

Electronic Supplementary Information

Structure and property exploration of two-dimensional, bulk, and cluster lithium sulfide using IM²ODE method

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S1. Atomic Coordinates of 2D Li₂S

S2. Atomic Coordinates of 3D Li₂S

S3. Atomic Coordinates of (Li₂S)_n clusters

S1. Atomic Coordinates of 2D Li₂S

Double-layer hexagonal structure

1.0000000000000000

3.9735300540999998	0.0000000000000000	0.0000000000000000
-1.9867650269999999	3.4411779695000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.2642822265999989

Li S

4 2

Direct

0.6666666870000029	0.3333333429999996	0.5322997122371408
0.3333333429999996	0.6666666870000029	0.4677002877628592
0.0000000000000000	0.0000000000000000	0.5954738478677918
0.0000000000000000	0.0000000000000000	0.4045261821322036
0.3333333429999996	0.6666666870000029	0.5685870039829538
0.6666666870000029	0.3333333429999996	0.4314129670170472

Single-layer hexagonal structure

1.0000000000000000

3.9316999911999999	0.0000000000000000	0.0000000000000000
-1.9658499956000000	3.4049520725000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	11.9525995255000002

Li S

2 1

Direct

0.3333333730000021	0.6666666870000029	0.5609500409999981
0.6666666269999979	0.3333333129999971	0.4390499889999973
0.0000000000000000	0.0000000000000000	0.5000000000000000

S2. Atomic Coordinates of 3D Li₂S

Fm $\bar{3}$ m- Li₂S

1.0000000000000000

5.7147959999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7176049999999998	-0.0000040000000000
0.0000000000000000	0.0000000000000000	5.7160299999999999

Li S

8 4

Direct

0.2500229999999998	0.7500420000000005	0.2500110000000006
0.7500229999999998	0.7499559999999974	0.7500130000000027
0.7500229999999998	0.2499570000000020	0.7499869999999973
0.2500229999999998	0.2500410000000031	0.2499880000000019
0.7499770000000012	0.2500410000000031	0.2499880000000019
0.2499770000000012	0.2499570000000020	0.7499869999999973
0.2499770000000012	0.7499559999999974	0.7500130000000027
0.7499770000000012	0.7500420000000005	0.2500110000000006
0.0000000000000000	0.9999960000000030	0.9996420000000015
0.0000000000000000	0.4999979999999979	0.5003590000000031
0.5000000000000000	0.5000080000000011	0.0003590000000031
0.5000000000000000	0.0000059999999991	0.4996399999999994

Pnma- Li₂S

1.0000000000000000

6.2965748469063945	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.8108583105460978	0.0000000000000000
0.0000000000000000	0.0000000000000000	7.2353406189558891

Li S

8 4

Direct

0.4788890643672981	0.2500000000000000	0.6654249923633647
0.0211109356327019	0.7500000000000000	0.1654249923633647
0.5211109356327019	0.7500000000000000	0.3345750076366352
0.9788890643672981	0.2500000000000000	0.8345750076366353
0.8577458222096654	0.2500000000000000	0.4287157560993083
0.6422541777903346	0.7500000000000000	0.9287157560993083
0.1422541777903346	0.7500000000000000	0.5712842439006917
0.3577458222096654	0.2500000000000000	0.0712842439006917
0.2456112005986677	0.2500000000000000	0.3906139244534804
0.2543887994013323	0.7500000000000000	0.8906139244534804
0.7543887994013323	0.7500000000000000	0.6093860755465196
0.7456112005986677	0.2500000000000000	0.1093860755465196

P6₃/mmc- Li₂S

1.0000000000000000

3.9406696216941870	0.0000000000000000	-0.0000000000000000
-1.9703348108470935	3.4127202154041267	0.0000000000000000
0.0000000000000000	0.0000000000000000	7.0860516454135549

Li S

4 2

Direct

0.3333330000000032	0.6666669999999968	0.5917880376474784
0.3333330000000032	0.6666669999999968	0.9082119623525216
0.6666669999999968	0.3333330000000032	0.4082119623525215
0.6666669999999968	0.3333330000000032	0.0917880376474785
0.3333330000000032	0.6666669999999968	0.2500000000000000
0.6666669999999968	0.3333330000000032	0.7500000000000000

P6₃mc

1.0000000000000000

3.9778925499822688	-0.0000000000000653	-0.0000000000000000
-1.9889462749412476	3.4449560018069096	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.7912492953888508

Li S

4 2

Direct

0.0000000000000000	-0.0000000000000000	0.2077051418209083
0.0000000000000000	0.0000000000000000	0.7077051568209060
0.3333333429999996	0.6666666870000029	0.9469165615453281
0.6666666269999979	0.3333333129999971	0.4469165615453281
0.3333333429999996	0.6666666870000029	0.3177382966337584
0.6666666269999979	0.3333333129999971	0.8177382966337584

S3. Atomic Coordinates of $(\text{Li}_2\text{S})_n$ ($n=1-12$) clusters

$n=1$: Li_2S

```
1.0000000000000000
15.0000000000000000  0.0000000000000000  0.0000000000000000
 0.0000000000000000  15.0000000000000000  0.0000000000000000
0.0000000000000000  0.0000000000000000  15.0000000000000000

  Li  S
    2   1

  Direct

0.56335700000000034  0.55061200000000010  0.54419000000000004
0.44143700000000005  0.39560900000000003  0.40349799999999990
0.49166799999999971  0.52266999999999980  0.42853900000000007
```

$n=2$: $(\text{Li}_2\text{S})_2$

```
1.0000000000000000
 15.0000000000000000  0.0000000000000000  0.0000000000000000
 0.0000000000000000  15.0000000000000000  0.0000000000000000
 0.0000000000000000  0.0000000000000000  15.0000000000000000

  Li  S
    4   2

  Direct

0.53209999999999998  0.43454100000000030  0.53022500000000015
0.51884700000000009  0.60212500000000009  0.54350300000000012
0.37974400000000023  0.50604400000000028  0.54582599999999981
0.46775800000000034  0.53235699999999975  0.27548699999999983
0.48448799999999989  0.50600699999999968  0.65214900000000014
0.46856600000000027  0.52308099999999977  0.41658400000000003
```

$n=3$: $(\text{Li}_2\text{S})_3$

```
1.0000000000000000
```

15.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

Li S

6 3

Direct

0.4641980000000032	0.5151189999999986	0.4227089999999976
0.4578950000000006	0.5205229999999972	0.5817010000000025
0.6965300000000028	0.3401879999999977	0.5307299999999984
0.4422199999999989	0.3579379999999972	0.5067960000000014
0.6110040000000012	0.5753070000000022	0.5062259999999981
0.3419600000000003	0.6102679999999978	0.4939910000000012
0.3365670000000023	0.4592150000000004	0.4988939999999999
0.4870949999999965	0.6527870000000036	0.4985879999999980
0.5830819999999974	0.4231320000000025	0.5117710000000031

n=4:(Li₂S)₄

1.0000000000000000

15.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

Li S

8 4

Direct

0.4894219999999976	0.5098550000000017	0.5091589999999968
0.5555719999999980	0.4648480000000035	0.6644649999999999
0.4431179999999983	0.6391640000000010	0.5947919999999982
0.6322339999999969	0.4613670000000027	0.5066720000000018
0.6052940000000007	0.6250720000000030	0.4481019999999987
0.3675100000000029	0.4177930000000032	0.5628659999999996

0.517099999999992	0.368318999999996	0.4116020000000020
0.4111639999999994	0.5552089999999978	0.3748549999999966
0.5598760000000027	0.5063869999999966	0.3635670000000033
0.5127590000000026	0.3591290000000029	0.5634780000000035
0.3431950000000015	0.5592850000000027	0.5113429999999966
0.5938179999999988	0.5960329999999985	0.5971529999999987

n=5:(Li₂S)₅

1.000000000000000

15.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	15.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	15.000000000000000

Li S

10 5

Direct

0.5148530000000022	0.4733450000000019	0.4636390000000006
0.3098659999999995	0.5142349999999993	0.6149610000000010
0.3879179999999991	0.5787779999999998	0.4792890000000014
0.4814259999999990	0.3738090000000014	0.5960419999999971
0.4670020000000008	0.7211759999999998	0.5271329999999992
0.6436410000000024	0.5739769999999993	0.5047899999999998
0.4271260000000012	0.3525210000000030	0.3842050000000015
0.5619399999999999	0.5296659999999989	0.3100340000000017
0.5034429999999972	0.5613389999999967	0.6345170000000024
0.6497469999999979	0.3697080000000028	0.4711550000000031
0.5699850000000026	0.3827119999999979	0.3447529999999972
0.3778470000000027	0.6475739999999988	0.6228029999999976
0.6124780000000030	0.4541210000000007	0.5962079999999972
0.5306780000000018	0.6318259999999967	0.4203100000000006
0.3656799999999976	0.4196120000000008	0.5080549999999988

n=6:(Li₂S)₆

1.0000000000000000

15.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

Li S

12 6

Direct

0.4941400893198049	0.5273393823730120	0.5849924663038997
0.3622051027878528	0.4529219664325890	0.4756472233611097
0.3725819073074836	0.6385960444150842	0.6313071930455940
0.5054158135313046	0.5116453522740146	0.4043805337433520
0.6126614467614282	0.4151135309889024	0.5202458391566956
0.6010189546008630	0.5889503156515921	0.7014589402171829
0.5210790059842162	0.4233056363179278	0.2525354793942977
0.3481541347351582	0.5791737547672775	0.3451197408549264
0.7041395644611502	0.5279607014184229	0.4229200094091841
0.4371206519560173	0.4234607841495537	0.7013490415137486
0.5462806071021206	0.6730889669356087	0.5098642529834108
0.4871272230137266	0.3428806963623636	0.4080100371891879
0.6511550064281754	0.5738680041182501	0.5570422141556969
0.4556096728082559	0.5700558413650202	0.7348361322745123
0.6273400280152738	0.4156724845823902	0.3599260093822162
0.4044374906895519	0.6232718625882628	0.4804176480863876
0.3859974592361283	0.4366369196790688	0.3195163109335528
0.4663008412614963	0.3732147555806620	0.5597039279950389

n=7:(Li₂S)₇

1.0000000000000000

15.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	15.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	15.000000000000000
Li	S	
14	7	
Direct		
0.623838999999967	0.514310000000018	0.3531570000000031
0.5109720000000024	0.3628140000000002	0.4522440000000003
0.526688999999975	0.637594999999975	0.687986999999997
0.725394999999989	0.415368999999983	0.4963460000000026
0.4338580000000007	0.538522999999979	0.4465450000000004
0.6376240000000024	0.3874380000000031	0.7049710000000005
0.3421900000000022	0.6894070000000028	0.4546479999999988
0.412388999999975	0.525576999999984	0.6257900000000021
0.5963100000000026	0.6666700000000034	0.4911549999999991
0.480604999999971	0.3656530000000018	0.6324650000000034
0.2559070000000006	0.502448999999986	0.493758999999972
0.3981410000000025	0.5539830000000023	0.267181999999983
0.350687999999981	0.422601999999977	0.372903999999983
0.5971990000000034	0.495353999999990	0.574911999999976
0.6201730000000012	0.330978999999992	0.564256999999978
0.494393999999998	0.449278999999971	0.3176750000000013
0.7008310000000009	0.5627300000000020	0.472929999999981
0.5298280000000020	0.492230999999968	0.724559999999968
0.2871790000000018	0.5782420000000030	0.3673620000000000
0.3678200000000018	0.407578999999984	0.5312520000000021
0.4560370000000020	0.664068999999978	0.552821999999990

n=8:(Li₂S)₈

1.000000000000000

15.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000
Li	S	
16	8	
Direct		
0.4525035659637136	0.4370660523545238	0.5226988164031496
0.4179093927394607	0.4063381152883628	0.3582903041960486
0.5658345601835707	0.3256785863837972	0.4636620532776243
0.5086898360750278	0.4906280404653927	0.6775261747443040
0.5483790363186722	0.5211344518037376	0.3588496433867027
0.6766192429188043	0.4936947280546637	0.5453282258715569
0.2935191484860875	0.3523759482364133	0.5440931872574872
0.3636744341300374	0.5625279219713885	0.7402152036013366
0.5337636688850708	0.6323075119657720	0.5074242260205991
0.4808016565589587	0.2452636271342886	0.3374568762285707
0.3655108808100861	0.5728353532225453	0.5678610439379657
0.6528622768726396	0.7245917429429602	0.4099686733068746
0.4556703709901616	0.3116406908821074	0.6219816680903539
0.4232876225007114	0.7010690683911432	0.3899065460991711
0.6956557070989557	0.4451138962858873	0.3412832690132913
0.4909179880949530	0.7766871061413529	0.5986610214584976
0.5683753193797898	0.3670225313972573	0.3098231547605181
0.5911577401017412	0.3858850966079773	0.6022467470871290
0.4071680770704674	0.5509149959668530	0.4188182243113214
0.3500865457041130	0.4350106567098597	0.6573412246685711
0.5253622127989793	0.7885615971060728	0.4540200415121683
0.4036665601151816	0.2847768328112548	0.4644163674218295
0.4685887292868574	0.6425487351923974	0.6662005360000466
0.6824664269159748	0.5761927126839834	0.4195627713448800

n=9:(Li₂S)₉

1.0000000000000000

15.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

Li S

18 9

Direct

0.4547725966013443	0.3512331720926729	0.4886591165713999
0.6163074282013261	0.6755024356640440	0.5414314794081397
0.3563868654499842	0.7534792804281959	0.5521211932512189
0.7444185751565721	0.5915812266997779	0.4048006301918118
0.4678808744165010	0.5940303335755962	0.3429018685219396
0.4022900049045260	0.3059445103737803	0.3282708436814924
0.5160574833157989	0.4158054776336664	0.6383179536936503
0.6204482005238897	0.3404540066402106	0.4128436217885910
0.4557106850836793	0.5914381196884344	0.5732299082781697
0.4890594400409446	0.7339653267787111	0.4482705770208538
0.4852321317349793	0.1892550170537868	0.5215166398373968
0.6950798797236212	0.4114476171435078	0.5613223151936590
0.2733495670836269	0.5674874493351966	0.5477521284775727
0.2964419196236392	0.3169389871940492	0.5497086269380604
0.3700604773082763	0.4896092011705832	0.4346698482015380
0.6276903357042694	0.5006388595620694	0.3086914135217719
0.5951346446593403	0.5115010767401211	0.4663585230434604
0.5585697472873530	0.6584344230068114	0.7049904128743463
0.6108831716854962	0.5411619387437065	0.6240318517351828
0.4940159861876589	0.7540281268560571	0.6073026921014177
0.3581778174894160	0.2279159701032419	0.4472135345320408

0.6071366213860973	0.6558735205428151	0.3819646312412217
0.5842473370039719	0.2977788507034757	0.5593780254385071
0.4869481363086323	0.4349397069658194	0.3459430061363112
0.3468078605517966	0.6484492192854361	0.4397232587310998
0.3599085164000247	0.4516187804325257	0.5893907055676143
0.7340766961672477	0.4436413655857099	0.4077171940215236

n=10:(Li₂S)₁₀

1.0000000000000000

15.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

Li S

20 10

Direct

0.5093015421443750	0.6875107552265634	0.3566363208884820
0.5285762550765726	0.5618945466561360	0.4792902404430869
0.3410499026897412	0.6262173737208246	0.5654879666122142
0.4099011344186128	0.3775802511650332	0.7050012442772710
0.5761978424555526	0.6270339567482653	0.2183352548680020
0.2376605131203772	0.3802338637066331	0.4810676457352914
0.6823620372791043	0.2792995897471188	0.5948170091245252
0.3449145596538142	0.6489079585230560	0.3883327302702860
0.5961848916335680	0.4214841320017638	0.5479167683020170
0.7307768169328035	0.5384281066679265	0.4821778410892026
0.6542243709428932	0.4008422253944091	0.3918820159812601
0.2644893465854430	0.4708173196315560	0.6324667362713760
0.3669006903491292	0.4843141524746982	0.3520359345553093
0.4583558913221264	0.2967564533978438	0.5539204337843896
0.6184976358977207	0.6927758241888118	0.4977949618832925

0.4978788358877607	0.6508743667954695	0.6368566312085150
0.5422342212460639	0.4926287663103165	0.7005225660580967
0.5297417812656858	0.5065888140451150	0.3176609835682068
0.3890344875222193	0.4536462295369807	0.5373569114085615
0.7168295908702917	0.4493349891045070	0.6468016647942643
0.3111975995983139	0.3231843119181833	0.5983950905155695
0.6489055061493667	0.6021109282165901	0.3572525122894562
0.5678886441981318	0.3388314737895678	0.6763423950408723
0.4967855600727926	0.4049975692355633	0.4267787146020515
0.2647559578608683	0.5306695543393135	0.4646651024183835
0.6391038180587308	0.5807719071621783	0.6089924218126697
0.4272819258026432	0.6014265793617057	0.2561764556061343
0.7506107340173586	0.3836961414073836	0.5080744807685268
0.4569901980206603	0.7100358458526015	0.4964145333307039
0.3953467089272770	0.5407320136738911	0.6861204324919793

n=11:(Li₂S)₁₁

1.0000000000000000

15.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

Li S

22 11

Direct

0.5445186549561026	0.4764626303547709	0.3793506976553024
0.6580254244033472	0.4083934007975843	0.6869193084099806
0.4818569300962930	0.3679441183045691	0.2760002322987346
0.6352355682939779	0.6601923481061976	0.5981207637034047
0.2091723454805319	0.4494785424668119	0.5587899910966566
0.3509320356805306	0.6369759872594154	0.3592323893012017

0.5522705572043314	0.5743928156705660	0.7317774789402718
0.7057220482986333	0.4515590547070501	0.3941617447975160
0.4926241653320093	0.8019236561258182	0.5390905224473310
0.5737176028408916	0.5023935349599998	0.2052810191092508
0.3253947045141082	0.2548042027647199	0.4910896961283531
0.3776806787768727	0.4080715397672814	0.5530767729480233
0.4828226809115921	0.6306534984831770	0.4950719641033794
0.3641320561548019	0.4597289031170547	0.3854721419743321
0.3595840756896020	0.3420256432224819	0.7124369577330252
0.7495179689441657	0.5082326812377080	0.5610210777351013
0.6110948941389063	0.3032834000723302	0.4009204298149415
0.3957920134627032	0.5583715258810916	0.6407771991377097
0.5904360824838062	0.4952925810257970	0.5704706333135035
0.3455257425715679	0.7044880869319333	0.5365968168790595
0.5356307455622573	0.3300233066245455	0.5614362800871133
0.5296799712705114	0.6642489642291723	0.3395822895316764
0.6980284277455754	0.5570437393056974	0.6930037321212565
0.4781588508427843	0.6906307824155961	0.6441209597644166
0.4399995113743337	0.5366853450188572	0.2726534346726951
0.6315590277122473	0.5915897291188964	0.4482191860450562
0.6840617661787111	0.3638502209388392	0.5310860577688578
0.6362971804125185	0.3852391664389104	0.2729800098432539
0.4259222047037386	0.7593583850226150	0.4124027672892023
0.3117632619620856	0.5520661755935444	0.5033227901251391
0.2560301843911802	0.3165451825364156	0.6080849191267403
0.4829841961863182	0.4285300874627426	0.6782187957142571
0.4459294414229596	0.3276547640378151	0.4271269403832600

n=12:(Li₂S)₁₂

1.0000000000000000

15.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

Li S

24 12

Direct

0.6043392649359747	0.4415088360441095	0.4358706793111218
0.3238130084762043	0.6367372172080199	0.4215987864130465
0.4638084682249446	0.4768671462246051	0.2593267001252056
0.2760770934629504	0.3427293991184505	0.4416417622412492
0.5421195624681577	0.5218385006483878	0.7171555898941301
0.7065240009063821	0.6375917343419628	0.5221539687849360
0.7225749041857940	0.3763655174155675	0.3655679545179605
0.6848986717124128	0.5058406936171478	0.6302788586368250
0.5280995854299105	0.6189476842393271	0.5104826235999009
0.3129610773843117	0.6037761398289485	0.5881409138916327
0.5355830250615169	0.2870577476518423	0.5781189245156213
0.4489848166118296	0.2607431427419000	0.4316329740392661
0.4459332451654121	0.3815617910336367	0.6855090616818053
0.3067373137782582	0.4933109189316476	0.3274270163605106
0.3349854474942686	0.5382335274153626	0.8559068707879982
0.5571367408984169	0.6140304848013730	0.2886075280911127
0.4661408641458276	0.7269558474379526	0.3831273488480942
0.5652683275510123	0.7644753557709769	0.5436234234237447
0.2922337960187621	0.4287773445859906	0.6102397442263576
0.4573773559061355	0.6695230341590200	0.6686957078252205
0.6951427070379047	0.3500316739136502	0.5553504655005418
0.5458869506847479	0.3328046617365013	0.3054528978924098
0.7069733697991122	0.5682124900526775	0.3622277094374597
0.4000902338617999	0.4307949984764659	0.4650741142623325

0.6101580929525164	0.6464729478485955	0.6492089523483435
0.2565110998308734	0.5038893556802067	0.4793461030897504
0.4042341691394334	0.7201195698296283	0.5319355263121691
0.3763176087018529	0.3048965703338890	0.5666897499469642
0.6012336525992490	0.3839107690980211	0.6808083605700334
0.3771303938532056	0.5288412237605840	0.7179247925513030
0.6097243779082413	0.2797438214041867	0.4390767264774813
0.6212098368516087	0.4681132718116704	0.2754771079212365
0.4000789750686946	0.6162496402485776	0.2886688125739392
0.6219971340461470	0.6994686771313735	0.4054499086197427
0.7502381259156671	0.4848130778632853	0.4885365808275916
0.3853437019304526	0.3542141875944699	0.3215177544529524