

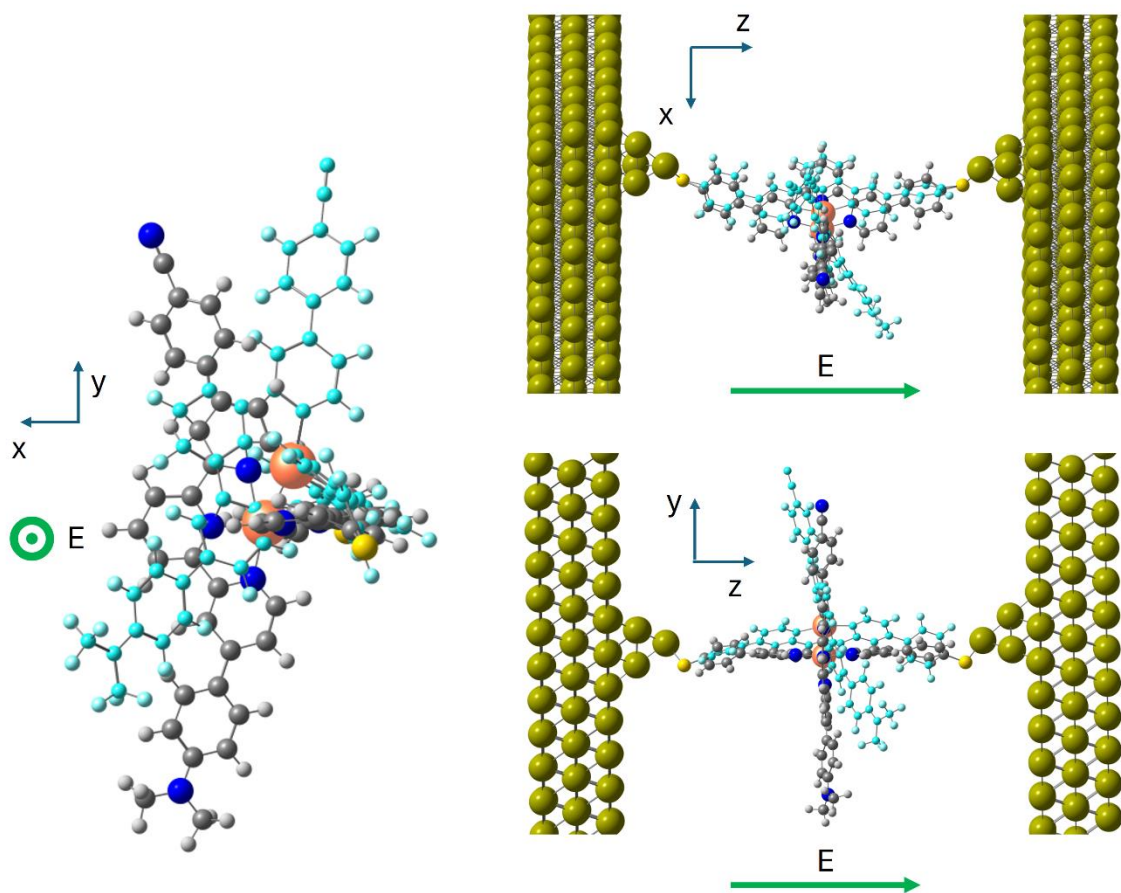
## Supporting Information

### **SPIN-STATE SWITCHING AT THE SINGLE-MOLECULE LEVEL BY DISTORTION OF THE COORDINATION SPHERE: VALIDATION BASED ON QUANTUM-CHEMISTRY CALCULATIONS**

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**Figure S1.** HS molecule optimized in the junction in presence of an external electric field along z axis  $E=0.1\text{V}/\text{\AA}$

Cartesian coordinates of the optimized molecular junction based on the HS molecule

Au	-4.702338	-14.463744	-20.831100
Au	-6.146139	-11.962984	-20.837801
Au	-7.591472	-9.458682	-20.847647
Au	-9.037894	-6.954881	-20.848483
Au	-10.479461	-4.461170	-20.846721
Au	-11.922741	-1.967860	-20.841084
Au	-13.361332	0.531400	-20.832310
Au	-14.799515	3.028860	-20.828500
Au	-16.238792	5.522810	-20.827949
Au	-17.678632	8.018200	-20.826697
Au	-19.119362	10.513180	-20.826314
Au	-20.561992	13.007810	-20.828047
Au	-1.819341	-14.464297	-20.829133
Au	-3.263431	-11.966058	-20.833445
Au	-4.707841	-9.460190	-20.851349
Au	-6.156492	-6.961297	-20.856820
Au	-7.588957	-4.465080	-20.847983
Au	-9.034392	-1.970520	-20.846811
Au	-10.472480	0.522330	-20.838792
Au	-11.912444	3.025070	-20.834523
Au	-13.354912	5.525110	-20.826214
Au	-14.793535	8.019270	-20.827143
Au	-16.235212	10.514660	-20.827181
Au	-17.677862	13.009990	-20.827800
Au	1.066192	-14.463054	-20.832227
Au	-0.378392	-11.966950	-20.833998
Au	-1.823354	-9.467438	-20.837428
Au	-3.270386	-6.965625	-20.847619
Au	-4.712509	-4.463940	-20.830608
Au	-6.158748	-1.980210	-20.822730
Au	-7.599401	0.515200	-20.834107
Au	-9.033048	3.020980	-20.830586
Au	-10.468687	5.519040	-20.835445
Au	-11.905537	8.015570	-20.834224
Au	-13.350900	10.514870	-20.829584
Au	-14.793475	13.011050	-20.830627
Au	3.950038	-14.460799	-20.835162
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Au	1.061924	-9.467224	-20.840564
Au	-0.385136	-6.963252	-20.842067
Au	-1.836138	-4.468100	-20.839145
Au	-3.274584	-1.976140	-20.815517
Au	-4.725810	0.513800	-20.818540
Au	-6.156404	3.017170	-20.828353

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Au	-11.909476	13.012470	-20.833036
Au	6.835098	-14.460941	-20.838509
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Au	3.948268	-9.467595	-20.842267
Au	2.500536	-6.968945	-20.841049
Au	1.050462	-4.469180	-20.838261
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Au	-4.710265	5.518540	-20.819774
Au	-6.143494	8.022230	-20.839515
Au	-7.585837	10.520040	-20.837500
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Au	2.486118	-1.971550	-20.835598
Au	1.040580	0.531700	-20.825754
Au	-0.393654	3.023350	-20.823456
Au	-1.829958	5.525720	-20.817317
Au	-3.262855	8.023110	-20.828911
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Au	12.604688	-14.458233	-20.843246
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Au	9.715698	-9.467813	-20.845785
Au	8.270278	-6.969497	-20.844866
Au	6.824098	-4.470350	-20.841388
Au	5.378438	-1.972110	-20.836896
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Au	1.059036	5.512680	-20.831615
Au	-0.377377	8.017370	-20.829074
Au	-1.816549	10.515840	-20.835777
Au	-3.257416	13.013170	-20.840599
Au	15.486948	-14.460631	-20.841857
Au	14.044228	-11.961110	-20.845660
Au	12.598278	-9.463722	-20.847180
Au	11.152348	-6.967636	-20.847027
Au	9.707748	-4.469930	-20.843247
Au	8.263648	-1.969720	-20.837494
Au	6.821358	0.527620	-20.832675

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Au	3.943178	5.519770	-20.824694
Au	2.504298	8.014420	-20.827137
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Au	16.926218	-11.962247	-20.842935
Au	15.480728	-9.461434	-20.846952
Au	14.034098	-6.962370	-20.846378
Au	12.589928	-4.467380	-20.844567
Au	11.145848	-1.969750	-20.839838
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Au	-16.260782	3.831330	-18.395339
Au	-17.698112	6.326690	-18.393993
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Au	-4.723634	-1.150550	-18.367648
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Au	-14.820276	-0.335420	-15.950188
Au	-16.261882	2.163550	-15.946150
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Au	-1.833186	-12.821391	-15.952966
Au	-3.276473	-10.323417	-15.964110
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Au	-13.369908	12.155940	-15.948102
Au	5.376908	-15.317247	-15.953209
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Au	2.497340	-10.330269	-15.960343
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Au	-1.748653	-2.882320	-15.898455
Au	-3.173889	-0.269160	-16.020638
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Au	-6.187449	4.702480	-15.935077
Au	-7.616933	7.176860	-15.945531
Au	-9.051943	9.666950	-15.946391
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Au	8.258028	-5.333330	-15.958611
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Au	1.051686	7.166990	-15.940179
Au	-0.391307	9.663080	-15.946923
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Au	16.910368	-15.314751	-15.956204
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Au	-4.676122	-2.740870	13.740070
Au	-6.089580	-0.300080	13.786900
Au	-3.047600	-0.269780	13.883650
Au	-4.661245	-14.410191	15.960720
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Au	-14.758409	3.082840	15.953330
Au	-16.194972	5.584980	15.960850
Au	-17.634192	8.082910	15.965580
Au	-19.076552	10.577070	15.966490
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Au	-7.579927	-4.474780	15.927490
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H	-4.659264	-0.179080	-2.238950
H	-5.955496	-0.232950	-0.099140
H	-4.727498	-0.249150	2.080170
H	-3.494643	-0.421590	3.783640
H	0.573286	-0.166280	5.248210
H	1.320793	0.000450	2.891770
H	-1.462461	2.876820	0.149050
H	-0.801718	5.264670	0.248030
H	3.319039	3.976690	-0.072460
H	4.608688	2.347060	-0.108890
H	5.952308	0.237460	-0.151100
H	4.775178	-1.967290	-0.113730
H	3.585963	-3.714390	-0.070340

H	-0.461403	-5.248400	0.083680
H	-1.263455	-2.893990	0.122040
N	3.288717	10.222690	0.205900
C	2.428146	11.335760	-0.162130
H	2.982518	12.278400	-0.020860
H	2.109216	11.276990	-1.224750
H	1.519199	11.372320	0.474110
C	4.665498	10.478180	0.600180
H	4.850778	10.192250	1.657820
H	5.379408	9.919580	-0.040840
H	4.877878	11.554430	0.491770
C	3.846348	-9.975970	-0.028550
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S	-3.596101	0.617540	-10.325420
S	-3.351314	0.619650	10.414960

Cartesian coordinates of the optimized junctions based on the LS molecule

Au	-4.558412	-14.278027	-20.551059
Au	-5.998109	-11.776643	-20.556984
Au	-7.439230	-9.274178	-20.566724
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Au	-20.419342	13.191680	-20.547712
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C	3.968338	-1.124390	-0.101940

C	2.568697	-1.140210	-0.048080
C	1.679032	-2.280670	-0.055190
C	2.072599	-3.623310	-0.069920
C	1.127661	-4.657680	-0.025120
C	-0.236733	-4.268010	0.039530
C	-0.574699	-2.924080	0.040100
H	1.730460	0.261150	-2.575090
H	1.224348	0.270630	-4.994170
H	-2.954951	-0.243950	-3.992560
H	-4.401188	-0.323410	-2.303140
H	-5.721289	-0.379570	-0.178270
H	-4.536326	-0.255070	2.023930
H	-3.216781	0.050180	3.771360
H	0.910918	0.226570	5.061480
H	1.578403	0.050780	2.683550
H	-1.719592	2.579070	0.046050
H	-1.205583	4.991610	0.206890
H	3.001838	3.956830	0.205620
H	4.444288	2.259100	0.089730
H	5.735238	0.126890	-0.094620
H	4.524888	-2.062600	-0.181540
H	3.140216	-3.864450	-0.068660
H	-1.036354	-5.015080	0.049450
H	-1.621564	-2.610460	0.077500
N	2.554723	10.200050	0.218630
C	1.691886	11.216750	-0.363170
H	2.162753	12.203950	-0.225450
H	1.538189	11.053510	-1.451220
H	0.696872	11.235650	0.128040
C	3.854450	10.583940	0.747170
H	3.929949	10.384300	1.836780
H	4.676218	10.040700	0.236990
H	4.001558	11.663320	0.579690
C	2.730932	-10.159524	0.036490
N	3.102488	-11.274280	0.066460
S	-2.574845	0.527060	-10.526240
S	-3.389889	1.100940	10.244600