Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

High-Spin Organic Diradical as a Spin Filter

Suranjan Shil,[a] Debojit Bhattacharya,[*b] Anirban Misra,[a] and Douglas J. Klein[b]

[a]Department of Chemistry, University of North Bengal, Darjeeling, PIN. 734013, West Bengal, INDIA

[b]Department of Marine Sciences, Texas A&M University at Galveston, Texas, 77553, USA

*Telephone: (409) 740-4538, *Email:debojitilora@gmail.com

Table 1S. The voltage and the respective BDSIC values of the aminoxyl diradical attached with the two Au electrodes.

Voltage	BDSIC
0.2	0.976
0.4	0.980
0.6	0.999
0.8	0.991
1.0	0.976
1.2	0.268
1.4	0.985
1.6	0.946
1.8	0.922
2.0	−0.996
2.2	0.966
2.4	0.131
2.6	0.977
2.8	0.770
3.0	0.893
3.2	0.261
3.4	−0.563
3.6	0.273
3.8	0.608
4.0	0.992

Table 2S. The voltage and the corresponding α-current (nA) and β-current (nA) in the range 2.1 V to 2.7 V.

Volt	α-current (nA)	β-current (nA)
2.1 V	0.691711379	0.0238698068
2.3 V	0.362052997	0.00139851046
2.5 V	0.007036514	0.135889983
2.7 V	0.382	0.0655

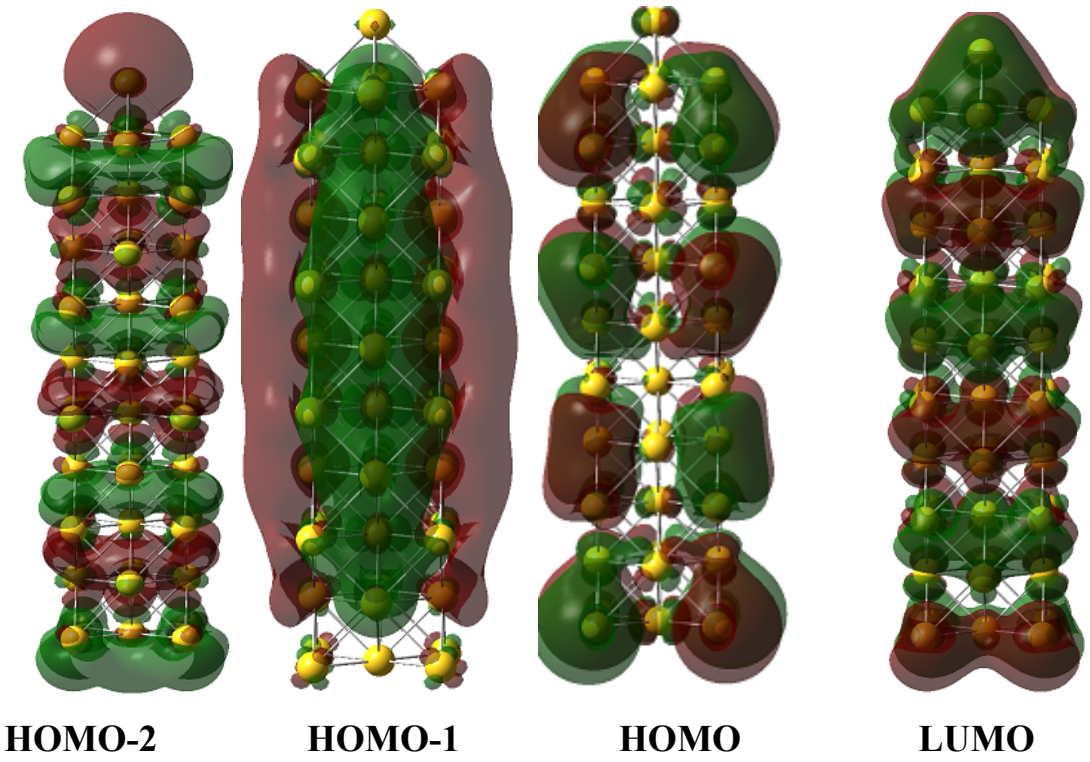


Figure 1S – The pictures (iso value 0.009) of frontier molecular orbitals of the gold electrode showing bonding character of the gold nano-structure taken in this work.

The complete reference of Gaussian'09W (Ref. 16):

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.;

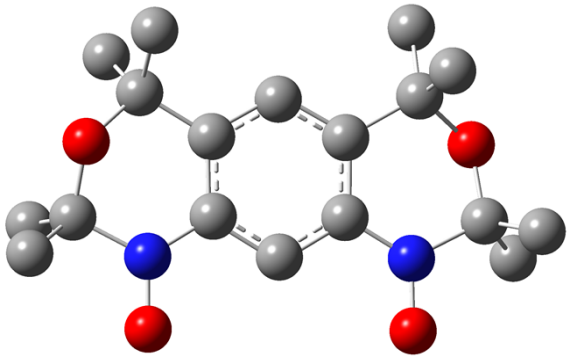
Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian'09W, Revision A.02; Gaussian, Inc.: Wallingford CT, 2009.

The XYZ coordinates and the respective figures of the optimized ferromagnetic aminoxyl diradical, aminoxyl diradical with two S-H bonds and the Au-Diradical-Au molecular junction. Here, the hydrogens are omitted due to picture clarity.

(I) Ferromagnetic Aminoxyl Diradical

O	1.07400000	8.98000000	16.85600000
O	4.88100000	10.33200000	14.27100000
O	0.60100000	5.50300000	16.58000000
O	6.82700000	7.47900000	13.43300000
N	1.33700000	7.74900000	16.61100000
N	5.21200000	9.10000000	14.11600000
C	2.46400000	7.39900000	15.86500000
C	0.51800000	6.71300000	17.30800000
C	1.87300000	4.94600000	16.17100000
C	2.76100000	6.04600000	15.63200000
C	3.89900000	5.74800000	14.88700000
H	4.11800000	4.83700000	14.73100000
C	4.73000000	6.73300000	14.36100000
C	5.85800000	6.40000000	13.41600000
C	6.44600000	8.83400000	13.31200000
C	4.40900000	8.07800000	14.62700000
C	3.28200000	8.41800000	15.37200000
H	3.07400000	9.32900000	15.54200000
C	0.99700000	6.62400000	18.74800000
H	1.95300000	6.41000000	18.76100000
H	0.49900000	5.92000000	19.21600000
H	0.84700000	7.48300000	19.19600000
C	-0.94200000	7.11000000	17.23800000
H	-1.19700000	7.25400000	16.30300000
H	-1.08100000	7.93600000	17.74500000

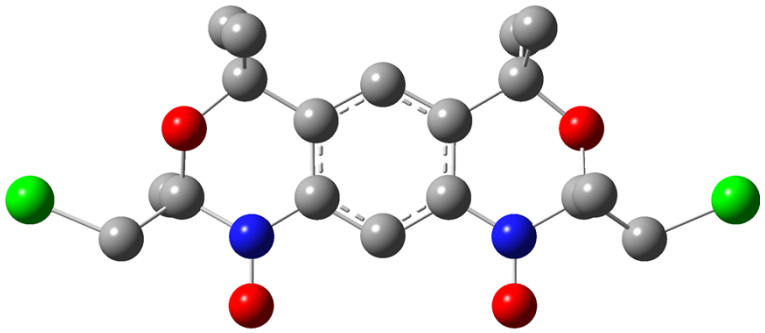
H	-1.49300000	6.39500000	17.62000000
C	2.57700000	4.17300000	17.28800000
H	2.91800000	4.80300000	17.95700000
H	3.32200000	3.66000000	16.91200000
H	1.94100000	3.56000000	17.71300000
C	1.46400000	3.97100000	15.06800000
H	1.00900000	4.46100000	14.35000000
H	0.85800000	3.29500000	15.43800000
H	2.26200000	3.53200000	14.70900000
C	5.28800000	6.14000000	12.02000000
H	4.70300000	6.88300000	11.76200000
H	4.77300000	5.30600000	12.02700000
H	6.02300000	6.06500000	11.37700000
C	6.68500000	5.20700000	13.86900000
H	7.05300000	5.38400000	14.76000000
H	7.41800000	5.05900000	13.23600000
H	6.11700000	4.41000000	13.90300000
C	6.19500000	9.29600000	11.87900000
H	5.42800000	8.81100000	11.51000000
H	6.99000000	9.11600000	11.33400000
H	6.00700000	10.25800000	11.87300000
C	7.60400000	9.60500000	13.92600000
H	7.74600000	9.30200000	14.84600000
H	7.39600000	10.56200000	13.92700000
H	8.41700000	9.44700000	13.40200000



(II) Ferromagnetic Aminoxyl Diradical with the S-H bonds

O	-2.41564100	-2.61390000	-0.06405600
O	2.41554800	-2.61381300	0.06529800
O	-3.64763900	0.65254000	0.34679700
O	3.64746100	0.65259700	-0.34704300
N	-2.40859100	-1.33594300	-0.00373300
N	2.40856100	-1.33587200	0.00430200
C	-1.20717200	-0.61746500	0.02197300
C	-3.68965700	-0.61198100	-0.28026500
C	-2.53531700	1.56292800	0.17901000
C	-1.22705400	0.79597500	0.04949500
C	-0.00006000	1.46103600	-0.00002500
H	-0.00005500	2.54666200	-0.00006900
C	1.22696900	0.79599200	-0.04941900
C	2.53520000	1.56299400	-0.17886600

C	3.68976100	-0.61184300	0.28011700
C	1.20715300	-0.61742100	-0.02160500
C	-0.00000800	-1.32144800	0.00025100
H	0.00002300	-2.40180600	0.00037300
C	-3.88850500	-0.57352700	-1.80021700
H	-3.02987100	-0.11767000	-2.29689600
H	-4.79230800	-0.01470200	-2.04673300
H	-3.98690600	-1.59683500	-2.17142400
C	-4.80300800	-1.38172400	0.45481600
H	-4.54414900	-1.43272300	1.51382700
H	-4.85561200	-2.39856100	0.06803700
C	-2.79238600	2.50366100	-1.01340600
H	-2.75257000	1.97925400	-1.96899500
H	-2.04633300	3.30349800	-1.03911500
H	-3.78052500	2.95993200	-0.90695900
C	-2.55401400	2.36999600	1.48953800
H	-2.39153200	1.70790700	2.34296900
H	-3.52651600	2.85718100	1.60484000
H	-1.77797200	3.13965500	1.48870300
C	2.79234300	2.50343100	1.01378100
H	2.75174900	1.97897800	1.96932000
H	2.04678500	3.30373800	1.03922400
H	3.78080600	2.95909700	0.90777600
C	2.55387200	2.37040300	-1.48918700
H	2.39159100	1.70848700	-2.34278600
H	3.52630600	2.85777900	-1.60427800
H	1.77770200	3.13992500	-1.48822000
C	3.88931700	-0.57307700	1.80000200
H	3.03046900	-0.11793800	2.29700300
H	4.79270400	-0.01338500	2.04601500
H	3.98884300	-1.59621000	2.17136300
C	4.80279200	-1.38164900	-0.45535200
H	4.54359900	-1.43258200	-1.51428600
H	4.85533300	-2.39849700	-0.06859900
S	-6.47903300	-0.66595300	0.26429900
S	6.47898700	-0.66619800	-0.26528200
H	-6.18705200	0.52955200	0.81339200
H	6.18727800	0.52929700	-0.81456500



(III) Diradical with the Au electrodes

Au	2.12773640	-0.41025746	-6.04135745
Au	2.46443518	0.33597666	-8.73535866
Au	3.82145369	-1.79562303	-8.10317830
Au	1.54346500	-2.86614901	-7.48443160
Au	0.16518524	-0.79821088	-8.24427885
Au	4.15019331	-0.72834971	-10.62174712
Au	1.88289914	-1.97066481	-10.06035687
Au	0.61443789	0.24592223	-10.75222550
Au	3.13488727	-4.18143352	-9.32832386
Au	-0.36311020	-3.23154481	-9.46208304
Au	2.24878288	-1.00516408	-12.63463500
Au	3.56168708	-3.16004643	-11.96753837
Au	-0.02483670	-2.17785589	-12.09093992
Au	1.29546336	-4.33415574	-11.46616208
Au	3.92893531	-2.06288495	-14.55538990
Au	0.35852923	-1.09184551	-14.66112628
Au	1.66056497	-3.28450064	-14.06437365
Au	2.92467122	-5.49673576	-13.44311070
Au	-0.58442079	-4.54332296	-13.55148478
Au	2.02972587	-2.20527837	-16.62038469
Au	3.33989379	-4.38065258	-15.99358545
Au	-0.22545249	-3.41014597	-16.09986661
Au	1.08169887	-5.60235840	-15.56190402
Au	3.76106559	-3.28910538	-18.53797314
Au	0.09969611	-2.28756011	-18.65077432
Au	1.46245325	-4.46281471	-18.06781828
Au	2.79851947	-6.64892828	-17.52805560
Au	-0.83305015	-5.65963632	-17.63787088
Au	1.84715967	-3.33213993	-20.58397126
Au	3.13412291	-5.53534809	-20.06212698
Au	-0.41426130	-4.56719261	-20.17778623
Au	0.88461995	-6.73672676	-19.56698906
Au	3.53117265	-4.36192118	-22.56313576
Au	0.00958067	-3.39423647	-22.67950628
Au	1.27435073	-5.62174717	-22.10998408
Au	2.53602229	-7.84569688	-21.50345757
Au	-0.97895101	-6.87763995	-21.61997868
Au	1.67705312	-4.47617399	-24.64520025
Au	2.99251728	-6.70377541	-24.01981563
Au	-0.63330511	-5.70545188	-24.13968287
Au	0.68008826	-7.95120817	-23.58056097
Au	3.40593517	-5.52283302	-26.36048533
Au	-0.24528826	-4.51819787	-26.48149071
Au	1.08277261	-6.77799063	-26.04305770
Au	2.42728088	-8.95499894	-25.30899473
Au	-1.22919032	-7.94698334	-25.42764774
O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	4.79618369
O	3.30650980	0.00000000	-1.20682513
O	3.22676598	-0.89202845	5.98825564
N	1.27503728	-0.13710027	-0.00620202
N	1.26074180	-0.24887568	4.79516788
C	1.98137695	-0.25994062	1.19177107
C	1.94246253	-0.35583786	-1.32398933

C	4.13606760	-0.50580622	-0.13374174
C	3.37377682	-0.44413257	1.17169845
C	4.03211837	-0.56680593	2.39252222
H	4.97218965	-0.70275730	2.39363164
C	3.36692343	-0.49829838	3.61329426
C	4.11303956	-0.46121454	4.92410831
C	1.91933589	-0.37676234	6.13301197
C	1.96934699	-0.32730017	3.59427560
C	1.27277428	-0.20509902	2.39402257
H	0.33039361	-0.08676188	2.39409888
C	1.69367368	-1.79522257	-1.74498550
H	2.03325261	-2.40054519	-1.05348592
H	2.15737848	-1.97394086	-2.59096518
H	0.73123819	-1.93940860	-1.86336336
C	1.37133112	0.61850384	-2.33323465
H	1.45929938	1.53239683	-1.99111306
H	0.42528412	0.41622668	-2.48398284
C	4.65967179	-1.91948417	-0.39486874
H	3.92457059	-2.56188476	-0.30717776
H	5.36095310	-2.13411347	0.25452237
H	5.02885637	-1.96953950	-1.30155899
C	5.31009076	0.47202791	-0.13874740
H	4.97968485	1.38120445	0.02520066
H	5.75885196	0.43892216	-1.00974072
H	5.94417968	0.22321750	0.56441020
C	4.66724231	0.94690341	5.15077812
H	3.94886958	1.60368179	5.03492996
H	5.38094827	1.12578318	4.50312402
H	5.02634692	1.01306098	6.05960486
C	5.23917113	-1.48025360	5.00009540
H	4.87557838	-2.37988020	4.86186988
H	5.66443393	-1.43132406	5.88136690
H	5.90243818	-1.28623193	4.30624999
C	1.84574514	0.97594759	6.83635702
H	2.29675590	1.65229093	6.28970906
H	2.28580184	0.91378813	7.71039150
H	0.90722815	1.22959728	6.96154362
C	1.18570092	-1.43752723	6.93859163
H	1.23620267	-2.29559569	6.47003952
H	0.24703284	-1.17834902	7.04272087
S	2.26201071	0.47196217	-3.86738438
S	1.94114405	-1.59428981	8.54268987
Au	2.04594424	-0.90442001	10.78670337
Au	1.87928441	-1.92635945	13.40504984
Au	4.02739393	-0.50634479	13.01255478
Au	2.43190131	1.45498170	12.44184688
Au	0.28263538	0.09176883	12.96691605
Au	3.73272060	-1.80280501	15.42557975
Au	2.21384856	0.30554206	14.92855956
Au	0.10776994	-1.23278033	15.37457672
Au	4.30504187	1.84847242	14.44160846
Au	0.72424424	2.42473318	14.39713142
Au	1.99125405	-0.91823199	17.40763179
Au	4.11093429	0.54382976	16.98150465

Au	0.43697880	1.12822891	16.92143986
Au	2.56134634	2.58528414	16.53774563
Au	3.83474991	-0.80097217	19.46159337
Au	0.18112861	-0.21178191	19.38541177
Au	2.30204720	1.28367206	19.03261001
Au	4.39800084	2.81445975	18.65633366
Au	0.80723655	3.39405469	18.58598271
Au	2.03693369	-0.04321870	21.48276688
Au	4.16002865	1.43548729	21.09862298
Au	0.51119622	2.02302464	21.02316039
Au	2.63294318	3.51147127	20.72894911
Au	3.93790878	0.07677277	23.53733724
Au	0.18856831	0.67540939	23.46301594
Au	2.35674921	2.12888910	23.12380264
Au	4.50241774	3.59997086	22.82794080
Au	0.78540331	4.19761365	22.75255681
Au	2.08715345	0.75193405	25.52978751
Au	4.19403996	2.25748167	25.25215907
Au	0.56102475	2.83941380	25.18667571
Au	2.67046251	4.31627325	24.81761930
Au	3.91908358	0.83779327	27.63931385
Au	0.31059679	1.40900670	27.57525116
Au	2.41021051	2.94942591	27.25193449
Au	4.50783882	4.49072260	26.89137686
Au	0.90521267	5.05884694	26.82759365
Au	2.14969878	1.55005159	29.67592155
Au	4.29894206	3.07383130	29.29828596
Au	0.58283052	3.66013516	29.23218931
Au	2.73352588	5.19618156	28.92217069
Au	4.04573909	1.65278993	31.52557210
Au	0.30385521	2.24379724	31.45937427
Au	2.46617032	3.77729047	31.27116052
Au	4.62783366	5.25145102	30.78128461
Au	0.87993425	5.84174403	30.71229336