

Interface-Protected Subsurface Vacancies for Room-Temperature Sub-ppm SO₂ and NO₂ Detection in MoS₂, MoSe₂, and MoTe₂ via Electron Irradiation

Maciej J. Szary^{a,*}

^a*Institute of Physics, Poznan University of Technology, ul. Piotrowo 3, 61-138 Poznan, Poland*

Supplementary Information

Contents

1	Optimized atomic structures of defective TMDs	3
1.1	v _S -MoS ₂	3
1.2	v _{Se} -MoSe ₂	4
1.3	v _{Te} -MoTe ₂	5
2	Optimized atomic structures of N₂ adsorption on defective TMDs	6
2.1	v _S -MoS ₂	6
2.2	v _{Se} -MoSe ₂	7
2.3	v _{Te} -MoTe ₂	8
3	Optimized atomic structures of O₂ adsorption on defective TMDs	9
3.1	v _S -MoS ₂	9
3.2	v _{Se} -MoSe ₂	10
3.3	v _{Te} -MoTe ₂	11
4	Optimized atomic structures of CH₄ adsorption on defective TMDs	12
4.1	v _S -MoS ₂	12
4.2	v _{Se} -MoSe ₂	13
4.3	v _{Te} -MoTe ₂	14
5	Optimized atomic structures of NH₃ adsorption on defective TMDs	15
5.1	v _S -MoS ₂	15
5.2	v _{Se} -MoSe ₂	16
5.3	v _{Te} -MoTe ₂	17
6	Optimized atomic structures of H₂S adsorption on defective TMDs	18
6.1	v _S -MoS ₂	18
6.2	v _{Se} -MoSe ₂	19
6.3	v _{Te} -MoTe ₂	20
7	Optimized atomic structures of CO₂ adsorption on defective TMDs	21
7.1	v _S -MoS ₂	21
7.2	v _{Se} -MoSe ₂	22
7.3	v _{Te} -MoTe ₂	23

*Corresponding author
Email address: maciej.szary@put.poznan.pl (Maciej J. Szary)

8	Optimized atomic structures of SO₂ adsorption on defective TMDs	24
8.1	v _S -MoS ₂	24
8.2	v _{Se} -MoSe ₂	25
8.3	v _{Te} -MoTe ₂	26
9	Optimized atomic structures of NO₂ adsorption on defective TMDs	27
9.1	v _S -MoS ₂	27
9.2	v _{Se} -MoSe ₂	28
9.3	v _{Te} -MoTe ₂	29

1. Optimized atomic structures of defective TMDs

1.1. v_S - MoS_2

Mo	-0.0062591479	1.8194570429	3.0592821321
Mo	4.7072583291	10.0362284826	3.1396501826
Mo	-4.7654332512	10.0625882581	3.0592823332
Mo	-1.5795882299	4.5712215067	3.0714643891
Mo	3.1689997698	7.3718860915	3.1396502809
Mo	-1.5725664020	10.0625882239	3.0592822475
Mo	1.6307409344	10.0362286324	3.1396501528
Mo	1.5901742114	4.5845609604	3.0592821573
Mo	-3.1689998074	7.3241630422	3.0714645298
Mo	3.1690000677	1.8296226564	3.0455749993
Mo	9.5069997083	1.7975888816	3.0983358715
Mo	6.3102577320	7.3345082120	3.0983361508
Mo	0.0277423084	7.3345085536	3.0983360868
Mo	6.3442593753	1.8194568394	3.0592821279
Mo	7.9175884233	4.5712213903	3.0714644063
Mo	4.7478257810	4.5845608929	3.0592821812
S	6.3341856213	9.1709601083	4.6651284388
S	1.5878058551	0.9167197998	4.6146779910
S	11.1093774683	0.9000851708	4.6651282755
S	6.2492703144	9.1447197235	1.5318695841
S	1.5744789637	0.9090253133	1.4852690524
S	11.0441950918	0.8396663179	1.5318693510
S	7.9208115708	6.4046549062	4.6388682724
S	3.1690000836	3.6554283272	4.6146779143
S	7.9046222607	0.9000852641	4.6651283214
S	7.9027490921	6.4150834993	1.5215004629
S	3.1690001364	3.6708171650	1.4852691528
S	7.9698047677	0.8396667291	1.5318690057
S	4.7501942374	0.9167198007	4.6146779603
S	4.7318079643	6.3955605303	4.6651284520
S	9.5070000633	3.6572957936	4.6388680763
S	4.7635212179	0.9090253557	1.4852690996
S	4.7120754707	6.4822194904	1.5318692863
S	9.5070001468	3.6364392068	1.5215002901
S	3.1690000833	9.1481148226	4.7189305428
S	-3.1689998221	9.1601753641	4.6251969698
S	0.0104450475	3.6532152662	4.6251969610
S	-3.1689997929	9.1430737040	1.4954869004
S	-0.0043653138	3.6617661985	1.4954866708
S	6.3275550235	3.6532151224	4.6251969729
S	6.3423652675	3.6617659571	1.4954867067
S	0.0038141280	9.1709599148	4.6651283142
S	-1.5828110758	6.4046551557	4.6388682690
S	1.6061916848	6.3955605975	4.6651282654
S	0.0887292771	9.1447194140	1.5318691496
S	-1.5647487314	6.4150835735	1.5215005391
S	1.6259243583	6.4822195167	1.5318692571

1.2. $v_{Se}-MoSe_2$

Se	1.6489745695	0.9520361378	5.2547869398
Se	11.5392798978	0.9325773468	5.3070185504
Se	6.5772751874	9.5270214595	5.3070182456
Se	0.0101815666	3.7953952824	5.2645559078
Se	3.2920015558	9.5031876659	5.4221980491
Se	-3.2920001757	9.5149429479	5.2645556727
Se	-1.6440651320	6.6533474021	5.2773213251
Se	1.6700025855	6.6461355917	5.3070184769
Se	0.0067243586	9.5270206595	5.3070179288
Se	4.9350254099	0.9520363150	5.2547868334
Se	9.8760003226	3.7990400701	5.2773203626
Se	4.9139977641	6.6461352875	5.3070189216
Se	8.2280655085	6.6533475250	5.2773209292
Se	8.2127205683	0.9325786041	5.3070187457
Se	3.2920001528	3.7978392263	5.2547870048
Se	6.5738184107	3.7953955267	5.2645559905
Mo	-0.0086543134	1.8880563828	3.5890330776
Mo	4.8572933005	10.4069087565	3.6878329233
Mo	-4.9532223474	10.4523000046	3.5890332153
Mo	-1.6398372869	4.7480355422	3.5990026470
Mo	3.2920007404	7.6957396679	3.6878356888
Mo	-1.6307784800	10.4523000494	3.5890332234
Mo	1.7267069227	10.4069095047	3.6878341163
Mo	1.6525673642	4.7653765648	3.5890334576
Mo	-3.2919996455	7.6096643773	3.5990027024
Mo	3.2920000373	1.9006372948	3.5734896733
Mo	9.8760006781	1.8614763283	3.6312967329
Mo	6.5500867926	7.6221296351	3.6312967924
Mo	0.0339129433	7.6221287291	3.6312966268
Mo	6.5926541602	1.8880571535	3.5890328964
Mo	8.2238375881	4.7480352869	3.5990026015
Mo	4.9314328206	4.7653767906	3.5890332574
Se	1.6334722053	0.9430858116	1.9029869662
Se	-0.0027157864	3.8028416690	1.9132311593
Se	6.4737879523	9.5045551814	1.9565349790
Se	-3.2920002108	9.5000502664	1.9132314295
Se	-1.6201763944	6.6671395980	1.9414459641
Se	1.7022905863	6.7469903578	1.9565366266
Se	4.8817099341	6.7469903701	1.9565359497
Se	0.1102112447	9.5045548972	1.9565359388
Se	3.2920001078	3.8157400217	1.9029872192
Se	4.9505277593	0.9430859390	1.9029869803
Se	8.2839204217	0.8541892209	1.9565346034
Se	11.4680797349	0.8541878949	1.9565343671
Se	9.8760003661	3.7714558708	1.9414468248
Se	8.2041768072	6.6671397385	1.9414463275
Se	6.5867158120	3.8028419825	1.9132308821

1.3. v_{Te} - $MoTe_2$

Mo	-0.0061275446	2.0566216690	3.8255341571
Mo	-1.7652053583	5.0703481323	3.8368624463
Mo	1.7241501585	5.0534391152	3.8256407677
Mo	-3.5399750708	8.1440943662	3.8368261819
Mo	3.5184674868	8.1260561918	3.9222829937
Mo	3.5186272399	2.0198356496	3.8107448104
Mo	-0.0235312159	8.1252228033	3.8669609329
Mo	7.0431992478	2.0566645922	3.8256022514
Mo	5.3132573288	5.0536161388	3.8256431703
Te	1.7623596555	1.0058088188	5.6249618245
Te	1.7492474161	0.9982447740	2.0077029230
Te	3.5187604328	4.0477439666	5.6250738799
Te	3.5187730270	4.0630531668	2.0078101828
Te	5.2747984710	1.0055846772	5.6249271390
Te	5.2879700208	0.9980254638	2.0077839852
Te	5.2919623809	7.0736518017	5.6851758021
Te	8.7822082100	1.0284422578	5.6850380006
Te	5.2586435543	7.1691329331	2.0521545277
Te	-0.0096556566	4.0564983883	5.6662734117
Te	-0.0209113515	4.0631268582	1.9884909615
Te	7.0468931872	4.0564524434	5.6663419136
Te	7.0581657163	4.0630630996	1.9884566810
Te	1.7450978687	7.0734705776	5.6851340454
Te	1.7783504383	7.1688829208	2.0521916121
Te	-1.7925694023	7.1038208394	5.6602516008
Te	-1.7694527707	7.1171494892	2.0317605191
Mo	5.2885608400	11.1919841590	3.9221305501
Mo	-5.2699297845	11.1744693813	3.8255188166
Mo	1.7486200919	11.1919773018	3.9220723535
Mo	-1.8097036102	11.1742432605	3.8255655257
Te	7.0869246205	10.1827796261	5.6848698627
Te	6.9877790039	10.1637833110	2.0521554399
Te	-3.5398706972	10.1712809357	5.6662812157
Te	-3.5398479596	10.1582172037	1.9883464034
Te	3.5185134702	10.1700160339	5.7160262941
Te	-0.0497281079	10.1826459257	5.6851665115
Te	0.0496110770	10.1636994166	2.0520043685
Te	12.3059580320	0.9518612518	2.0520256864
Te	12.3719027017	1.0282483433	5.6849239679
Mo	10.5771139781	2.0346537612	3.8668137087
Te	10.5771576525	4.0772564840	5.6603287726
Te	10.5771731490	4.0507373426	2.0316159176
Mo	8.8024442448	5.0701288939	3.8368596991
Te	8.8296358593	7.1036165882	5.6602585903
Te	8.8065227838	7.1169534554	2.0317438011
Mo	7.0606697030	8.1251290522	3.8669119152

2. Optimized atomic structures of N₂ adsorption on defective TMDs

2.1. *v_S*-MoS₂

N	2.5884425057	9.1548890538	8.2832738295
N	3.6970602790	9.1516513439	8.3392397380
Mo	-0.0057834696	1.8195730430	3.0302420487
Mo	4.7086973365	10.0366318701	3.1074158198
Mo	-4.7648970032	10.0623791519	3.0300833521
Mo	-1.5792615771	4.5711493624	3.0423010452
Mo	3.1692604802	7.3705395716	3.1074451679
Mo	-1.5725604629	10.0623927305	3.0301605396
Mo	1.6297856936	10.0366392789	3.1076330364
Mo	1.5903399748	4.5841167053	3.0302514907
Mo	-3.1687080261	7.3240245497	3.0422210724
Mo	3.1692815960	1.8294050093	3.0156850506
Mo	9.5072652806	1.7969366484	3.0693339359
Mo	6.3100951145	7.3347254649	3.0692664500
Mo	0.0284706442	7.3347549075	3.0693721733
Mo	6.3443437555	1.8196092278	3.0303611402
Mo	7.9178754304	4.5711683820	3.0423003337
Mo	4.7482495133	4.5841310112	3.0302723966
S	6.3332729181	9.1715199975	4.6359518213
S	1.5882504292	0.9164999964	4.5852623627
S	11.1096431077	0.8983934219	4.6359167046
S	6.2513924217	9.1441165758	1.5016725351
S	1.5744036335	0.9086893668	1.4557297270
S	11.0450399026	0.8414001463	1.5018964346
S	7.9209877031	6.4047168587	4.6099002272
S	3.1692893386	3.6550084367	4.5853262555
S	7.9049144362	0.8984468877	4.6360710188
S	7.9024085735	6.4153194093	1.4925393074
S	3.1693115546	3.6710328457	1.4558085304
S	7.9694209441	0.8413668318	1.5020240148
S	4.7502635241	0.9165327889	4.5853480373
S	4.7308793511	6.3962669697	4.6358822034
S	9.5073075747	3.6571112127	4.6099284580
S	4.7642035183	0.9087086972	1.4558099469
S	4.7136444213	6.4806390606	1.5018663988
S	9.5073030233	3.6356440847	1.4926444190
S	3.1693563156	9.1479731823	4.6804576874
S	-3.1687582204	9.1597240711	4.5959557490
S	0.0105054789	3.6532117729	4.5960236299
S	-3.1686970386	9.1429652628	1.4660388304
S	-0.0039879103	3.6615901789	1.4661685997
S	6.3281107947	3.6533049819	4.5960744334
S	6.3425856810	3.6615865461	1.4662203665
S	0.0051781586	9.1715339184	4.6361260821
S	-1.5824217150	6.4046892489	4.6099449383
S	1.6076963657	6.3962218395	4.6359217488
S	0.0871516763	9.1441519613	1.5018020450
S	-1.5637718162	6.4153357202	1.4925897273
S	1.6248620513	6.4806671917	1.5018938735

2.2. $v_{Se}-MoSe_2$

N	1.9396535752	10.7661305566	9.2249056259
N	2.8131588234	11.1133111147	8.6330563051
Se	1.6799743676	0.8992047325	5.2597142051
Se	11.5678797201	0.8799353887	5.3137074111
Se	6.6083648960	9.4733633864	5.3135615857
Se	0.0437018946	3.7412106931	5.2719816589
Se	3.3241912306	9.4502227258	5.4237137364
Se	-3.2593014358	9.4614167783	5.2710484377
Se	-1.6109994875	6.5996480563	5.2840797894
Se	1.7017066441	6.5975241323	5.3150537863
Se	0.0394085471	9.4753615769	5.3141862209
Se	4.9656979736	0.9016082378	5.2596582928
Se	9.9083708747	3.7444593631	5.2823460803
Se	4.9465511355	6.5963088701	5.3131286817
Se	8.2601238092	6.5997602502	5.2822494977
Se	8.2445093244	0.8819706667	5.3092844472
Se	3.3251951609	3.7479334761	5.2602980615
Se	6.6068503696	3.7428751757	5.2693728240
Mo	0.0218457056	1.8346817398	3.5954512635
Mo	4.8897963069	10.3556570209	3.6930487097
Mo	-4.9209037008	10.3976962666	3.5956572675
Mo	-1.6058066532	4.6942514238	3.6062612082
Mo	3.3235103467	7.6435171848	3.6923673482
Mo	-1.5999278266	10.3998084239	3.5957030687
Mo	1.7575375657	10.3554634518	3.6924828474
Mo	1.6847316131	4.7156360765	3.5970869584
Mo	-3.2588313586	7.5558136731	3.6057248911
Mo	3.3224683628	1.8501114414	3.5779992079
Mo	9.9079246051	1.8088695078	3.6352002284
Mo	6.5823230485	7.5700435417	3.6368453131
Mo	0.0657195814	7.5706230331	3.6385272191
Mo	6.6233179164	1.8370081193	3.5932244310
Mo	8.2570106754	4.6949621439	3.6039588229
Mo	4.9646349623	4.7156999534	3.5949345856
Se	1.6632628494	0.8879625731	1.9093202003
Se	0.0321190676	3.7506005883	1.9210428174
Se	6.5063671394	9.4520143605	1.9627495430
Se	-3.2601733266	9.4444420535	1.9192398002
Se	-1.5864572814	6.6129835436	1.9489064362
Se	1.7323311481	6.6960933644	1.9631528479
Se	4.9143353507	6.6969608798	1.9617072889
Se	0.1399486232	9.4525208198	1.9633863455
Se	3.3236723856	3.7684910205	1.9093399942
Se	4.9809020781	0.8901089429	1.9088151493
Se	8.3139774727	0.8034238738	1.9610991263
Se	11.4998651344	0.8024570331	1.9613501998
Se	9.9107065566	3.7194692509	1.9467903254
Se	8.2373005834	6.6145515033	1.9475938681
Se	6.6186344228	3.7529434085	1.9182152723

2.3. ν_{Te} - $MoTe_2$

N	3.3455660838	11.9892081680	9.1505528816
N	4.1554304463	11.5420556618	9.7646332689
Mo	-0.0136667505	1.9983780158	3.7911632124
Mo	-1.7732814016	5.0121372094	3.8037140075
Mo	1.7167073448	4.9943770339	3.7929447627
Mo	-3.5483298459	8.0862972073	3.8044307799
Mo	3.5102560959	8.0678411654	3.8879829742
Mo	3.5101691685	1.9614698282	3.7771204324
Mo	-0.0326667642	8.0667046319	3.8349880505
Mo	7.0338248089	1.9988856373	3.7896678582
Mo	5.3037681637	4.9947107756	3.7924433498
Te	1.7538413833	0.9475781735	5.5918913960
Te	1.7411466657	0.9397073968	1.9734794877
Te	3.5105599015	3.9887354665	5.5926199554
Te	3.5101705512	4.0046029431	1.9740237530
Te	5.2670690509	0.9481363433	5.5914390074
Te	5.2787512409	0.9397344329	1.9729443536
Te	5.2829645784	7.0153916852	5.6517579794
Te	8.7719642497	0.9708741230	5.6490873563
Te	5.2503634400	7.1106632202	2.0201773473
Te	8.8391636339	0.8939855519	2.0173797573
Te	-0.0176850379	3.9973624473	5.6325386422
Te	-0.0285222079	4.0058707486	1.9549529031
Te	7.0382836825	3.9974589537	5.6318140057
Te	7.0492747619	4.0067700776	1.9540338640
Te	1.7369595676	7.0152604252	5.6520015427
Te	1.7692791717	7.1101922985	2.0205212761
Te	-1.8016145000	7.0447434794	5.6281090484
Te	-1.7778282781	7.0596136484	1.9994327092
Mo	5.2795230746	11.1332461839	3.8868410003
Mo	-5.2785112583	11.1167771312	3.7926653381
Mo	1.7400800515	11.1344985446	3.8872361102
Mo	-1.8186820500	11.1171082603	3.7926064030
Te	7.0765943296	10.1252920666	5.6514235640
Te	6.9804491342	10.1054766062	2.0194348530
Te	-3.5484839415	10.1134905722	5.6332519646
Te	-3.5484216389	10.1005906460	1.9555512379
Te	3.5095161845	10.1111807669	5.6797374018
Te	-0.0570623156	10.1256230105	5.6516673731
Te	0.0395449978	10.1055688149	2.0199878406
Te	12.2981678986	0.8942188726	2.0180444364
Te	12.3633344342	0.9696767284	5.6488787763
Mo	10.5681062640	1.9767784846	3.8322221555
Te	10.5684751555	4.0183282162	5.6267851042
Te	10.5688787372	3.9931801171	1.9982303152
Mo	8.7940168831	5.0124676765	3.8033382982
Te	8.8215195240	7.0448816378	5.6277846631
Te	8.7980854436	7.0599537157	1.9992812588
Mo	7.0528095057	8.0666462620	3.8346381582

3. Optimized atomic structures of O₂ adsorption on defective TMDs

3.1. *v_S*-MoS₂

O	2.5237704277	9.1514396152	8.1770362915
O	3.7517352169	9.1487505613	8.2129200055
Mo	-0.0056318379	1.8196165830	3.0350578244
Mo	4.7085811306	10.0366438697	3.1126638416
Mo	-4.7647618649	10.0625710697	3.0350247957
Mo	-1.5790679000	4.5712380496	3.0472721236
Mo	3.1694794771	7.3710020808	3.1128011884
Mo	-1.5722819141	10.0625936637	3.0351313344
Mo	1.6303618638	10.0366526201	3.1128759892
Mo	1.5906057758	4.5843458015	3.0351173450
Mo	-3.1684947683	7.3241517270	3.0472686194
Mo	3.1694821689	1.8295904699	3.0199730385
Mo	9.5074831498	1.7970996400	3.0742206614
Mo	6.3103527618	7.3347845118	3.0742497433
Mo	0.0286356735	7.3348002376	3.0743867435
Mo	6.3446059920	1.8196469429	3.0351646997
Mo	7.9181046735	4.5712525910	3.0472591020
Mo	4.7484053232	4.5843500434	3.0351092080
S	6.3334557865	9.1716010423	4.6408800573
S	1.5885878317	0.9168300745	4.5898138597
S	11.1098239861	0.8986255682	4.6408192478
S	6.2514259436	9.1442639189	1.5068284975
S	1.5742826265	0.9086134975	1.4603537866
S	11.0451527025	0.8413234995	1.5068904508
S	7.9211629031	6.4047775465	4.6148632727
S	3.1695057539	3.6550121693	4.5898688443
S	7.9051666431	0.8986899065	4.6409585821
S	7.9026970900	6.4154254779	1.4975310237
S	3.1695058606	3.6716027074	1.4604062706
S	7.9697447219	0.8412823918	1.5070169343
S	4.7503291552	0.9168836856	4.5898981787
S	4.7311854438	6.3963174569	4.6408664000
S	9.5075162435	3.6571190335	4.6148405054
S	4.7647251179	0.9086212302	1.4604367969
S	4.7137246698	6.4809907685	1.5069659399
S	9.5075197129	3.6358098481	1.4975428706
S	3.1695852210	9.1481601626	4.6865829226
S	-3.1685636369	9.1600415655	4.6008399660
S	0.0108474174	3.6532340450	4.6008296613
S	-3.1684738566	9.1431876507	1.4712150213
S	-0.0037202520	3.6617129040	1.4712244121
S	6.3281835879	3.6533254656	4.6008616576
S	6.3427498555	3.6616941973	1.4712547327
S	0.0054537941	9.1716163717	4.6410689309
S	-1.5821933537	6.4047421965	4.6149230506
S	1.6078384438	6.3962914211	4.6409313160
S	0.0875467025	9.1442936475	1.5070009919
S	-1.5636274391	6.4154439260	1.4975913908
S	1.6251992370	6.4810233207	1.5070166070

3.2. $v_{Se}-MoSe_2$

O	2.6278100143	9.5653677479	8.9461223089
O	3.8509826137	9.5606468312	9.0620258931
Se	1.6490292183	0.9511788682	5.2254839563
Se	11.5393702173	0.9305220364	5.2784698454
Se	6.5762322220	9.5268381758	5.2785017986
Se	0.0107545606	3.7948204013	5.2357551198
Se	3.2924942787	9.5025364927	5.3849298608
Se	-3.2916497644	9.5143714719	5.2357780317
Se	-1.6430289831	6.6531294669	5.2483747835
Se	1.6715174004	6.6466964742	5.2784763720
Se	0.0085421418	9.5268574827	5.2788127596
Se	4.9357512050	0.9512230631	5.2255865642
Se	9.8764313828	3.7977857722	5.2483102898
Se	4.9133863730	6.6467227959	5.2783531760
Se	8.2278453475	6.6531540696	5.2482732998
Se	8.2134971146	0.9305781203	5.2787052104
Se	3.2924335529	3.7977098306	5.2254915015
Se	6.5741112553	3.7949085181	5.2357650046
Mo	-0.0084503232	1.8876399935	3.5601749400
Mo	4.8589749648	10.4071064290	3.6558203238
Mo	-4.9528623646	10.4513943485	3.5601325922
Mo	-1.6391615131	4.7473691415	3.5702223492
Mo	3.2923719391	7.6938783149	3.6558636609
Mo	-1.6303063427	10.4513938968	3.5602835945
Mo	1.7258431546	10.4070652315	3.6561711362
Mo	1.6528203629	4.7650188313	3.5601610075
Mo	-3.2915605046	7.6092747657	3.5701956806
Mo	3.2924155762	1.9000582516	3.5442510542
Mo	9.8764063804	1.8599125674	3.6024744682
Mo	6.5496829884	7.6221299335	3.6023436016
Mo	0.0351742783	7.6221496597	3.6025508631
Mo	6.5933073756	1.8876358204	3.5603103780
Mo	8.2240448320	4.7473687921	3.5701840394
Mo	4.9320285017	4.7650181257	3.5601286351
Se	1.6337052042	0.9423808106	1.8739584653
Se	-0.0023264240	3.8023659774	1.8839848163
Se	6.4756102040	9.5040758624	1.9263971761
Se	-3.2915248159	9.4993342288	1.8840090507
Se	-1.6192170545	6.6668483887	1.9130219727
Se	1.7019975653	6.7452896977	1.9265436349
Se	4.8827459778	6.7452676948	1.9264703848
Se	0.1092624409	9.5040908732	1.9266473589
Se	3.2924182282	3.8154041626	1.8739322601
Se	4.9511832940	0.9423551236	1.8740725646
Se	8.2835159327	0.8547857756	1.9267061352
Se	11.4692633714	0.8548999492	1.9265305539
Se	9.8764512518	3.7703484664	1.9130201879
Se	8.2041870782	6.6668063428	1.9129274292
Se	6.5871956544	3.8023028605	1.8840096429

3.3. ν_{Te} - $MoTe_2$

O	3.2930108054	11.5030663187	8.9487060651
O	4.1109433488	10.9857847133	9.7125785405
Mo	-0.0082555899	2.0191352049	3.7978799477
Mo	-1.7724594403	5.0362797084	3.8100914633
Mo	1.7166078777	5.0189427744	3.7986328583
Mo	-3.5445805685	8.1023307972	3.8097341086
Mo	3.5124516610	8.0875127935	3.8924538949
Mo	3.5140149094	1.9834294350	3.7810851593
Mo	-0.0297336122	8.0902534395	3.8398732461
Mo	7.0342023220	2.0189769324	3.799263675
Mo	5.3051417729	5.0184262934	3.7977507405
Te	1.7627153024	0.9716509523	5.5988724807
Te	1.7445361977	0.9614635901	1.9784498944
Te	3.5103877555	4.0124151861	5.5954890254
Te	3.5109971109	4.0273681743	1.9793676841
Te	5.2657931812	0.9680039730	5.5996374952
Te	5.2821295949	0.9592155166	1.9795885966
Te	5.2889050817	7.0423106570	5.6564867445
Te	8.7790713694	0.9952811740	5.6582443679
Te	5.2533150451	7.1316098935	2.0243367968
Te	8.8412953968	0.9178004962	2.0263882640
Te	-0.0158247342	4.0205121763	5.6386885085
Te	-0.0288474332	4.0266349645	1.9629500552
Te	7.0324807011	4.0172875845	5.6408061019
Te	7.0488204548	4.0249719659	1.9609465603
Te	1.7398052620	7.0423442213	5.6583920092
Te	1.7701078807	7.1302237680	2.0254960944
Te	-1.7970638309	7.0669613857	5.6352085022
Te	-1.7717351604	7.0819382641	2.0025653686
Mo	5.2809511177	11.1572927494	3.8842946677
Mo	-5.2770673269	11.1407015815	3.7980522167
Mo	1.7409403610	11.1587179748	3.8950578241
Mo	-1.8159764812	11.1377397295	3.8007601277
Te	7.0764704580	10.1511970222	5.6519900666
Te	6.9833778094	10.1282449015	2.0194583869
Te	-3.5478070977	10.1308335238	5.6381729212
Te	-3.5466890739	10.1196478701	1.9654536258
Te	3.5143799853	10.1346838406	5.6752718202
Te	-0.0528017046	10.1474257577	5.6598579429
Te	0.0410441725	10.1294527486	2.0266564229
Te	12.3003993959	0.9202845057	2.0207597637
Te	12.3677183641	0.9896095481	5.6526748284
Mo	10.5726822279	2.0008851856	3.8387595656
Te	10.5679420300	4.0432663204	5.6329708049
Te	10.5691577374	4.0158221067	2.0051214558
Mo	8.7902428892	5.0310029976	3.8100696016
Te	8.8210835815	7.0645922463	5.6313967084
Te	8.7997536091	7.0786040269	2.0041365687
Mo	7.0558249025	8.0915940729	3.836572646

4. Optimized atomic structures of CH₄ adsorption on defective TMDs

4.1. *v_S*-MoS₂

H	3.2006265467	8.8213674472	9.3067465061
C	3.1953327027	8.8891833470	8.2129542698
H	2.2998683806	8.3961889497	7.8175597079
H	4.0876973432	8.3974602212	7.8090550755
H	3.1931263229	9.9420724117	7.9088540470
Mo	-0.0066097705	1.8215331000	3.0374543674
Mo	4.7086535287	10.0388048803	3.1124775802
Mo	-4.7653489657	10.0641948254	3.0374830560
Mo	-1.5796795812	4.5729323193	3.0499423571
Mo	3.1688627291	7.3720068483	3.1140609433
Mo	-1.5729232274	10.0641826085	3.0373697241
Mo	1.6290602893	10.0388104634	3.1122793842
Mo	1.5896364128	4.5862317516	3.0383618190
Mo	-3.1691525327	7.3262727267	3.0501015920
Mo	3.1688438388	1.8314595444	3.0242450743
Mo	9.5068549988	1.7983559881	3.0759310839
Mo	6.3093135464	7.3367009903	3.0771189709
Mo	0.0283957118	7.3367013392	3.0769972517
Mo	6.3443040729	1.8215095785	3.0373249773
Mo	7.9173386508	4.5729124797	3.0499500129
Mo	4.7480435040	4.5862085391	3.0383451550
S	6.3313616886	9.1738739938	4.6427772396
S	1.5869493216	0.9181921140	4.5930138961
S	11.1084081898	0.8989672021	4.6422829908
S	6.2513044217	9.1455145605	1.5086598850
S	1.5743899246	0.9109837718	1.4636542874
S	11.0447368199	0.8433279398	1.5081914671
S	7.9203082546	6.4066735007	4.6177215522
S	3.1688408824	3.6575705081	4.593738960
S	7.9052567483	0.8989184916	4.6421405719
S	7.9019500864	6.4173544069	1.5006295348
S	3.1688213471	3.6729105120	1.4643722419
S	7.9690381673	0.8433703873	1.5080640747
S	4.7507999614	0.9181541120	4.5929142783
S	4.7298013235	6.3991019047	4.6437866895
S	9.5068294642	3.6581109913	4.6171896003
S	4.7632485103	0.9109878531	1.4635570876
S	4.7132309920	6.4824207581	1.5096013593
S	9.5068310697	3.6378289216	1.5000391598
S	3.1687257682	9.1512496646	4.6841009037
S	-3.1690870442	9.1621096733	4.6036508147
S	0.0096723219	3.6548082683	4.6039209079
S	-3.1691798396	9.1447578711	1.4730869529
S	-0.0044489572	3.6638203268	1.473433594
S	6.3279819928	3.6547090502	4.6038727948
S	6.3421223636	3.6638388487	1.4733754696
S	0.0064087764	9.1738798520	4.6425956830
S	-1.5825787115	6.4067131698	4.6176682588
S	1.6078806968	6.3991686493	4.6437522258
S	0.0864139559	9.1454948514	1.5084943376
S	-1.5643070636	6.4173422609	1.5005708615
S	1.6245357692	6.4824020777	1.5095650726

4.2. $v_{Se}-MoSe_2$

H	3.2949915177	9.1775155155	10.0620831467
C	3.2941445351	9.2730565277	8.9703687861
H	2.4003102741	8.7903208528	8.5586978178
H	4.1880575551	8.7915590549	8.5574161048
H	3.2932109890	10.3334450453	8.6929946379
Se	1.6484795843	0.9552300711	5.1844657815
Se	11.5382515794	0.9339507415	5.2360840202
Se	6.5748902458	9.5308835226	5.2365898686
Se	0.0097298779	3.7987744085	5.1943762770
Se	3.2919602930	9.5081198771	5.3396709567
Se	-3.2920225807	9.5182320839	5.1941833789
Se	-1.6434686209	6.6571339248	5.2068565898
Se	1.6711330534	6.6516055340	5.2375573635
Se	0.0090580418	9.5308861233	5.2365746674
Se	4.9354721630	0.9552286390	5.1844592640
Se	9.8759748950	3.8013389242	5.2064876183
Se	4.9128141547	6.6516039336	5.2375618343
Se	8.2274218390	6.6571317474	5.2068601852
Se	8.2136931722	0.9339491497	5.2360733754
Se	3.2919749596	3.8015239236	5.1850697469
Se	6.5742194617	3.7987715870	5.1943736356
Mo	-0.0088125887	1.8915859002	3.5187604175
Mo	4.8591348826	10.4114207238	3.6124033394
Mo	-4.9533185137	10.4555572711	3.5188812852
Mo	-1.6398969641	4.7514828080	3.5286005085
Mo	3.2919749172	7.6973394102	3.6139502659
Mo	-1.6307347085	10.4555581007	3.5188721409
Mo	1.7248107800	10.4114229831	3.6123870223
Mo	1.6524542435	4.7691090770	3.5196213015
Mo	-3.2920252001	7.6130830416	3.5286582325
Mo	3.2919742693	1.9041066656	3.5032612774
Mo	9.8759747620	1.8641271752	3.5597548474
Mo	6.5493746231	7.6259607777	3.5607039998
Mo	0.0345746266	7.6259612157	3.5606946355
Mo	6.5927604504	1.8915874499	3.5187521210
Mo	8.2238468803	4.7514827663	3.5286006562
Mo	4.9314951820	4.7691101742	3.5196215656
Se	1.6334561357	0.9465090783	1.8326314873
Se	-0.0023359270	3.8065381228	1.8432032597
Se	6.4763138977	9.5076600754	1.8843296834
Se	-3.2920299359	9.5035613318	1.8429906055
Se	-1.6199149355	6.6707305989	1.8710799942
Se	1.7013735367	6.7485005329	1.8852184848
Se	4.8825803882	6.7485027510	1.8852214185
Se	0.1076311563	9.5076596523	1.8843165047
Se	3.2919746982	3.8196323273	1.8332616719
Se	4.9504887200	0.9465118000	1.8326246245
Se	8.2825210461	0.8597109573	1.8839537933
Se	11.4694305265	0.8597038376	1.8839633278
Se	9.8759752863	3.7749243721	1.8706892066
Se	8.2038615730	6.6707327425	1.8710836919
Se	6.5862850082	3.8065431056	1.8432002806

4.3. v_{Te} - $MoTe_2$

H	3.4847848603	9.9417315401	10.6464198570
C	3.4911571065	9.9890811171	9.5514926244
H	2.5998740044	9.4889545283	9.1553034395
H	4.3875399069	9.4899540402	9.1657250057
H	3.4924853564	11.0360636718	9.2272436835
Mo	-0.0049734510	2.0582248886	3.8003892754
Mo	-1.7651163528	5.0721539105	3.8109375366
Mo	1.7249942947	5.0548813980	3.8011922489
Mo	-3.5396627633	8.1455556492	3.8109862841
Mo	3.5188545792	8.1273230322	3.8915303834
Mo	3.5188924727	2.0214968616	3.7863486055
Mo	-0.0238528049	8.1265154030	3.8405681245
Mo	7.0426794108	2.0582622363	3.8005049022
Mo	5.3128628168	5.0549703441	3.8011800410
Te	1.7623480000	1.0073943783	5.6006939152
Te	1.7499801418	1.0002101001	1.9825255202
Te	3.5189609386	4.0495462202	5.6011454290
Te	3.5189598120	4.0645458569	1.9831932026
Te	5.2753557053	1.0072945062	5.6007451723
Te	5.2878239303	1.0000733548	1.9826379023
Te	5.2906552257	7.0779231592	5.6584638356
Te	8.7836809848	1.0274129660	5.6571345011
Te	5.2603066671	7.1685141117	2.0257673534
Te	8.8469054636	0.9563921641	2.0247596416
Te	-0.0099774277	4.0584014139	5.6409035670
Te	-0.0198987574	4.0649087623	1.9636386242
Te	7.0477615862	4.0584568916	5.6409630777
Te	7.0577004040	4.0648470398	1.9636547669
Te	1.7470848130	7.0778329614	5.6585001388
Te	1.7773486571	7.1684323544	2.0258390886
Te	-1.7923169013	7.1054533012	5.6342611153
Te	-1.7694849224	7.1186509199	2.0056398462
Mo	5.2895296138	11.1940773624	3.8897606270
Mo	-5.2696250164	11.1770263946	3.8004923903
Mo	1.7482273016	11.1941190983	3.8900364150
Mo	-1.8095209643	11.1768672116	3.8005901406
Te	7.0841078343	10.1849485453	5.6573897907
Te	6.9911397522	10.1650214811	2.0249086275
Te	-3.5396583139	10.1726148771	5.6407104679
Te	-3.5395711131	10.1604998914	1.9635187191
Te	3.5190245940	10.1729180515	5.6787488270
Te	-0.0463041016	10.1849015883	5.6576404475
Te	0.0467919955	10.1650181648	2.0250329398
Te	12.3077505417	0.9563841304	2.0245815580
Te	12.3710788072	1.0272928752	5.6570101087
Mo	10.5774103125	2.0369911042	3.8396959764
Te	10.5774230764	4.0786492238	5.6339465462
Te	10.5774171818	4.0530333603	2.0052690357
Mo	8.8029290839	5.0720605889	3.8109390129
Te	8.8299707064	7.1053852735	5.6342176429
Te	8.8072237816	7.1185258467	2.0055989925
Mo	7.0615892285	8.1264969887	3.8404562135

5. Optimized atomic structures of NH₃ adsorption on defective TMDs

5.1. *v_S*-MoS₂

N	3.1632765537	7.1307928820	7.6185713089
H	2.3269390146	6.8877331854	8.1529497047
H	3.9708646372	6.9430151231	8.2157758326
H	3.1353269663	8.1400192966	7.4578833307
Mo	-0.0021312144	1.9585612599	3.0635469050
Mo	4.7113364705	10.1747948516	3.1434918984
Mo	-4.7613785732	10.2017550694	3.0622997350
Mo	-1.5758804047	4.7098461103	3.0747150782
Mo	3.1729336167	7.5052792075	3.1505537336
Mo	-1.5688722109	10.2017847301	3.0624937527
Mo	1.6344324323	10.1748252599	3.1435571448
Mo	1.5934764256	4.7244884972	3.0636401876
Mo	-3.1653237616	7.4629576143	3.0735012193
Mo	3.1729690970	1.9693841154	3.0473139484
Mo	9.5109682221	1.9359308518	3.1034434215
Mo	6.3124229001	7.4729906622	3.0991819408
Mo	0.0327992238	7.4730814513	3.0991363481
Mo	6.3480516278	1.9585889584	3.0637742921
Mo	7.9214752972	4.7098859116	3.0748243794
Mo	4.7521040183	4.7247446427	3.0637166352
S	6.3377630554	9.3082600710	4.6683416580
S	1.5928893190	1.0559958620	4.6173263530
S	11.1139887682	1.0378438438	4.6695639120
S	6.2526906318	9.2842065639	1.5347215037
S	1.5774135925	1.0482035993	1.4880353307
S	11.0481928853	0.9790747127	1.5366297932
S	7.9235581834	6.5440396657	4.6411347481
S	3.1728225828	3.7947447823	4.6188586542
S	7.9080882628	1.0378686398	4.6697319494
S	7.9056723469	6.5536560449	1.5237990965
S	3.1728884709	3.8121076081	1.4888111808
S	7.9737287969	0.9790749203	1.5367663281
S	4.7529855448	1.0560723373	4.6175001995
S	4.7386333218	6.5332300483	4.6718470493
S	9.5108682813	3.7967592118	4.6427287687
S	4.7686803874	1.0482007807	1.4882103637
S	4.7134851031	6.6202501815	1.5357763554
S	9.5107745167	3.7736244005	1.5256095264
S	3.1729013068	9.2862169412	4.7207614759
S	-3.1652396966	9.2986087811	4.6271836488
S	0.0137907303	3.7927860120	4.6290486574
S	-3.1650736164	9.2826626786	1.4982728371
S	-0.0000657353	3.8005352096	1.4993269835
S	6.3318298972	3.7929542303	4.6292210535
S	6.3457111677	3.8005389518	1.4995539468
S	0.0079472056	9.3082115579	4.6684785004
S	-1.5782810483	6.5439801654	4.6410596685
S	1.6066409712	6.5331341652	4.6713877161
S	0.0929589963	9.2843282895	1.5348386118
S	-1.5604107824	6.5536657684	1.5237416010
S	1.6319404255	6.6202218524	1.5359721162

5.2. $v_{Se}-MoSe_2$

N	3.3247713335	7.4731480851	8.6475225055
H	2.4985894700	7.0270877103	8.2420931179
H	4.1378013642	7.0264914432	8.2169260030
H	3.3202648851	8.4433354557	8.3240893009
Se	1.6498511316	0.9658460839	5.2243665409
Se	11.5404062039	0.9455901642	5.2778110492
Se	6.5780353819	9.5409373268	5.2782672313
Se	0.0110021880	3.8089754054	5.2346466372
Se	3.2929882628	9.5193172474	5.3900470150
Se	-3.2911044206	9.5291785464	5.2346713415
Se	-1.6432259687	6.6672336968	5.2478878564
Se	1.6688294380	6.6581853674	5.2773859514
Se	0.0079107625	9.5411037198	5.2784793389
Se	4.9360511637	0.9658159380	5.2243305079
Se	9.8769314165	3.8121895948	5.2475002363
Se	4.9177331097	6.6578998904	5.2762942471
Se	8.2290603813	6.6671192256	5.2476313289
Se	8.2134520791	0.9456756861	5.2778548820
Se	3.2931365671	3.8108040252	5.2247497650
Se	6.5749411278	3.8089419661	5.2344121986
Mo	-0.0077737378	1.9019333282	3.5590591944
Mo	4.8591616078	10.4208778987	3.6570721214
Mo	-4.9522543865	10.4661620113	3.5591698245
Mo	-1.6388256237	4.7617910205	3.5691360899
Mo	3.2929796207	7.7081339588	3.6621217533
Mo	-1.6298474557	10.4660795397	3.5592347584
Mo	1.7267641335	10.4209349133	3.6571817200
Mo	1.6535212799	4.7781250691	3.5588116738
Mo	-3.2910277911	7.6236253532	3.5693650020
Mo	3.2929408241	1.9140622605	3.5425013690
Mo	9.8769494440	1.8742012812	3.6018451050
Mo	6.5516378182	7.6366173671	3.6012051432
Mo	0.0345905978	7.6365674657	3.6017847908
Mo	6.5936864402	1.9018583272	3.5589598185
Mo	8.2248099704	4.7616809040	3.5689090215
Mo	4.9325525910	4.7778835424	3.5583244788
Se	1.6338952504	0.9566060215	1.8723286065
Se	-0.0020061393	3.8167886820	1.8828079900
Se	6.4754786026	9.5187034938	1.9264410324
Se	-3.2910443278	9.5137436227	1.8831784444
Se	-1.6189828062	6.6813753596	1.9119257765
Se	1.7043728127	6.7607844873	1.9285415922
Se	4.8815308166	6.7608252037	1.9282249808
Se	0.1105369007	9.5184938973	1.9267370484
Se	3.2928131640	3.8293284275	1.8719866456
Se	4.9519363137	0.9564687748	1.8723274996
Se	8.2842409260	0.8680074732	1.9266668369
Se	11.4696738077	0.8680602012	1.9266908297
Se	9.8771021516	3.7841989624	1.9119055602
Se	8.2052220510	6.6812193285	1.9116047870
Se	6.5880893844	3.8165308497	1.8824731087

5.3. ν_{Te} - $MoTe_2$

N	3.5160631933	7.8729706407	8.7846688084
H	2.6622057268	7.6142265263	9.2833802438
H	4.3052332465	7.5815524738	9.3652752159
H	3.5380893018	8.8943436207	8.7388355543
Mo	-0.0103904172	2.0701294927	3.8427553729
Mo	-1.7698057669	5.0838298081	3.8533259385
Mo	1.7179143653	5.0678750558	3.8433375400
Mo	-3.5442504146	8.1573130544	3.8520265005
Mo	3.5147274407	8.1348898332	3.9540427234
Mo	3.5141904476	2.0342199354	3.8270335746
Mo	-0.0282075613	8.1391495156	3.8809935191
Mo	7.0387283299	2.0699353601	3.8427280071
Mo	5.3106465125	5.0682176164	3.8431471918
Te	1.7586348654	1.0200476624	5.6415854161
Te	1.7444634090	1.0132593216	2.0237147000
Te	3.5144208057	4.0627845453	5.6425305066
Te	3.5142673786	4.0792105521	2.0257888083
Te	5.2696947142	1.0199646546	5.6415589140
Te	5.2838370213	1.0131466115	2.0237116478
Te	5.2932309096	7.0860299306	5.7101961351
Te	8.7774677804	1.0407509048	5.7008274567
Te	5.2504246660	7.1840532289	2.0729703962
Te	8.8436183396	0.9659917400	2.0698140517
Te	-0.0148042851	4.0708615516	5.6829667509
Te	-0.0252070296	4.0771134712	2.0053567130
Te	7.0432590687	4.0709142041	5.6827815080
Te	7.0537555812	4.0770160943	2.0054132259
Te	1.7355678533	7.0861012478	5.7093296168
Te	1.7783741955	7.1840291716	2.0734319777
Te	-1.7962140106	7.1181104483	5.6751205550
Te	-1.7734807131	7.1305878355	2.0469742417
Mo	5.2832507300	11.2058360630	3.9379923169
Mo	-5.2752936471	11.1900861063	3.8416789594
Mo	1.7453241666	11.2058513790	3.9379385460
Mo	-1.8130986357	11.1899806637	3.8416961080
Te	7.0813692296	10.1949102430	5.6995223517
Te	6.9830068553	10.1785519201	2.0684532807
Te	-3.5442608172	10.1854312110	5.6803117280
Te	-3.5442500671	10.1732772991	2.0053593706
Te	3.5143406992	10.1858067331	5.7327133213
Te	-0.0527257329	10.1950964015	5.6995994580
Te	0.0456040996	10.1786278836	2.0684003267
Te	12.3017215521	0.9659754938	2.0698386217
Te	12.3678598851	1.0407675343	5.7008153800
Mo	10.5726567886	2.0481548997	3.8845207378
Te	10.5727513747	4.0915349916	5.6766359116
Te	10.5727982140	4.0637079292	2.0488212372
Mo	8.7984866048	5.0838078354	3.8532659018
Te	8.8246943746	7.1179946435	5.6751431161
Te	8.8020897756	7.1305047207	2.0468540536
Mo	7.0566819468	8.1388255202	3.8808909701

6. Optimized atomic structures of H₂S adsorption on defective TMDs

6.1. *v_S*-MoS₂

S	3.2354534906	7.3198194092	8.0687790743
H	2.2798038336	8.1795516479	7.6497962714
H	4.2106001238	8.1066328672	7.5606476800
Mo	-0.0089627864	1.8881342568	3.0429546305
Mo	4.7047234591	10.1051971647	3.1216887199
Mo	-4.7680414225	10.1313190959	3.0431713554
Mo	-1.5824899889	4.6396122012	3.0551525796
Mo	3.1660509351	7.4370339192	3.1279187583
Mo	-1.5759770693	10.1312720670	3.0431034375
Mo	1.6271141269	10.1051869599	3.1216434916
Mo	1.5871269272	4.6529949147	3.0432586740
Mo	-3.1719392442	7.3927323746	3.0549337636
Mo	3.1659628919	1.8982370458	3.0271305391
Mo	9.5039758928	1.8657863027	3.0821801530
Mo	6.3064658824	7.4027844239	3.0806519206
Mo	0.0258206008	7.4028058939	3.0815630107
Mo	6.3409896799	1.8880481472	3.0426059269
Mo	7.9145246492	4.6395531788	3.0547516885
Mo	4.7450283251	4.6525874383	3.0423970335
S	6.3300231013	9.2389496270	4.6488583231
S	1.5856704275	0.9858593103	4.5975864483
S	11.1066440036	0.9678616538	4.6486837869
S	6.2471863726	9.2132109637	1.5151590350
S	1.5705465337	0.9769431043	1.4679172929
S	11.0415443123	0.9092723469	1.5152211336
S	7.9172010460	6.4731279594	4.6222995715
S	3.1662407054	3.7231603827	4.5981352965
S	7.9011868069	0.9679029120	4.6485585234
S	7.8993314734	6.4838056041	1.5047818153
S	3.1656743884	3.7404981736	1.4679263544
S	7.9665364367	0.9091287834	1.5150365461
S	4.7464238012	0.9858757550	4.5974071935
S	4.7312994519	6.4614202416	4.6492677542
S	9.5038548638	3.7259443242	4.6225927432
S	4.7612808771	0.9768528609	1.4677715474
S	4.7077444852	6.5499584170	1.5159549008
S	9.5041718428	3.7042861541	1.5052544496
S	3.1658162089	9.2187515446	4.6979022215
S	-3.1719902871	9.2286597140	4.6086284863
S	0.0072701357	3.7217644224	4.6090523899
S	-3.1720313550	9.2119762558	1.4790964111
S	-0.0070295649	3.7302521077	1.4790876983
S	6.3247384065	3.7216701936	4.6085411988
S	6.3392629531	3.7299522775	1.4784321874
S	0.0018483721	9.2393059563	4.6490670903
S	-1.5853367242	6.4731791956	4.6227183496
S	1.6016338383	6.4621748873	4.6510099074
S	0.0847515951	9.2128208148	1.5153902331
S	-1.5668629537	6.4838550945	1.5052658487
S	1.6241449778	6.5500004292	1.5166020246

6.2. $v_{Se}-MoSe_2$

S	3.2954910511	7.5247446416	8.8353221287
H	2.3456899190	8.3107719902	8.2797145310
H	4.2787477933	8.3034390174	8.3301202415
Se	1.6487957822	1.0416444654	5.2367594189
Se	11.5385524081	1.0210793160	5.2898484733
Se	6.5753645445	9.6152233099	5.2897499721
Se	0.0096613515	3.8843973588	5.2469155081
Se	3.2912195412	9.5937430730	5.3992837058
Se	-3.2926929591	9.6037797686	5.2468812706
Se	-1.6436738239	6.7426684995	5.2588622858
Se	1.6663582706	6.7329013673	5.2903112061
Se	0.0072246515	9.6152562692	5.2897073630
Se	4.9338705582	1.0416586591	5.2367171608
Se	9.8752302022	3.8883457086	5.2596163589
Se	4.9161693967	6.7329165445	5.2903946953
Se	8.2261382054	6.7426866649	5.2588212925
Se	8.2120206995	1.0210351097	5.2897892673
Se	3.2913359133	3.8873400313	5.2373516754
Se	6.5728469867	3.8844491054	5.2468164081
Mo	-0.0093153611	1.9770349962	3.5715157497
Mo	4.8575321763	10.4968985876	3.6686573976
Mo	-4.9537506026	10.5414053207	3.5718039536
Mo	-1.6403235503	4.8368576088	3.5809955411
Mo	3.2913338298	7.7803342560	3.6738475995
Mo	-1.6316588455	10.5414157448	3.5717686977
Mo	1.7250485519	10.4968765265	3.6685461597
Mo	1.6517045079	4.8540318481	3.5708887529
Mo	-3.2927323761	7.6987513211	3.5808565671
Mo	3.2913166697	1.9901779192	3.5546001822
Mo	9.8752890732	1.9502617677	3.6140782813
Mo	6.5483089778	7.7114520411	3.6118961548
Mo	0.0341379986	7.7114463378	3.6119301853
Mo	6.5919199476	1.9770347308	3.5714316238
Mo	8.2228566621	4.8368893244	3.5809422073
Mo	4.9308256047	4.8541549984	3.5707909377
Se	1.6324168826	1.0316841199	1.8848198165
Se	-0.0034187774	3.8914774983	1.8950300361
Se	6.4735402631	9.5946718865	1.9382962031
Se	-3.2927189135	9.5893092771	1.8955300236
Se	-1.6204059173	6.7562795571	1.9231788057
Se	1.7030918901	6.8350299907	1.9390065544
Se	4.8794284491	6.8351131621	1.9388625390
Se	0.1089994476	9.5946056342	1.9382599255
Se	3.2912489821	3.9053322652	1.8840444262
Se	4.9501848880	1.0316905805	1.8847608556
Se	8.2827090347	0.9442033887	1.9386683284
Se	11.4679312489	0.9442128859	1.9387386117
Se	9.8752797474	3.8600678167	1.9237452470
Se	8.2029159711	6.7563389691	1.9231524758
Se	6.5859639896	3.8915206755	1.8949696668

6.3. v_{Te} - $MoTe_2$

S	3.5155482863	12.2019539972	9.2813044391
H	2.5094168072	11.4586784564	8.7672057557
H	4.4361650554	11.3186448492	8.8323873740
Mo	-0.0031353348	1.9915331243	3.7988796831
Mo	-1.7649823224	5.0048680786	3.8151726395
Mo	1.7251795064	4.9877911624	3.7999513531
Mo	-3.5392308868	8.0789990710	3.8167315828
Mo	3.5190166525	8.0592952687	3.8926220420
Mo	3.5190787185	1.9534277463	3.7852913166
Mo	-0.0226659528	8.0598480976	3.8452976207
Mo	7.0408969424	1.9916988748	3.7988896271
Mo	5.3130090684	4.9877788629	3.7999963022
Te	1.7627464978	0.9421788441	5.6014995635
Te	1.7500954343	0.9308018858	1.9822363151
Te	3.5189927070	3.9818541654	5.5992511014
Te	3.5190960387	3.9969646980	1.9819272903
Te	5.2750649628	0.9422454086	5.6016517913
Te	5.2880532077	0.9308042823	1.9820906856
Te	5.2899089485	7.0075848124	5.6591124921
Te	8.7764909470	0.9675094161	5.6613223883
Te	5.2616607460	7.1030619243	2.0269518937
Te	8.8503843335	0.8875140117	2.0310429992
Te	-0.0076461099	3.9904274859	5.6417602010
Te	-0.0217759917	3.9989429582	1.9636541361
Te	7.0458901454	3.9906480563	5.6417899548
Te	7.0600213351	3.9989782272	1.9636174572
Te	1.7482618139	7.0075333866	5.6590986820
Te	1.7764804532	7.1030611119	2.0269803925
Te	-1.7913172799	7.0377878172	5.6392166810
Te	-1.7693904457	7.0523646951	2.0112275322
Mo	5.2881829569	11.1293474542	3.9017062456
Mo	-5.2695133451	11.1102658919	3.8043357153
Mo	1.7500161373	11.1289878769	3.9015329579
Mo	-1.8089693559	11.1103595438	3.8043076897
Te	7.0860032142	10.1181398705	5.6633974898
Te	6.9873116836	10.1002165439	2.0329827444
Te	-3.5392567941	10.1068723828	5.6448090433
Te	-3.5392063271	10.0925951866	1.9679435728
Te	3.5193118482	10.0972819885	5.6872953122
Te	-0.0477518423	10.1182804540	5.6633568735
Te	0.0509606470	10.1001221288	2.0327292730
Te	12.3048652236	0.8873422277	2.0308509711
Te	12.3784804554	0.9672422970	5.6626556850
Mo	10.5779232854	1.9696144628	3.8493625224
Te	10.5777463820	4.0127151963	5.6416652769
Te	10.5777120865	3.9837152376	2.0115278039
Mo	8.8033438874	5.0047648673	3.8151513907
Te	8.8297167121	7.0377798770	5.6391828467
Te	8.8079618824	7.0522854380	2.0111751696
Mo	7.0610101742	8.0596453618	3.8452030744

7. Optimized atomic structures of CO₂ adsorption on defective TMDs

7.1. *v_S*-MoS₂

C	3.1686809152	9.2268809153	7.9957967960
O	4.3432117730	9.2269068227	8.0006802105
O	1.9942184252	9.2268981967	8.0000867392
Mo	-0.0062417983	1.8193106281	3.0321007113
Mo	4.7107792567	10.0367555290	3.1073047480
Mo	-4.7649895373	10.0611269611	3.0306912171
Mo	-1.5791337597	4.5705361529	3.0445332951
Mo	3.1690002126	7.3677096633	3.1076191985
Mo	-1.5730094298	10.0611257372	3.0306937721
Mo	1.6272244338	10.0367532332	3.1073126351
Mo	1.5896218274	4.5832774074	3.0321077133
Mo	-3.1690015833	7.3237747457	3.0438858487
Mo	3.1689987374	1.8284380188	3.0184509461
Mo	9.5069992918	1.7958973542	3.0708152962
Mo	6.3093833835	7.3345750227	3.0704907562
Mo	0.0286152872	7.3345752213	3.0704941087
Mo	6.3442405585	1.8193077461	3.0321041906
Mo	7.9171286063	4.5705349696	3.0445335665
Mo	4.7483746400	4.5832759974	3.0321077327
S	6.3334802029	9.1712347990	4.6369059626
S	1.5870556891	0.9145178184	4.5869360199
S	11.1093403466	0.8971009794	4.6375045637
S	6.2519414353	9.1432916164	1.5017947566
S	1.5742575286	0.9085288945	1.4578885868
S	11.0453705685	0.8417233301	1.5030973444
S	7.9200204917	6.4049697676	4.6115682134
S	3.1689976707	3.6549939130	4.5874100386
S	7.9046611691	0.8971002928	4.6375086891
S	7.9020384344	6.4145616670	1.4946823269
S	3.1689979924	3.6698069464	1.4584680829
S	7.9686282376	0.8417187416	1.5031015294
S	4.7509409546	0.9145168160	4.5869383404
S	4.7306283474	6.3957734869	4.6373150640
S	9.5069975787	3.6560038815	4.6117500676
S	4.7637419846	0.9085269752	1.4578914394
S	4.7136512770	6.4789612447	1.5029289505
S	9.5069971263	3.6353988584	1.4952021242
S	3.1690082096	9.1478257951	4.6744389861
S	-3.1690004948	9.1595063911	4.5973697792
S	0.0104307890	3.6524250335	4.5984987949
S	-3.1689983963	9.1416957406	1.4660781684
S	-0.0044384836	3.6610429999	1.4674576907
S	6.3275645291	3.6524231294	4.5985001214
S	6.3424339735	3.6610383971	1.4674593708
S	0.0045202109	9.1712334248	4.6369102300
S	-1.5820249518	6.4049701168	4.6115693232
S	1.6073714672	6.3957740065	4.6373164781
S	0.0860618838	9.1432918058	1.5017998549
S	-1.5640408898	6.4145637175	1.4946838179
S	1.6243461404	6.4789627283	1.5029305369

7.2. $v_{Se}-MoSe_2$

O	4.5482192167	10.6543945620	8.6429564243
O	2.2027005231	10.7785907966	8.6554811325
C	3.3753565888	10.7147336814	8.6466968228
Se	1.6419781733	0.8874000986	5.2229376300
Se	11.5318847570	0.8685182568	5.2745234114
Se	6.5694704282	9.4631452268	5.2774852858
Se	0.0034985418	3.7305934509	5.2327043706
Se	3.2848818393	9.4362032735	5.3800720695
Se	-3.2988428423	9.4506719727	5.2333340555
Se	-1.6500744254	6.5892178831	5.2460183828
Se	1.6637436366	6.5813132686	5.2756810458
Se	0.0009797195	9.4634032696	5.2774024813
Se	4.9284435028	0.8875868115	5.2227917020
Se	9.8691532712	3.7334221648	5.2452174315
Se	4.9068993298	6.5813613706	5.2756872446
Se	8.2205653262	6.5892585588	5.2459755185
Se	8.2059177649	0.8687516680	5.2744916042
Se	3.2852992751	3.7329072760	5.2221858125
Se	6.5669714274	3.7305748077	5.2325021438
Mo	-0.0153822182	1.8237599592	3.5570287638
Mo	4.8530287647	10.3433049277	3.6545487290
Mo	-4.9605552574	10.3874318549	3.5578477201
Mo	-1.6463527144	4.6835507567	3.5673439072
Mo	3.2853319274	7.6273791666	3.6534718739
Mo	-1.6372063367	10.3875320370	3.5578319751
Mo	1.7172881930	10.3437135686	3.6543562512
Mo	1.6454870642	4.7005173605	3.5570919370
Mo	-3.2987371184	7.5453659589	3.5679572013
Mo	3.2851312360	1.8356289530	3.5407317185
Mo	9.8689732933	1.7964363257	3.5978242276
Mo	6.5424220865	7.5585702015	3.6000431551
Mo	0.0281023951	7.5585426341	3.6001525317
Mo	6.5857402579	1.8238143777	3.5566320159
Mo	8.2168585173	4.6836364069	3.5672571049
Mo	4.9249707353	4.7006092610	3.5569664616
Se	1.6262047364	0.8778020653	1.8707295067
Se	-0.0096476595	3.7383236301	1.8809977822
Se	6.4682248148	9.4402325580	1.9242350840
Se	-3.2988259028	9.4354800967	1.8820348731
Se	-1.6264095783	6.6033456504	1.9105501201
Se	1.6945769662	6.6808791652	1.9239669098
Se	4.8759488552	6.6809703926	1.9238216438
Se	0.1020796419	9.4402517495	1.9243328507
Se	3.2851685853	3.7512198322	1.8705588497
Se	4.9438995613	0.8778237215	1.8705836633
Se	8.2758201533	0.7903719345	1.9233213664
Se	11.4624978863	0.7902143416	1.9237279228
Se	9.8692621193	3.7073823628	1.9094111336
Se	8.1970178695	6.6033999700	1.9104638043
Se	6.5801214364	3.7385351809	1.8808100804

7.3. v_{Te} - $MoTe_2$

C	3.5346261446	10.2708825854	9.2818613499
O	4.7092230960	10.2707662021	9.2772401571
O	2.3601534142	10.2710817195	9.2979252193
Mo	-0.0056115029	2.0549357744	3.7864985945
Mo	-1.7646712860	5.0687315512	3.7973486185
Mo	1.7247422597	5.0517615795	3.7860029136
Mo	-3.5395991813	8.1424445614	3.7969916121
Mo	3.5188385273	8.1219899735	3.8756697368
Mo	3.5188671645	2.0178504766	3.7715642200
Mo	-0.0230199542	8.1240281647	3.8257850573
Mo	7.0433179097	2.0549833906	3.7863765041
Mo	5.3130139976	5.0518083211	3.7860009811
Te	1.7623858102	1.0032510306	5.5860186027
Te	1.7493785335	0.9965532351	1.9684037164
Te	3.5188940653	4.0461772830	5.5858738461
Te	3.5188872843	4.0608778749	1.9682935547
Te	5.2753800935	1.0032733555	5.5859479789
Te	5.2882923567	0.9965949332	1.9683157076
Te	5.2908093667	7.0740547028	5.6433427530
Te	8.7832683370	1.0239295863	5.6441418769
Te	5.2608044418	7.1649342428	2.0100789269
Te	8.8469547309	0.9528824531	2.0106063479
Te	-0.0092667325	4.0551665925	5.6268912651
Te	-0.0205134234	4.0612814645	1.9492653667
Te	7.0470487409	4.0551790223	5.6268370892
Te	7.0582838452	4.0613999344	1.9492215496
Te	1.7468912233	7.0740278538	5.6433000174
Te	1.7769562670	7.1648730586	2.0100465299
Te	-1.7916426586	7.1028286391	5.6202011820
Te	-1.7695604908	7.1151002153	1.9918535646
Mo	5.2919440522	11.1910519490	3.8766299352
Mo	-5.2701999497	11.1725782493	3.7856164221
Mo	1.7456735836	11.1911216868	3.8763325046
Mo	-1.8090920822	11.1726150302	3.7855331636
Te	7.0854329691	10.1813005029	5.6451031725
Te	6.9906972204	10.1616401473	2.0096805624
Te	-3.5396070467	10.1696514653	5.6264149301
Te	-3.5396785599	10.1566433924	1.9487385460
Te	3.5185856122	10.1685549806	5.6562715256
Te	-0.0476917123	10.1813427524	5.6448966235
Te	0.0468927214	10.1616209822	2.0095207879
Te	12.3077476884	0.9527306701	2.0107646060
Te	12.3713509368	1.0239292864	5.6443136622
Mo	10.5773443305	2.0322649318	3.8260666231
Te	10.5773739474	4.0749170087	5.6200852714
Te	10.5773894950	4.0494063586	1.9923066701
Mo	8.8024758158	5.0687531856	3.7973349326
Te	8.8294317256	7.1028246379	5.6202291971
Te	8.8072788544	7.1151540912	1.9918872938
Mo	7.0607566361	8.1240368391	3.8258809452

8. Optimized atomic structures of SO₂ adsorption on defective TMDs

8.1. *v_S*-MoS₂

S	3.1948926715	8.5527147184	7.7314055530
O	1.9258806930	9.2057859092	8.0459762309
O	4.4414987349	9.2424890255	8.0572319639
Mo	-0.0059971805	1.8186255715	3.0355641055
Mo	4.7166424695	10.0385052842	3.1124898001
Mo	-4.7638683025	10.0604488884	3.0336619064
Mo	-1.5794813507	4.5697939024	3.0456327339
Mo	3.1696986429	7.3636437341	3.1094739365
Mo	-1.5728688961	10.0603520249	3.0339690855
Mo	1.6229394083	10.0384076987	3.1132262821
Mo	1.5900066234	4.5818152306	3.0335684164
Mo	-3.1685437357	7.3227779423	3.0438883085
Mo	3.1693138118	1.8274479841	3.0185782271
Mo	9.5074248628	1.7938114920	3.0753117574
Mo	6.3100384092	7.3338953352	3.0709636983
Mo	0.0291184003	7.3340560458	3.0713945053
Mo	6.3447709409	1.8183076268	3.0358065583
Mo	7.9181352663	4.5695869031	3.0455939632
Mo	4.7487326732	4.5815121758	3.0334467645
S	6.3385131201	9.1689035783	4.6406281730
S	1.5893143858	0.9149546762	4.5896205274
S	11.1117829165	0.8991923794	4.6435868464
S	6.2531446839	9.1437114235	1.5040041835
S	1.5731118009	0.9072627979	1.4600298532
S	11.0459987339	0.8411881071	1.5068953785
S	7.9209620272	6.4043328816	4.6117536407
S	3.1692806102	3.6519917216	4.5883560660
S	7.9032792014	0.8992229597	4.6439440729
S	7.9021944968	6.4133991371	1.4944882360
S	3.1692184490	3.6694174538	1.4588841128
S	7.9688739935	0.8408015644	1.5072463995
S	4.7492227535	0.9148764273	4.5898104039
S	4.7327816609	6.3927926813	4.6386069313
S	9.5073198678	3.6557937243	4.6141802795
S	4.7656728976	0.9070347041	1.4602425422
S	4.7138974368	6.4773240209	1.5040360043
S	9.5073320041	3.6317228954	1.4972610883
S	3.1705312982	9.1458205391	4.6660620452
S	-3.1684899930	9.1566537303	4.5998808936
S	0.0096269149	3.6528642702	4.6005540801
S	-3.1682317214	9.1424398916	1.4691199307
S	-0.0046551340	3.6591888752	1.4705263706
S	6.3289921537	3.6525928547	4.6005646047
S	6.3433289567	3.6586302649	1.4705666795
S	0.0008512819	9.1689222074	4.6412279299
S	-1.5821875806	6.4044736091	4.6118854141
S	1.6065258443	6.3930756447	4.6389034198
S	0.0864843907	9.1438171194	1.5045591567
S	-1.5631210304	6.4137092278	1.4946765230
S	1.6251162765	6.4776219146	1.5042498865

8.2. $v_{Se}-MoSe_2$

S	3.2976172053	9.9739505327	8.5043711376
O	2.0468887062	10.7329688910	8.5465831014
O	4.5615981452	10.7108947959	8.5419323726
Se	1.6483250631	0.8885186877	5.2366880805
Se	11.5404990759	0.8768352781	5.2929711405
Se	6.5809722691	9.4630822680	5.2939784866
Se	0.0098228632	3.7309184667	5.2462660666
Se	3.2914371443	9.4365734091	5.3702248540
Se	-3.2924333230	9.4509616799	5.2480585336
Se	-1.6434686706	6.5895624102	5.2590087739
Se	1.6679637651	6.5785323403	5.2894698127
Se	0.0022382944	9.4631728665	5.2938941610
Se	4.9348128092	0.8885613846	5.2366621529
Se	9.8755916776	3.7340065810	5.2584847294
Se	4.9152095047	6.5785412737	5.2894926319
Se	8.2266553659	6.5895713000	5.2590132523
Se	8.2105774362	0.8768791076	5.2928772299
Se	3.2915774132	3.7327074931	5.2350739833
Se	6.5733505104	3.7309410150	5.2462658449
Mo	-0.0094737945	1.8249332867	3.5697588297
Mo	4.8691762810	10.3521311456	3.6705937195
Mo	-4.9530702748	10.3874050997	3.5717401750
Mo	-1.6396481730	4.6839784851	3.5803207415
Mo	3.2915915922	7.6178120503	3.6650128743
Mo	-1.6318190984	10.3874400123	3.5717327546
Mo	1.7139427355	10.3522013024	3.6704402297
Mo	1.6511332877	4.7002159447	3.5695454893
Mo	-3.2924058019	7.5464698254	3.5816195919
Mo	3.2915603766	1.8358442756	3.5539524924
Mo	9.8755640963	1.7952731550	3.6119969710
Mo	6.5479649026	7.5598827043	3.6130190771
Mo	0.0351990932	7.5598854261	3.6130119249
Mo	6.5925964624	1.8249807207	3.5697003769
Mo	8.2228349436	4.6839881418	3.5803215406
Mo	4.9320295044	4.7002274702	3.5695521873
Se	1.6329055009	0.8778205090	1.8842527908
Se	-0.0037097301	3.7388026033	1.8934282718
Se	6.4764371719	9.4422481351	1.9381079291
Se	-3.2924346483	9.4358760534	1.8954002844
Se	-1.6202681105	6.6042013969	1.9241039894
Se	1.6991881201	6.6793018923	1.9355365672
Se	4.8839874130	6.6793046496	1.9355406072
Se	0.1066410497	9.4422538155	1.9380699845
Se	3.2915815165	3.7507496778	1.8833765180
Se	4.9502042161	0.8778446388	1.8842331270
Se	8.2814677433	0.7931276510	1.9360287604
Se	11.4696734067	0.7930405778	1.9361234039
Se	9.8755931021	3.7071448437	1.9232397474
Se	8.2034537537	6.6042106439	1.9241083966
Se	6.5868790489	3.7388660220	1.8934107712

8.3. v_{Te} - $MoTe_2$

S	3.4929219408	10.6804879977	8.8569776517
O	2.2400130810	11.4460143370	8.8943417101
O	4.7554312346	11.4279635036	8.9216947563
Mo	-0.0076730095	1.9981519408	3.8209761512
Mo	-1.7635694639	5.0122334737	3.8325520262
Mo	1.7244182737	4.9955795322	3.8204430586
Mo	-3.5399765807	8.0883859292	3.8348486157
Mo	3.5184336661	8.0550457370	3.9129281538
Mo	3.5186127688	1.9599471963	3.8064967538
Mo	-0.0174945086	8.0702636908	3.8641121414
Mo	7.0446262011	1.9982354773	3.8205542777
Mo	5.3127501597	4.9957579860	3.8203155853
Te	1.7613954116	0.9479245084	5.6226139054
Te	1.7481546456	0.9370877957	2.0052793568
Te	3.5186842702	3.9879879670	5.6202023201
Te	3.5185799319	4.0030433025	2.0032327129
Te	5.2758755641	0.9478842545	5.6225316916
Te	5.2887980906	0.9369637084	2.0050410343
Te	5.2922289304	7.0113354663	5.6822631495
Te	8.7806484867	0.9804763452	5.6896647759
Te	5.2605311796	7.1077808842	2.0452736264
Te	8.8469507513	0.8940754014	2.0476471823
Te	-0.0092883682	3.9978319026	5.6623901781
Te	-0.0211181594	4.0044905186	1.9836843718
Te	7.0464191641	3.9977827800	5.6621776865
Te	7.0582533532	4.0046643136	1.9834453703
Te	1.7446908586	7.0113013604	5.6822494427
Te	1.7764195804	7.1075720134	2.0453500397
Te	-1.7907550846	7.0462491665	5.6558878597
Te	-1.7680229734	7.0614177289	2.0310618716
Mo	5.2987080740	11.1419227653	3.9243514504
Mo	-5.2710649797	11.1139936013	3.8246307294
Mo	1.7383376914	11.1419822203	3.9243778173
Mo	-1.8086924911	11.1139545319	3.8245376505
Te	7.0901654462	10.1237467751	5.6908164105
Te	6.9880893233	10.1077639463	2.0507929624
Te	-3.5398520359	10.1131882447	5.6662472151
Te	-3.5399276406	10.1006580151	1.9866205604
Te	3.5183981700	10.1062263186	5.6609069587
Te	-0.0530235115	10.1237761923	5.6908898228
Te	0.0491624926	10.1077795414	2.0506925989
Te	12.3072451283	0.8939642134	2.0477399115
Te	12.3732341538	0.9799398410	5.6900942865
Mo	10.5771728581	1.9706509250	3.8624451406
Te	10.5770757904	4.0177405810	5.6547759439
Te	10.5771430402	3.9912155542	2.0295899503
Mo	8.8007601867	5.0121565009	3.8324608526
Te	8.8277852134	7.0461279312	5.6558610185
Te	8.8050274451	7.0614086119	2.0310783216
Mo	7.0544794451	8.0702225339	3.8641858918

9. Optimized atomic structures of NO₂ adsorption on defective TMDs

9.1. *v_S*-MoS₂

N	3.1914988394	8.9682112415	8.1160869074
O	2.0757164914	8.9212124138	7.6306499030
O	4.2972082594	8.9218892823	7.6077862889
Mo	-0.0056978632	1.8226774970	3.0436336801
Mo	4.7131284190	10.0404083176	3.1194259842
Mo	-4.7639535956	10.0644068316	3.0420143575
Mo	-1.5787132981	4.5734863281	3.0574439253
Mo	3.1694357303	7.3689929623	3.1228111303
Mo	-1.5732856500	10.0644768749	3.0420738277
Mo	1.6254783375	10.0405779851	3.1193319916
Mo	1.5898244318	4.5858599846	3.0449145241
Mo	-3.1685016583	7.3270877406	3.0569970981
Mo	3.1694662592	1.8317225707	3.0295459950
Mo	9.5074618935	1.7988383817	3.0830573121
Mo	6.3097750728	7.3374224294	3.0842994686
Mo	0.0291577682	7.3374307988	3.0843483382
Mo	6.3446163859	1.8228654085	3.0435948115
Mo	7.9178781910	4.5735742659	3.0573981974
Mo	4.7492367717	4.5859477001	3.0448865248
S	6.3349437392	9.1754356462	4.6486484547
S	1.5878498136	0.9179194259	4.5980056675
S	11.1105708052	0.9007872976	4.6493600585
S	6.2531683234	9.1456397143	1.5142525644
S	1.5745813992	0.9118543995	1.4691183255
S	11.0461771327	0.8450983019	1.5149788160
S	7.9208099409	6.4078890222	4.6249467585
S	3.1695651924	3.6571347520	4.5996205175
S	7.9042314166	0.9009448869	4.6493080603
S	7.9023340314	6.4178994501	1.5081815990
S	3.1695418058	3.6735912425	1.4707049131
S	7.9686515528	0.8452789531	1.5149125276
S	4.7510719815	0.9180627251	4.5980123342
S	4.7315541388	6.3972591966	4.6514747094
S	9.5075685595	3.6585340186	4.6244447902
S	4.7643124867	0.9119338216	1.4691289048
S	4.7139280957	6.4815764733	1.5169107393
S	9.5076034731	3.6385552828	1.5078543317
S	3.1691626615	9.1528080800	4.6793841536
S	-3.1686415501	9.1633758421	4.6095668499
S	0.0105326151	3.6548269088	4.6111470188
S	-3.1685982329	9.1442469797	1.4778351796
S	-0.0042142870	3.6645871996	1.4798364706
S	6.3286133028	3.6550474666	4.6111060607
S	6.3433352535	3.6647905095	1.4797957372
S	0.0038163995	9.1754971893	4.6487738716
S	-1.5817905103	6.4078328316	4.6249748890
S	1.6073910298	6.3971823436	4.6515029670
S	0.0854864688	9.1456747768	1.5142652209
S	-1.5632725868	6.4178249902	1.5082340122
S	1.6249916012	6.4815320335	1.5169487013

9.2. $v_{Se}-MoSe_2$

N	3.2947992040	9.4562748449	8.8311745487
O	2.1874039652	9.4454438997	8.3132671118
O	4.4014264494	9.4450916708	8.3116016412
Se	1.6497901553	0.9532624120	5.2383099097
Se	11.5414100603	0.9345585693	5.2935134965
Se	6.5794719004	9.5299020772	5.2935832447
Se	0.0108313386	3.7964930833	5.2509432149
Se	3.2920761911	9.5080759737	5.3697572029
Se	-3.2919477018	9.5167308682	5.2503829617
Se	-1.6433161635	6.6552009432	5.2636705015
Se	1.6693525351	6.6461649112	5.2945755818
Se	0.0046603935	9.5298887957	5.2936008828
Se	4.9343085015	0.9532534918	5.2383153046
Se	9.8760385578	3.7989084171	5.2633614814
Se	4.9147532719	6.6461598707	5.2945767102
Se	8.2274050579	6.6551950771	5.2636726352
Se	8.2107012139	0.9345533679	5.2935141915
Se	3.2920398798	3.7989462379	5.2386941173
Se	6.5732470701	3.7964781561	5.2509479098
Mo	-0.0082676215	1.8909876810	3.5735382682
Mo	4.8709152802	10.4142954283	3.6676137435
Mo	-4.9517860767	10.4527908587	3.5727257551
Mo	-1.6390744906	4.7488598239	3.5854277136
Mo	3.2920594840	7.6850273500	3.6699982352
Mo	-1.6320941513	10.4527791223	3.5727392278
Mo	1.7132125959	10.4142942513	3.6676178971
Mo	1.6513956342	4.7667401724	3.5739850369
Mo	-3.2919547919	7.6114632019	3.5852284041
Mo	3.2920498691	1.9023127657	3.5565256800
Mo	9.8760505401	1.8606943995	3.6167028854
Mo	6.5488619543	7.6248043939	3.6171595219
Mo	0.0352412728	7.6248025581	3.6171617232
Mo	6.5923665006	1.8909737224	3.5735429410
Mo	8.2231497406	4.7488517897	3.5854296650
Mo	4.9326901238	4.7667324208	3.5739863478
Se	1.6336007077	0.9447847212	1.8867443127
Se	-0.0030023930	3.8049895734	1.8977398883
Se	6.4803121664	9.5052350603	1.9379210983
Se	-3.2919389081	9.5000404629	1.8969419303
Se	-1.6197617648	6.6682952027	1.9284045552
Se	1.7000179923	6.7447828286	1.9398076471
Se	4.8840866451	6.7447764435	1.9398063205
Se	0.1038109068	9.5052324254	1.9379299977
Se	3.2920414005	3.8180777817	1.8874025541
Se	4.9505029279	0.9447671730	1.8867527897
Se	8.2808902796	0.8604951606	1.9388833777
Se	11.4712155679	0.8605037682	1.9388810029
Se	9.8760370167	3.7724108087	1.9283885805
Se	8.2038514673	6.6682868684	1.9284040820
Se	6.5870791855	3.8049710503	1.8977426388

9.3. v_{Te} - $MoTe_2$

N	3.5000640448	10.3124756281	9.1147349453
O	2.4053185584	10.2855563168	8.5413471355
O	4.6000501519	10.2894320114	8.5515155555
Mo	-0.0073923957	2.0582895950	3.8322382129
Mo	-1.7633168775	5.0695405465	3.8459674171
Mo	1.7223681151	5.0549937424	3.8333650722
Mo	-3.5402891375	8.1472768486	3.8451735634
Mo	3.5181575039	8.1127602365	3.9289689338
Mo	3.5182299113	2.0204028207	3.8165437931
Mo	-0.0172265465	8.1302293131	3.8759176113
Mo	7.0437793962	2.0582324198	3.8321909146
Mo	5.3140550878	5.0549999146	3.8334024494
Te	1.7622612870	1.0054657624	5.6311056028
Te	1.7483745123	0.9990711937	2.0146427326
Te	3.5182057082	4.0475210922	5.6322329985
Te	3.5182283452	4.0648614664	2.0160509620
Te	5.2741697150	1.0053775161	5.6310619371
Te	5.2880056848	0.9991423436	2.0145041507
Te	5.2925929980	7.0706407474	5.6975494362
Te	8.7784937837	1.0281775402	5.6953777845
Te	5.2592552183	7.1655479212	2.0590215574
Te	8.8440349171	0.9570957343	2.0563575234
Te	-0.0096286776	4.0562090347	5.6762163984
Te	-0.0214689662	4.0646390696	1.9956205542
Te	7.0460552967	4.0561203041	5.6762076395
Te	7.0578876450	4.0646411355	1.9956353382
Te	1.7437113461	7.0706590855	5.6974999331
Te	1.7771639192	7.1655269548	2.0589533504
Te	-1.7910524600	7.1061855790	5.6677706720
Te	-1.7673913128	7.1186170216	2.0434973160
Mo	5.3025174092	11.1984150590	3.9234375268
Mo	-5.2701805483	11.1733216603	3.8305262827
Mo	1.7338693968	11.1983288719	3.9232305688
Mo	-1.8104921227	11.1733786020	3.8302962610
Te	7.0887158149	10.1870527029	5.6960996376
Te	6.9932833449	10.1640150604	2.0552153130
Te	-3.5402164123	10.1732839779	5.6746027948
Te	-3.5403967967	10.1576376314	1.9936341199
Te	3.5179932366	10.1761177610	5.6594362858
Te	-0.0524371019	10.1871423865	5.6957736897
Te	0.0430426797	10.1640001712	2.0550069936
Te	12.3093616921	0.9570580280	2.0564523607
Te	12.3748470175	1.0283464140	5.6954478834
Mo	10.5766776788	2.0267164650	3.8750793731
Te	10.5766989069	4.0744234364	5.6674232112
Te	10.5766897231	4.0489108102	2.0435513406
Mo	8.7997313741	5.0695093776	3.8459875091
Te	8.8274924992	7.1061347368	5.6677952741
Te	8.8037047048	7.1186282224	2.0435820379
Mo	7.0535639261	8.1302447930	3.8760829967