

Supporting Information:

**Goldene monolayer as a highly effective catalyst
for polysulfide anchoring and conversion: A
theoretical study**

Nicolas F. Martins,^{*,†} José A. S. Laranjeira,[†] Bill D. Aparicio-Huacarpuma,[‡]
Kleuton A. L. Lima,[¶] Luiz A. Ribeiro Junior,^{*,‡} and Julio R. Sambrano^{*,†}

[†]*Modeling and Molecular Simulation Group, São Paulo State University (UNESP), School
of Sciences, Bauru, 17033-360, SP, Brazil*

[‡]*Computational Materials Laboratory, LCCMat, Institute of Physics, University of Brasília,
70919-970, Brasília, DF, Brazil*

[¶]*Department of Applied Physics and Center for Computational Engineering and Sciences,
University of Campinas, Brazil.*

E-mail: nicolas.ferreira@unesp.br; ribeirojr.fis@gmail.com; jr.sambrano@unesp.br

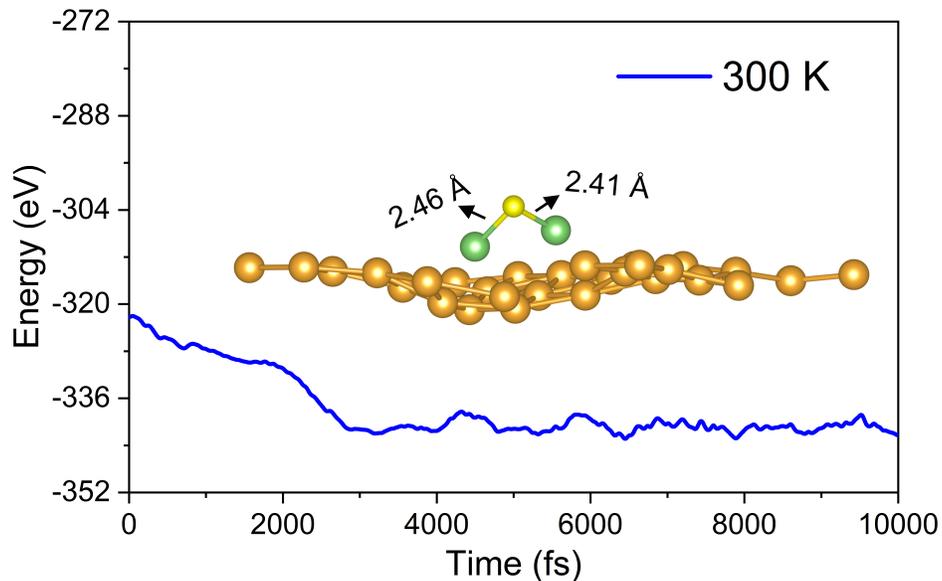


Figure S1: Enter Caption

POSCAR file

Li₂S@Goldene

Au

1.0

13.5388193130	0.0000000000	0.0000000000
-6.7694112178	11.7249605609	0.0000000000
0.0000000000	0.0000000000	19.8669948578

Au S Li

25 1 2

Cartesian

1.357434650	2.256910925	9.733455776
0.017725671	4.582516772	9.718179281
-1.330106040	6.924240364	10.050711588
-2.712243998	9.274807875	10.150910555

-4.065378781	11.623676346	9.891106157
4.028725110	2.256753911	9.748146090
2.667762575	4.431959275	10.866607679
1.367068756	6.931422426	9.605712236
-0.004970820	9.281306667	9.954203377
-1.361214984	11.625655396	9.959530912
6.748954616	2.251479987	9.902890573
5.353363945	4.582051388	9.756503325
4.029466061	6.938876803	9.589161613
2.703517773	9.280626573	9.870635925
1.352338696	11.627431769	10.048961835
9.469687086	2.245194314	10.050918643
8.107199220	4.594891108	9.995515329
6.715719796	6.920927688	10.098623993
5.407589162	9.283624674	10.044693874
4.057512903	11.628958868	10.052506123
12.186512126	2.247692316	9.887293908
10.825692464	4.591211110	9.987009929
9.471253113	6.935556400	10.167091458
8.121025236	9.271847559	10.156053116
6.767759495	11.627044538	9.978013579
2.648817678	5.658564137	12.819591205
0.507990075	6.003033599	11.953927018
4.790787358	6.029656246	11.967858703

Li₂S₂@Goldene

Au

1.0000000000000000
13.5388193129999994 0.0000000000000000 0.0000000000000000
-6.7694112178000001 11.7249605608999996 0.0000000000000000
0.0000000000000000 0.0000000000000000 19.8669948578000017

Au S Li
25 2 2

Direct

0.2049441779742153 0.2008791902904075 0.5033680060988319
0.2015552456111502 0.3984486009433043 0.4876111157043262
0.2005713274225202 0.5998229219545685 0.4998766190163452
0.2011766764970398 0.7994128077762159 0.5093252445073330
0.2032864136375996 0.9996928130921984 0.5067671846511628
0.4030929443833697 0.1981460190976615 0.4928578456267115
0.4020180220401101 0.3988077659912427 0.4713207287873742
0.4014678242156926 0.5987414809306750 0.4905475476968801
0.4018178714964071 0.7979341788123969 0.5077540840204008
0.4023965512115160 0.9981007598545607 0.5072320778238261
0.6030463971302924 0.1971107140563724 0.5028044129819365
0.6033541534678886 0.3970263095156764 0.4916257606729862
0.5988278206705718 0.5938336321923477 0.5075292749165028
0.6013126268213341 0.7964158888471145 0.5062724114384528
0.6025247108611270 0.9970596686345676 0.5072360997298611
0.8030820298192198 0.1972725564650628 0.5063393065570406
0.8026121801361816 0.3972834928190609 0.5069827693651687
0.8009436625817272 0.5969902071627889 0.5068736223674626
0.8008237565408449 0.7965783497473118 0.5066851352888173
0.8023270256778587 0.9971727790501580 0.5050111445559765

0.0033874227408057	0.1985187712475934	0.5037102057488011
0.0029794932864129	0.3982984092899158	0.5070682402818488
0.0009563039809960	0.5988148580211620	0.5092743322527263
0.0012319853565986	0.7990030339113338	0.5085757711959361
0.0031973183565282	0.9990220410575266	0.5041664672710310
0.4386118223006981	0.5108476283914301	0.6426010518265762
0.2908421875549350	0.3580470486447263	0.6424758835058345
0.2710814760539578	0.5192152383943780	0.6028972845968781
0.4543505520480649	0.3543558133901839	0.5928667024455211

Li₂S₄@Goldene

Au

1.0000000000000000		
13.5388193129999994	0.0000000000000000	0.0000000000000000
-6.7694112178000001	11.7249605608999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.8669948578000017

Au	S	Li
25	4	2

Direct

0.2058178026381666	0.2163504226541911	0.4982176283408693
0.1928803165098523	0.4006756959070306	0.5536156983018733
0.1983217424231520	0.6006464709844175	0.5091323046390214
0.1987047142779699	0.8037899049698694	0.5088311325076764
0.2006480991138086	0.0067643786797638	0.5071436097595416
0.3989388423517898	0.2055393489615241	0.4925282576881287
0.4035491809576982	0.4057436788177648	0.4515709625909685
0.3918658030540671	0.5910820019315712	0.4959294655381948

0.3976686369839249	0.7990037886107463	0.5085145447949042
0.3990715453171228	0.0032232700233960	0.5090018994795582
0.5973380123556654	0.2027296753569871	0.5105618799235229
0.5955501874655942	0.4032387258627779	0.5057249117015534
0.5951631385957915	0.6002487130034776	0.4987464107537988
0.5961911924603174	0.7997097907447964	0.5032091145559729
0.5975657785384436	0.0008091331001929	0.5095028921897343
0.7978783995095617	0.2026415007057359	0.5091280587473732
0.7977988008924692	0.4032438172868336	0.5092246221913554
0.7975518750181246	0.6036571530811836	0.5105860866307691
0.7986480491748851	0.8035777673349581	0.5099192455376205
0.7991942986059196	0.0032673543384734	0.5086507189341580
0.0019407597890736	0.2067339513374201	0.5080099511970345
0.9996066500759142	0.4029751201394052	0.5089423144081420
0.9982723082472551	0.6033729310868005	0.5092825290857308
0.9993325548180494	0.8055758467470002	0.5109148128587438
0.0026092816713744	0.0082430316153508	0.5103210438469118
0.2382401037906022	0.2978523958684782	0.7115916548246530
0.2985807806069360	0.2005634515574705	0.6642879029237889
0.4744336895613672	0.2969578291789302	0.6629141043452015
0.3010174394040432	0.4496346346210482	0.6560983131059823
0.4471347534453870	0.4347353365527218	0.7178934934697413
0.3925181232443358	0.3674678493832859	0.5781805366149375

Li₂S₆@Goldene

Au

1.0000000000000000

13.5388193129999994	0.0000000000000000	0.0000000000000000
-6.7694112178000001	11.7249605608999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.8669948578000017

Au	S	Li
25	6	2

Direct

0.1995339390971311	0.1954495510965151	0.4918879988510280
0.2016115413486441	0.3953433695009482	0.4966573513052095
0.1985505850489942	0.5950475935194128	0.5057571828167184
0.1974978483845700	0.7957656851338264	0.5075169531025996
0.1969173642213243	0.9963120919839679	0.5086769805842156
0.3960997146163063	0.1960051056250065	0.5381599058706429
0.3981903418734226	0.3898460541305012	0.4642632103505164
0.3983582571055388	0.5950905553125289	0.4887575388963055
0.3972067401915991	0.7953464184025306	0.5058375270105040
0.3964766673782975	0.9969795015415325	0.5075753877206151
0.5950042320238355	0.1955375328367269	0.5098045953094239
0.5932675994072453	0.3937143647596361	0.5040325345403126
0.5939404885872687	0.5926953993158868	0.5016748390246379
0.5970647804666580	0.7955681098472105	0.5086751441198615
0.5970008888890863	0.9965545989095029	0.5089030092740441
0.7979419812485548	0.1971678765813462	0.5087484762816823
0.7958443251303683	0.3952089003712752	0.5116962466618327
0.7951940772434805	0.5945703598449972	0.5109992899933306
0.7957719678299415	0.7949760493741247	0.5143073540120086
0.7976774469683664	0.9965958769353824	0.5095117220425184
0.9984822558764784	0.1972851334757943	0.5004731073153409

0.9994821211087428	0.3970587091874204	0.5085967789118506
0.9969798254414269	0.5952194464365621	0.5115920502157543
0.9961446381092642	0.7949025715467117	0.5118202259900891
0.9977459400137355	0.9969391154568759	0.5086222235430683
0.4529762232886915	0.6383287811876645	0.6621316702918872
0.5489872363281634	0.5977547917540452	0.7240582654478880
0.6058168210107382	0.4990639536875602	0.6671824181012850
0.5078415356982502	0.3330707613446971	0.6982733640761263
0.3556024095395661	0.2602662524726633	0.6455529667152236
0.2895758008998735	0.5019984264630634	0.6577692447054576
0.4108760458960669	0.4537694464372134	0.5875594731683818
0.3594057639278141	0.4026747286773989	0.7239706483723696

Li₂S₈@Goldene

Au

1.0000000000000000		
13.5388193129999994	0.0000000000000000	0.0000000000000000
-6.7694112178000001	11.7249605608999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.8669948578000017

Au	S	Li
25	8	2

Direct

0.2125674683738754	0.2141742771311153	0.4976457747042659
0.2116745530376696	0.4124689313914968	0.5004178935191869
0.2083640140186802	0.6106487321509003	0.5106339579658619
0.2076895542376458	0.8109146402046359	0.5107296091771055
0.2076579233802032	0.0102771903025303	0.5017034202564801

0.4088099652464928	0.2103939237762086	0.4805655704470785
0.4105250881633623	0.4166857180705737	0.4654170659324015
0.4104384096024608	0.6125246332978354	0.4884352859931902
0.4077586818993757	0.8097943886431794	0.5105418763208110
0.4072208205407482	0.0108784153874862	0.5069041639099976
0.6063247012859512	0.2101993917585353	0.5099005168210563
0.6052597823359837	0.4113322385215124	0.4961831851402612
0.6054749470917441	0.6069417353090113	0.5385702199085355
0.6068495681360166	0.8093797163378457	0.5080209170417488
0.6078668717080874	0.0111514790131041	0.5137024334193667
0.8085560198773992	0.2115355008367983	0.5194717154107222
0.8056230040923659	0.4102189770198527	0.5158093226828782
0.8052087648922455	0.6094670584629179	0.5072924504141914
0.8047011902605068	0.8080660613419423	0.5069158035452772
0.8081263405926408	0.0103150726989083	0.5150819207428012
0.0103735411149129	0.2121255868728079	0.5155636761779798
0.0099208341496084	0.4111058341961943	0.5181535836517013
0.0071149000333195	0.6100757983077782	0.5143669471681565
0.0058948164834402	0.8093972382333323	0.5087323260555292
0.0086964468172903	0.0115541708069158	0.5087643834600456
0.2446997199999114	0.1851577731543206	0.6437071443643295
0.2155377827837560	0.2360666986517590	0.7476175481269109
0.1675781303879186	0.3539698132086932	0.7289158666343647
0.3082634727392788	0.5182871207299440	0.7426356078707156
0.3834514719270322	0.5835425459891496	0.6524475716748988
0.5075317288889029	0.5344665445833178	0.6454339529080696
0.5210553236974147	0.2742532649859935	0.6615748953610218

0.3611856986502864	0.1343676119112299	0.6586389820026147
0.4253922987009103	0.3653661823980983	0.7182081296840921
0.4256011690726103	0.3461958468713353	0.5849320108306643

S₈@Goldene

Au

1.0000000000000000		
13.5388193129999994	0.0000000000000000	0.0000000000000000
-6.7694112178000001	11.7249605608999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.8669948578000017

Au S

25 8

Direct

0.1999897546953175	0.1999938444810562	0.4900719534639444
0.1987545039340289	0.3997398285736972	0.4868974939022141
0.1994964469414917	0.6001059360556538	0.4991655270959642
0.1993360293951911	0.8003185229139802	0.5044377569186055
0.1998674507982117	0.0000589267215753	0.5000962157920740
0.3995001681420831	0.2000527304466429	0.4903469895881739
0.3994619050278823	0.4010574223277177	0.4843439070403738
0.3999988123159979	0.6007425846167125	0.4826088470455586
0.3991915801611688	0.7994744518167022	0.5001013681828932
0.3995778687120803	0.0005731944334092	0.5041911649209840
0.5992880547798628	0.1995349496044919	0.5000947807167647
0.5999540572523357	0.4001644933253590	0.4900843199803576
0.6000420630884008	0.6000124370141491	0.4823618461720957
0.5991455250431870	0.7990384413679282	0.4993870071836574

0.5991605334512242	0.9990064464360031	0.5046009343312896
0.7994905547454363	0.1983992612812809	0.5063035107858054
0.7986829365025722	0.3983372840805078	0.5025617824748583
0.7992191998674668	0.5993745922213002	0.4999329302112333
0.7992932888702807	0.7992442146312125	0.5000202429276731
0.7992741363671456	0.9983440775356046	0.5060290047226486
0.0000012365294837	0.1998824983541438	0.5002263087584231
0.0001070824472634	0.3993156618216150	0.5042040797909136
0.9990305705213716	0.5986171341880019	0.5045570646326560
0.9987128091096248	0.7991938332077878	0.5044554344448621
0.0000206677296873	0.0000689582574547	0.5000721529051777
0.3149696751653459	0.5415315850626490	0.6420716708454078
0.4719472212869380	0.6322752752487875	0.6879762163627489
0.5903026347181126	0.6053639368358471	0.6379483229627767
0.6080406594163005	0.4810858734709208	0.6874997069482320
0.5094166720081550	0.3251400959474954	0.6415643622770641
0.3523355896957394	0.2340264868984469	0.6878242322437585
0.2332873843463212	0.2610738225602415	0.6391265083433533
0.2164365073944004	0.3862946336098282	0.6886615598616331