4985000      1.4425000     -7.0312000      1  Au     18
     2.4985000      1.4425000     -7.0312000      1  Au     19
     0.0000000      2.8850000     -7.0312000      1  Au     20
%endblock AtomicCoordinatesAndAtomicSpecies



=====================================================
=====================================================
# General variables

ElectronicTemperature  300 K
MeshCutoff           200. Ry
xc.functional         GGA         # Exchange-correlation functional
xc.authors            PBE
SpinPolarized .false.
SolutionMethod Diagon

=====================================================
```

```
=====================================================

# SCF variables

DM.MixSCF1   T
MaxSCFIterations      10000           # Maximum number of SCF iter
DM.MixingWeight       0.1         # New DM amount for next SCF cycle
DM.Tolerance          5.d-5         # Tolerance in maximum difference
DM.UseSaveDM          true          # to use continuation files
DM.NumberPulay         5
Diag.DivideAndConquer  no
Diag.ParallelOverK    yes

=====================================================
=====================================================
# MD variables

MD.FinalTimeStep 1
MD.TypeOfRun CG
MD.NumCGsteps     000
MD.UseSaveXV      .true.

=====================================================
=====================================================
# Output variables

WriteMullikenPop                1
WriteBands                      .true.
```

```
SaveRho                         .false.
SaveDeltaRho                    .false.
SaveHS                          .false.
SaveElectrostaticPotential      True
SaveTotalPotential              no
WriteCoorXmol                   .true.
WriteMDXmol                     .true.
WriteMDhistory                  .false.
WriteEigenvalues                yes

================================================
================================================
# Band structure analysis

BandLinesScale pi/a
%block BandLines
1       0.00    0.00    0.00    \Gamma
160     0.00    0.50    0.00    X
120     0.25    0.50    0.00    W
120     0.25    0.25    0.25    L
120     0.00    0.00    0.00    \Gamma
%endblock BandLines

================================================
================================================
```

Sample TranSIESTA Input File for Molecular Junction

```
SystemName  BenzDA_DZP

SystemLabel BenzDA_DZP

================================================

================================================

# SPECIES AND BASIS


# Number of species

NumberOfSpecies 6

%block ChemicalSpeciesLabel

  1   79  Au

  2   16  S

  3    6  C

  4    1  H

  5    7  N

  6    8  O

%endblock ChemicalSpeciesLabel


%block    PAO.BasisSizes

  Au        DZ

   S        DZP

   C        DZP

   H        DZP

   N        DZP

   O        DZP

%endblock PAO.BasisSizes
```

```
PAO.BasisType split

PAO.SplitNorm 0.15

PAO.EnergyShift 0.01 eV

=================================================

=================================================

# K-points

%block kgrid_Monkhorst_Pack

1   0   0   0.0

0   1   0   0.0

0   0   1   0.0

%endblock kgrid_Monkhorst_Pack

T CELL AND ATOMIC POSITIONS

# UNIT CELL

LatticeConstant       1.00 Ang

%block LatticeVectors

30.00000000   0.00000000000   0.0000000000

0.000000000   30.0000000000   0.0000000000

0.000000000   0.00000000000   50.161980000

%endblock LatticeVectors

# Atomic coordinates

NumberOfAtoms 111

AtomicCoordinatesFormat ScaledCartesian

%block AtomicCoordinatesAndAtomicSpecies
```

```
-0.8328000  -1.4425000  -14.0980000 1   Au  1
 1.6656000   0.0000000  -14.0980000 1   Au  2
-0.8328000   1.4425000  -14.0980000 1   Au  3
 0.0000000  -2.8850000  -11.7424000 1   Au  4
-2.4985000  -1.4425000  -11.7424000 1   Au  5
 2.4985000  -1.4425000  -11.7424000 1   Au  6
 0.0000000   0.0000000  -11.7424000 1   Au  7
-2.4985000   1.4425000  -11.7424000 1   Au  8
 2.4985000   1.4425000  -11.7424000 1   Au  9
 0.0000000   2.8850000  -11.7424000 1   Au  10
-0.8328000  -1.4425000  -9.3868000  1   Au  11
 1.6656000   0.0000000  -9.3868000  1   Au  12
-0.8328000   1.4425000  -9.3868000  1   Au  13
 0.0000000  -2.8850000  -7.0312000  1   Au  14
-2.4985000  -1.4425000  -7.0312000  1   Au  15
 2.4985000  -1.4425000  -7.0312000  1   Au  16
 0.0000000   0.0000000  -7.0312000  1   Au  17
-2.4985000   1.4425000  -7.0312000  1   Au  18
 2.4985000   1.4425000  -7.0312000  1   Au  19
 0.0000000   2.8850000  -7.0312000  1   Au  20
-0.8328000  -1.4425000  -4.6756000  1   Au  21
 1.6656000   0.0000000  -4.6756000  1   Au  22
-0.8328000   1.4425000  -4.6756000  1   Au  23
 0.0000000  -2.8850000  -2.3200000  1   Au  24
-2.4985000  -1.4425000  -2.3200000  1   Au  25
 2.4985000  -1.4425000  -2.3200000  1   Au  26
 0.0000000   0.0000000  -2.3200000  1   Au  27
```

-2.4985000	1.4425000	-2.3200000	1	Au	28
2.4985000	1.4425000	-2.3200000	1	Au	29
0.0000000	2.8850000	-2.3200000	1	Au	30
0.0000000	0.0000000	0.0000000	2	S	31
2.9079800	0.1548400	0.5082900	4	H	32
2.3774200	0.0961300	1.4534300	3	C	33
0.9841500	0.0030300	1.4902400	3	C	34
4.9101500	0.5450100	1.8024900	4	H	35
4.4869000	0.1491900	2.6285100	5	N	36
3.1050300	0.1050000	2.6500900	3	C	37
0.2946600	-0.0798000	2.7018100	3	C	38
-0.7872100	-0.1678100	2.7166000	4	H	39
4.9304700	0.4264300	3.4929800	4	H	40
2.4234200	0.0316900	3.8964100	3	C	41
1.0030800	-0.0694500	3.9098200	3	C	42
3.1487800	0.0679900	5.1113600	3	C	43
0.3387900	-0.1979900	5.1116000	5	N	44
-0.6379600	0.0527800	5.1233000	4	H	45
0.8511200	0.0668000	5.9406200	4	H	46
3.7701300	0.1115600	6.1615600	3	C	47
6.4381900	0.1319500	6.4548400	4	H	48
4.4910300	0.1464400	7.3878300	3	C	49
5.9032000	0.1567700	7.3984600	3	C	50
7.6911500	0.2019900	8.5868500	4	H	51
6.6056200	0.1940000	8.6005300	3	C	52
3.8097000	0.1720500	8.6170400	3	C	53
2.7259200	0.1663100	8.6389200	4	H	54

5.9301000	0.2199200	9.8172400	3	C	55
4.5203300	0.2081000	9.8287800	3	C	56
6.4688200	0.2514300	10.7578300	4	H	57
3.8117900	0.2371900	11.0593200	3	C	58
0.6985000	0.7541100	11.1406600	6	O	59
3.1975000	0.2758800	12.1077000	3	C	60
0.2489900	0.1763400	12.1245400	5	N	61
-0.8425300	-0.3923600	12.1715700	6	O	62
2.4711100	0.2698600	13.3171000	3	C	63
1.0536200	0.1785800	13.3637100	3	C	64
5.1977700	0.8625300	13.8352700	6	O	65
-0.7480500	0.0031600	14.4754100	4	H	66
0.3300100	0.0851600	14.5433500	3	C	67
3.0878500	0.2537700	14.5955500	3	C	68
4.5563600	0.3334500	14.7360400	5	N	69
5.0420400	-0.1241700	15.7722900	6	O	70
0.9859800	0.0903200	15.7781200	3	C	71
2.3797400	0.1660700	15.7876400	3	C	72
2.9473100	0.1520500	16.7095500	4	H	73
0.0000000	0.0000000	17.2547800	2	S	74
0.0000000	-2.8850000	19.5747800	1	Au	75
-2.4985000	-1.4425000	19.5747800	1	Au	76
2.4985000	-1.4425000	19.5747800	1	Au	77
0.0000000	0.0000000	19.5747800	1	Au	78
-2.4985000	1.4425000	19.5747800	1	Au	79
2.4985000	1.4425000	19.5747800	1	Au	80
0.0000000	2.8850000	19.5747800	1	Au	81

```
-0.8328000  -1.4425000   21.9303800 1   Au  82
 1.6656000   0.0000000   21.9303800 1   Au  83
-0.8328000   1.4425000   21.9303800 1   Au  84
 0.0000000  -2.8850000   24.2859800 1   Au  85
-2.4985000  -1.4425000   24.2859800 1   Au  86
 2.4985000  -1.4425000   24.2859800 1   Au  87
 0.0000000   0.0000000   24.2859800 1   Au  88
-2.4985000   1.4425000   24.2859800 1   Au  89
 2.4985000   1.4425000   24.2859800 1   Au  90
 0.0000000   2.8850000   24.2859800 1   Au  91
-0.8328000  -1.4425000   26.6415800 1   Au  92
 1.6656000   0.0000000   26.6415800 1   Au  93
-0.8328000   1.4425000   26.6415800 1   Au  94
 0.0000000  -2.8850000   28.9971800 1   Au  95
-2.4985000  -1.4425000   28.9971800 1   Au  96
 2.4985000  -1.4425000   28.9971800 1   Au  97
 0.0000000   0.0000000   28.9971800 1   Au  98
-2.4985000   1.4425000   28.9971800 1   Au  99
 2.4985000   1.4425000   28.9971800 1   Au  100
 0.0000000   2.8850000   28.9971800 1   Au  101
-0.8328000  -1.4425000   31.3527800 1   Au  102
 1.6656000   0.0000000   31.3527800 1   Au  103
-0.8328000   1.4425000   31.3527800 1   Au  104
 0.0000000  -2.8850000   33.7083800 1   Au  105
-2.4985000  -1.4425000   33.7083800 1   Au  106
 2.4985000  -1.4425000   33.7083800 1   Au  107
 0.0000000   0.0000000   33.7083800 1   Au  108
```

```
-2.4985000   1.4425000   33.7083800 1   Au  109
 2.4985000   1.4425000   33.7083800 1   Au  110
 0.0000000   2.8850000   33.7083800 1   Au  111
%endblock AtomicCoordinatesAndAtomicSpecies
================================================
================================================
# General variables

#ElectronicTemperature  300 K
MeshCutoff           200. Ry
xc.functional         GGA           # Exchange-correlation functional
xc.authors            PBE
SpinPolarized .false.
SolutionMethod Transiesta
================================================
================================================
# SCF variables

DM.MixSCF1   T
MaxSCFIterations      10000         # Maximum number of SCF iter
DM.MixingWeight       0.1           # New DM amount for next SCF cycle
DM.Tolerance          5.d-5         # Tolerance in maximum difference
DM.UseSaveDM          true          # to use continuation files
DM.NumberPulay         5
Diag.DivideAndConquer  no
Diag.ParallelOverK     yes
================================================
```

```
================================================

# MD variables

MD.FinalTimeStep 1

MD.TypeOfRun CG

MD.NumCGsteps     000

MD.UseSaveXV      .true.

================================================

================================================

# Output variables

WriteMullikenPop                1

WriteBands                      .false.

SaveRho                         .false.

SaveDeltaRho                    .false.

SaveHS                          .false.

SaveElectrostaticPotential      True

SaveTotalPotential              no

WriteCoorXmol                   .true.

WriteMDXmol                     .true.

WriteMDhistory                  .false.

WriteEigenvalues                yes

================================================

================================================

# Transiesta information

# GF OPTIONS
```

```
TS.ComplexContour.Emin    -30.0 eV
TS.ComplexContour.NPoles       10
TS.ComplexContour.NCircle      100
TS.ComplexContour.NLine        10
# BIAS OPTIONS
TS.biasContour.NumPoints       100

# TS OPTIONS
TS.Voltage 0.000000 eV

# TBT OPTIONS
TS.TBT.Emin -3.0 eV
TS.TBT.Emax +3.0 eV
TS.TBT.NPoints 3000
TS.TBT.NEigen 3
TS.TBT.Eta        0.000001 Ry

# Write hamiltonian
TS.SaveHS   .true.

# LEFT ELECTRODE
TS.HSFileLeft  ./Elec_ABC_Au.TSHS
#TS.ReplicateA1Left    1
#TS.ReplicateA2Left    1
TS.NumUsedAtomsLeft   20
TS.BufferAtomsLeft    0
```

```
# RIGHT ELECTRODE

TS.HSFileRight  ./Elec_ABC_Au.TSHS

#TS.ReplicateA1Right   1

#TS.ReplicateA2Right   1

TS.NumUsedAtomsRight  20

TS.BufferAtomsRight   0

================================================

================================================
```