

RESEARCH ARTICLE

Mechanical properties of lateral transition metal dichalcogenide heterostructuresSadegh Imani Yengejeh, William Wen, Yun Wang[†]*Centre for Clean Environment and Energy, School of Environment and Science, Griffith University,
Gold Coast Campus, Southport 4222, Australia**Corresponding author. E-mail: [†]yun.wang@griffith.edu.au**Received June 11, 2020; accepted September 8, 2020***Supplemental Material****MoS₂****1H**

3.1642264856087907	-0.0000000000008834	0.0000000000000000
-1.5821132427551616	2.7403005198520272	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Mo S

1 2

Direct

0.3333333469999999	0.6666666939999999	0.1250000000000000
0.6666666249999977	0.3333333249999981	0.2034565851457129
0.6666666249999977	0.3333333249999981	0.0465434208542876

1T'

6.3896450466670984	0.0000000000000008	-0.0000000000000001
-3.1948225233335488	5.7334302035443461	-0.0046169662032723
0.0000000000000004	-0.0103329515007108	23.4132840728015736

Mo S

4 8

Direct

0.0249100683464289	0.5498201366928580	0.2475882893824575
0.9750899316535711	0.9501798633071420	0.2524117106175425
0.5249100683464289	0.5498201366928580	0.2475882893824575
0.4750899316535711	0.9501798633071420	0.2524117106175425
0.3312301382877739	0.6624602766755567	0.1778975077928305
0.6687698617122262	0.8375397233244433	0.3221024922071695
0.8312301382877738	0.6624602766755567	0.1778975077928305
0.1687698617122261	0.8375397233244433	0.3221024922071695
0.1642746424836223	0.3285492848672356	0.3067632573104915
0.8357253575163779	0.1714507151327644	0.1932367426895085
0.6642746424836221	0.3285492848672356	0.3067632573104915

0.3357253575163777 0.1714507151327644 0.1932367426895085

1H/1T'

25.5759436178227482 0.1682233317418700 0.0000000000000000
-6.3211515988713884 10.9494844568903442 0.0000000000000000
0.0000000000000000 0.0000000000000000 19.9999904633000014

Mo S
32 64

Direct

0.1043673993974805 0.1045217461901515 0.6267229936839160
0.5796591778902342 0.0795512751208206 0.5792287813112840
0.2031746788858645 0.0784691308586338 0.5995158587265226
0.7016550737082868 0.0763230652845815 0.6006005664746286
0.1043343866530911 0.3544091097968128 0.6268500121568398
0.5796593449216561 0.3295502984341406 0.5792102623033500
0.2032295640848328 0.3285458150214079 0.5998832546349330
0.7016528210770896 0.3263333793311841 0.6005885380725089
0.3566892779300095 0.1071381356507445 0.5826614803314173
0.8228641828906567 0.0725210600918182 0.6244516677465805
0.4553552100776020 0.0807721500703764 0.5617143246338558
0.9452862691808589 0.0702914476946121 0.6497770020560302
0.3567231089933344 0.3571291715031607 0.5829127415985761
0.8228478652526185 0.3224643615098272 0.6244241631490501
0.4553444910236939 0.3307250057800134 0.5617488107184577
0.9452907516852822 0.3200597686617762 0.6495902835428907
0.1043182388898031 0.6044047285958869 0.6265894820941388
0.5796659091154417 0.5795444617236807 0.5792595463383445
0.2032100603264959 0.5784437261769610 0.5997788801218552
0.7016617972350485 0.5763177739306922 0.6006465443173566
0.1043084020922254 0.8544557374787874 0.6264152458959042
0.5796682482724459 0.8295656510643238 0.5792862041723684
0.2031426762927752 0.8283818361699631 0.5994078220587015
0.7016602312481218 0.8263342806591850 0.6006554136874417
0.3567527029800509 0.6071685965724478 0.5830990702814293
0.8228780189282648 0.5724839039829683 0.6244240893375336
0.4553494639419526 0.5807152892971723 0.5619363249559403
0.9452857996944521 0.5696971981496500 0.6495417692958886
0.3567176419389689 0.8572036287305334 0.5828276513895853
0.8228391696389682 0.8224844164132314 0.6245112073079039
0.4553522920648237 0.8307676577588143 0.5619184568725361
0.9452998772136338 0.8199635430209794 0.6497089134944257
0.0352060456878201 0.1603768548886654 0.5707497958451658
0.5478921273098937 0.1728418796683648 0.4950151299141783
0.1597603464900739 0.1603192059705059 0.5235824352351570
0.6716786931318174 0.1713595364330490 0.5158705682702993
0.0352479569960743 0.4101966494555337 0.5706017918179169
0.5478838922760502 0.4228957266017611 0.4950481583065627
0.1597195230469627 0.4099083645954840 0.5237173512376327
0.6716890385117703 0.4214280102793921 0.5158874688718874
0.2897008999737950 0.1653621066976225 0.5202231028588592

0.7947967969057920 0.1693946836982078 0.5391041802566230
0.4193233384319981 0.1698198269688754 0.4838490716362894
0.9167334570888954 0.1663713609465967 0.5634697063826490
0.2896664499982547 0.4152396369982208 0.5205642672938313
0.7947944309616783 0.4194270957353397 0.5390933903489356
0.4192705555893878 0.4198666946701909 0.4840351583012374
0.9166582203145508 0.4163482568606611 0.5633429414746165
0.0351992143385227 0.6601265474493860 0.5703970943788252
0.5478340422276630 0.6728211977943721 0.4951170242284152
0.1597376881171506 0.6597239965251509 0.5234321088647171
0.6716998200297282 0.6713757619200786 0.5159376261377022
0.0351683281536236 0.9104244918250347 0.5705540139419880
0.5478500999926365 0.9227853278545249 0.4951139945952370
0.1597363757018421 0.9100705336954698 0.5232828627546346
0.6716806659805530 0.9213350100126854 0.5159110809555372
0.2896685935150858 0.6649039723871164 0.5205231894145095
0.7948115949085895 0.6694710950698837 0.5391539649165747
0.4192390295098565 0.6696926712915342 0.4841778492868992
0.9167249112436725 0.6665148886038613 0.5634441336063127
0.2897093117055203 0.9150409013897951 0.5201752272764855
0.7948033289658648 0.9194032384416259 0.5391529845146612
0.4193175235769869 0.9196631984107899 0.4839936483518879
0.9166881141795159 0.9164733357289215 0.5635888930179430
0.0160606429691732 0.0158697013343997 0.7026481259107480
0.0160717637043751 0.2660123947004755 0.7028522679397123
0.0161280701462791 0.5159840059926688 0.7026982976516439
0.0160954491752588 0.7657904342656552 0.7024580161856065
0.1458439225176142 0.0207454385121572 0.7027738067505359
0.1457863638202951 0.2708332227727390 0.7031091637855524
0.1457939110698732 0.5210383879696850 0.7029882673531470
0.1458382690782416 0.7710668914221379 0.7026622756507312
0.2682816299875840 0.0185098815884790 0.6600052843167207
0.2683056989310388 0.2684045377277222 0.6603136896662112
0.2682999815171676 0.5186288402241950 0.6605100157594052
0.2682897615623061 0.7687699882967450 0.6601748691764617
0.3925944268290130 0.0181570207706078 0.6608485351056343
0.3925754815251123 0.2678280387128010 0.6609114032387396
0.3926221606125664 0.5179261193668270 0.6611272402142622
0.3926122336962523 0.7682467515338893 0.6610810708997837
0.5293515114073650 0.1543172197442821 0.6497303989080794
0.6499919825096052 0.1496886294015448 0.6707180334053692
0.7700523826505036 0.1447163886890471 0.6937644102588469
0.8903549984022229 0.1401975421903266 0.7189305597894895
0.5293439166373934 0.4042661600449693 0.6497352604061134
0.6499560293610567 0.3996110237672567 0.6707312938262365
0.7700700230643264 0.3946935156016775 0.6937534517223232
0.8903974851087030 0.3900000979698011 0.7188774211258071
0.5294270275078630 0.6543781524363740 0.6498471957491287
0.6499874055604836 0.6496560926962610 0.6707743960292112
0.7700889676636938 0.6446308743761238 0.6938116277905221

0.8904366798031406 0.6398793137739606 0.7188406927627462
0.5294202468783711 0.9043908560293746 0.6498360945237218
0.6499903749937289 0.8997077414949219 0.6707571075049688
0.7700638192074416 0.8947560650610518 0.6938193087662580
0.8903992527142396 0.8900909179377922 0.7189178067699132

MoSe₂

1H

3.2939483216371750 0.0000000000012434 0.0000000000000000
-1.6469741607654622 2.8526429252755445 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

Mo Se
1 2

Direct

0.3333333469999999 0.6666666939999999 0.1250000000000000
0.6666666249999977 0.3333333249999981 0.2088978669335304
0.6666666249999977 0.3333333249999981 0.0411021390664701

1T'

6.5160954181412833 0.0016154178772311 0.0000000000000000
-3.2590998656914452 5.9371422612993472 0.0000000000000000
-1.6292750222007388 -2.6664386338671164 20.0000000000000000

Mo Se
4 8

Direct

0.2136634458486526 0.4832795298120303 0.8881009769341830
0.1585426466964677 0.8688342659065498 0.8961475895658140
0.7136648366684213 0.4832768559780334 0.8881000260485052
0.6585413603742509 0.8688369814216230 0.8961485409515006
0.4754879696733170 0.5521033913529081 0.7982005836467181
0.8967181695671016 0.8000104485161472 0.9860479888532794
0.9754885763776571 0.5521065445914957 0.7982015130980713
0.3967175378458521 0.8000071860741258 0.9860470474019323
0.3818386703258767 0.2821763656693719 0.9630389539492725
0.9903674563684746 0.0699374273553133 0.8212096065507311
0.8818356205872533 0.2821751527141316 0.9630387734888259
0.4903704830098690 0.0699386249700495 0.8212097990111715

1H/1T'

26.6274572685277384 0.2696157302960449 0.0000000000000000
-6.5401037631586121 11.3265211364951259 0.0000000000000000
0.0000000000000000 0.0000000000000000 19.9999904633000014

Mo Se
32 64

Direct

0.1065700793080676 0.1065638270690190 0.6270719316073515
0.5790996949763964 0.0790658271735481 0.5793430903772907
0.2012884357879054 0.0764763859547796 0.5997117036613953
0.7011648161502341 0.0760205911709465 0.6007295785074351

0.1065597334573434 0.3565471746981975 0.6271142243273713
0.5791051028043522 0.3290694086429001 0.5793191953289804
0.2013044308699460 0.3264817502478047 0.5998293842474864
0.7011764702628280 0.3260217362527867 0.6007129614738042
0.3597059630542435 0.1100033237709679 0.5826518322586648
0.8227171526603115 0.0725382919433902 0.6245495255693118
0.4541746816195997 0.0793988778381920 0.5617978206299390
0.9444950142584816 0.0695407496153205 0.6486585242107950
0.3597196383050740 0.3600243269078949 0.5827639499404564
0.8227096517937741 0.3224979539166921 0.6245340588483569
0.4541973779483399 0.3293952870908010 0.5618154284494544
0.9444765443952653 0.3193362776573443 0.6486432067682277
0.1065514403566189 0.6065275865277762 0.6270425635003372
0.5791060848679384 0.5790646941243683 0.5793448728532347
0.2012995287735132 0.5764732665433923 0.5997934772451209
0.7011947027882619 0.5760421938298734 0.6007161236591935
0.1065676029110982 0.8565484794817509 0.6270032354354340
0.5790994303792619 0.8290567660547131 0.5793709448307908
0.2012847648167999 0.8264743296468410 0.5996900498223182
0.7011821593591906 0.8260348661689909 0.6007354443735879
0.3597111139742753 0.6099766922501105 0.5828055420644764
0.8227156179031493 0.5725026745592805 0.6245156519350848
0.4541846677582383 0.5793734097751645 0.5618925396398334
0.9444922991231927 0.5691255120756713 0.6486465007688358
0.3596899101768744 0.8599808892813979 0.5827078251079176
0.8227135102439794 0.8225224711272461 0.6245204469525563
0.4541717687497847 0.8293916859874600 0.5618802561047549
0.9445077212737764 0.8192991472052854 0.6486724254792046
0.0351777388010288 0.1601136519299128 0.5664729359951127
0.5465079897432394 0.1715125789507552 0.4897682057602925
0.1604993168808428 0.1607874421793604 0.5166491160224274
0.6706277682589179 0.1704653224078130 0.5103288884111294
0.0351640281507628 0.4100020527891056 0.5664740744266754
0.5465136280979060 0.4215470080691624 0.4897205125880173
0.1605248172289951 0.4106717116564937 0.5167049458755756
0.6706304709431743 0.4205350096873119 0.5103418993944869
0.2895941376679441 0.1649564711762757 0.5164606171343448
0.7939301539753491 0.1687333983000141 0.5335635010065346
0.4192088897922360 0.1694194144452454 0.4769552738546549
0.9162727282852468 0.1661632938439219 0.5569164705836495
0.2895700432398582 0.4148131873716964 0.5165661556663663
0.7939432646283464 0.4187292954071674 0.5335491906212184
0.4191766150916716 0.4194397173771074 0.4770064427152664
0.9162817724069331 0.4160874803904911 0.5568929983198702
0.0351593985472517 0.6600004524337831 0.5664220726307413
0.5464796595615362 0.6715137666416124 0.4898105305508817
0.1605185860896131 0.6606447202159810 0.5166065169112217
0.6706413353907236 0.6704957850155009 0.5103401272818339
0.0351438735678523 0.9100144599901655 0.5664519698761340
0.5464803865865888 0.9214827359859912 0.4897730905569803

0.1605206706868474	0.9107113303202868	0.5165677522722244
0.6706132868239096	0.9205090724153747	0.5103637173937018
0.2895846120172280	0.6647477293687386	0.5165428434343711
0.7939637329637205	0.6687821381204894	0.5335396263338864
0.4191623855089220	0.6693445609943782	0.4770833288533918
0.9162956193460294	0.6661094220899698	0.5569527117605449
0.2895814187950219	0.9148155801931968	0.5164356031772432
0.7939499318365604	0.9187748358460692	0.5335721878373308
0.4191783981411976	0.9193644893243863	0.4769747457518132
0.9163234105237050	0.9161670828642672	0.5569560700642304
0.0180204771780555	0.0179101454404081	0.7072462147243985
0.0180486343490459	0.2679722221430278	0.7073589784597641
0.0180595648854706	0.5178915304732674	0.7073338698826747
0.0180567456282033	0.7678845350651886	0.7072326482746768
0.1466003370327563	0.0215242965251407	0.7103448741742117
0.1465684159618030	0.2715264295900838	0.7104233631564545
0.1465921271263725	0.5216184418921651	0.7104048966718458
0.1465992433318095	0.7715978957876786	0.7102998867026042
0.2697100166108869	0.0199615301197371	0.6630339562755498
0.2697044439855663	0.2698513905362129	0.6631609158671763
0.2697158377887348	0.5199924135611771	0.6632032317306952
0.2697001585723885	0.7699761046534119	0.6631088470511279
0.3930221562331312	0.0183529989205091	0.6681826823136520
0.3930555786168811	0.2683253003004428	0.6682188995379260
0.3930526716747327	0.5183314435522631	0.6683171140717750
0.3930463087709635	0.7684370887325748	0.6682732405831654
0.5284763031890579	0.1534577333741132	0.6553974716951739
0.6494122160051161	0.1492582849603764	0.6765226634312480
0.7697984220563806	0.1445827811503518	0.6994042708260785
0.8904917617433786	0.1403839248464874	0.7248213029560365
0.5285010943424200	0.4034721983654705	0.6554100839717703
0.6494231921832234	0.3992857168503247	0.6764904608401817
0.7698251402310418	0.3946110548487342	0.6993922157114327
0.8904707191582576	0.3902026943003818	0.7248196530920602
0.5285090372845656	0.6534434147314253	0.6554618154853245
0.6494314643818710	0.6492266863745171	0.6765193956487219
0.7698354346696987	0.6445996118972469	0.6993965720419639
0.8905142786023351	0.6402566804005300	0.7247503610042662
0.5285066077026682	0.9035148284226986	0.6554503209494819
0.6494222421359035	0.8992780499506771	0.6765310899528483
0.7698323835059361	0.8946086793387500	0.6994105162807218
0.8905062233740347	0.8903438965026398	0.7247347135938710

WS₂

IH

3.1719554180786913	-0.0000000000007492	0.0000000000000000
-1.5859777089898734	2.7469939717149319	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

W S

1 2

Direct

0.3333333469999999	0.6666666939999999	0.1250000000000000
0.6666666249999977	0.3333333249999981	0.2038514151992352
0.6666666249999977	0.3333333249999981	0.0461485908007653

1T'

6.3690321811705841	0.0008107876818742	0.0000000000000000
-3.1862279507456384	5.7027963808348510	0.0000000000000000
-1.5921966873704134	-2.5608395956785288	20.0000000000000000

W S

4 8

Direct

0.2102621359224040	0.4765119271362118	0.8889172867426229
0.1619439566227163	0.8756018685823683	0.8953312797573740
0.7102605138550142	0.4765133051123636	0.8889176448531405
0.6619456831876580	0.8756005322872927	0.8953309221468654
0.4757377742841048	0.5491456622265672	0.8047146523641058
0.8964683649563138	0.8029681776424881	0.9795339201358917
0.9757378495601706	0.5491436417586770	0.8047145282337380
0.3964682646633386	0.8029700889069444	0.9795340322662656
0.3827049763304633	0.2856512785252860	0.9588796537948541
0.9895011503638880	0.0664625144993992	0.8253689067051495
0.8827048283877388	0.2856513198605304	0.9588798381428362
0.4895012752093835	0.0664624578236507	0.8253687343571613

1H/1T'

25.6563972179522466	0.1612278578834141	0.0000000000000000
-6.3442873815591927	10.9882864662826698	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.9999904633000014

W S

32 64

Direct

0.1041848335911624	0.1043377351830088	0.6258853587901854
0.5794376049303622	0.0793585187250088	0.5795979984630293
0.2034202240679690	0.0785769028460663	0.5999763532001197
0.7015313360754618	0.0763532804220404	0.6007099113935439
0.1041744017294519	0.3542998691532091	0.6259811059960327
0.5794392763494329	0.3293432392377440	0.5795824569433989
0.2034503253743267	0.3286162556422099	0.6001455668737279
0.7015563934423454	0.3263800507771180	0.6007084857609684
0.3561328482832522	0.1063379808777256	0.5819023537251411
0.8226044669391896	0.0723710492242162	0.6244762535138904
0.4557438882101366	0.0809334718141344	0.5621814691226064
0.9455764956278685	0.0707801207257575	0.6499213510896524
0.3561351176938601	0.3563482141116125	0.5820121274324137
0.8226257852279701	0.3223398067562258	0.6244468426186529
0.4557319536136362	0.3309313140026688	0.5621986956437723
0.9455920932518254	0.3203582852324729	0.6498769238878523

0.1041756504556446 0.6042679786308724 0.6258606910695264
0.5794353757654989 0.5793454653260071 0.5796117052248846
0.2034603697009985 0.5785883022686633 0.6000967422099706
0.7015598111927872 0.5763776975184811 0.6007215838573785
0.1041715301449102 0.8542854964874493 0.6257516918328960
0.5794280100104174 0.8293528507341321 0.5796250716790112
0.2034331386167096 0.8285502213205262 0.5999474542583556
0.7015398621133002 0.8263486505408864 0.6007272649485458
0.3561615896279307 0.6063875542387009 0.5820907243055871
0.8226258609259460 0.5723517949554306 0.6244456220816375
0.4557279559846563 0.5809514503547319 0.5622880271985196
0.9456179057841538 0.5701020355182251 0.6498756270179058
0.3561383323703637 0.8563706269563696 0.5819809353596810
0.8226123814134567 0.8223780445566149 0.6244778979638284
0.4557463824033974 0.8309836406630495 0.5622567641176417
0.9456108554749960 0.8205466191813784 0.6499288697900454
0.0360293450109879 0.1612059732072169 0.5701069830878964
0.5479097609685297 0.1728840816786885 0.4949038103180854
0.1607410178261830 0.1610070301581743 0.5226205768201382
0.6715549067003224 0.1714029894892946 0.5157228828540994
0.0360442586682908 0.4110412947203201 0.5700735807066266
0.5479017817481449 0.4229096713424880 0.4949275142540657
0.1607195608684080 0.4108455233866408 0.5227062036801939
0.6715682992546661 0.4214205620055438 0.5157302145810476
0.2894269017797484 0.1647518527321878 0.5195982696283252
0.7947200783325101 0.1694607617073061 0.5387865101218594
0.4188306920460434 0.1690950136084481 0.4830289260274796
0.9166835976797785 0.1665096016288174 0.5636904275341195
0.2894060706401689 0.4147380056769663 0.5197343389373259
0.7947548578905810 0.4195070923108375 0.5387765012428432
0.4187994582825993 0.4191424260270438 0.4830974098004077
0.9167039167302633 0.4164558999855004 0.5636541600536660
0.0360255653039090 0.6609986404764001 0.5699672739588451
0.5478622783536977 0.6728639634576368 0.4949719794587608
0.1607507080384494 0.6607851136396121 0.5225754426915969
0.6715571819659587 0.6713969818625571 0.5157447198352045
0.0360159566935891 0.9111879359459820 0.5700100954130178
0.5478799898828086 0.9228565701474949 0.4949550684545301
0.1607631509022127 0.9109316623190509 0.5224843658923461
0.6715448567327584 0.9213697722118894 0.5157438350570089
0.2894073711481155 0.6645988196972894 0.5196962321388838
0.7947642927260148 0.6695371483081942 0.5388021639720719
0.4187700430127208 0.6690603018796821 0.4831552291516559
0.9167258469877169 0.6665506002432409 0.5637573493433194
0.2894390953349273 0.9146499133294981 0.5195617086847264
0.7947312541073757 0.9194916785552536 0.5388183534096171
0.4187926883502939 0.9190181889888365 0.4830744801520268
0.9166969270535859 0.9165701744635300 0.5637658267507888
0.0159699353374521 0.0159928575115771 0.7027987652054648
0.0160178141705813 0.2660359873706781 0.7030704478249916

0.0160419798607379	0.5159657243329434	0.7029422704866661
0.0159910836862736	0.7659248769611082	0.7026657507474283
0.1450512329364528	0.0201349430196487	0.7033682927260969
0.1450232328972447	0.2701569761624611	0.7035414024145439
0.1450632679367487	0.5203219102405470	0.7034996882255413
0.1450783665198614	0.7703100381385113	0.7033338602730623
0.2684371132349384	0.0185442186890867	0.6602967119173044
0.2684520394032575	0.2684742984102613	0.6604400717764918
0.2684613974952654	0.5185894138814504	0.6605307199368227
0.2684587443369892	0.7686692267562449	0.6603946377543437
0.3923612895962520	0.0176549724788799	0.6613008485190548
0.3923622808678573	0.2675194476842933	0.6613002384199902
0.3923929162571653	0.5175551218669625	0.6614094828541965
0.3923969402832057	0.7677329813578879	0.6613884548399867
0.5297163196690278	0.1546470571333458	0.65092831111168642
0.6500495805387629	0.1498810613760568	0.6711880609993983
0.7700551033850118	0.1448053374107943	0.6941964043174735
0.8902937490174239	0.1402095503715444	0.7192447771520847
0.5297213723536842	0.4046207242142330	0.6509386683589611
0.6500505244241097	0.3998569818278668	0.6711871816090280
0.7700889358890066	0.3948108116450229	0.6941924630835601
0.8903494973620312	0.3900171026084678	0.7191864008934985
0.5297415233209151	0.6546646559786069	0.6509902199834485
0.6500461139216185	0.6498311711262588	0.6712085048401093
0.7700939847729842	0.6448061664016009	0.6942277458229782
0.8903915943090439	0.6400613628973346	0.7191183626804616
0.5297408180886620	0.9046985358085777	0.6509770914573707
0.6500432454521814	0.8998590526042562	0.6712063488579076
0.7700681341366931	0.8948107270932937	0.6942291849945974
0.8903525201237343	0.8902485934658344	0.7191712345273160

WSe₂

1H

3.2893786429240466	0.0000000000011301	0.0000000000000000
-1.6446893214090681	2.8486854674229720	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

W Se

1 2

Direct

0.3333333469999999	0.6666666939999999	0.1250000000000000
0.6666666249999977	0.3333333249999981	0.2094859074881157
0.6666666249999977	0.3333333249999981	0.0405140985118848

1T'

6.5445272597339113	0.0010766054489618	0.0000000000000000
-3.2738138139446686	5.9192411158180107	0.0000000000000000
-1.6361625342316324	-2.6581456143309481	20.0000000000000000

W Se

4 8

Direct

0.2142630300658234	0.4842798075191905	0.8881102633159692
0.1579430624792968	0.8678339881993895	0.8961383031840278
0.7142618219367742	0.4842782773828884	0.8881100098886314
0.6579443751058980	0.8678355600167680	0.8961385571113745
0.4740540773779524	0.5493415941547394	0.7971450749041740
0.8981520618624661	0.8027722457143159	0.9871034975958235
0.9740551586803032	0.5493397839032493	0.7971450600424834
0.3981509555432060	0.8027739467623721	0.9871035004575202
0.3825346982614191	0.2834838590370329	0.9630684851921447
0.9896714284329322	0.0686299339876523	0.8211800753078589
0.8825364921116430	0.2834852341519881	0.9630689116630566
0.4896696114854793	0.0686285435321931	0.8211796608369408

1H/1T'

Building Supercell From POSCAR File

1.0000000000000000

26.6151225484966787	0.2662940728087042	0.0000000000000000
-6.5384880593161920	11.3258433373408192	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.9999904633000014

W Se

32 64

Direct

0.1066336591990630	0.1065772491844240	0.6239440334869814
0.578885299158718	0.0791381633264100	0.5804138655970374
0.2013629735964687	0.0764767765510396	0.5989471618229704
0.7004670746663321	0.0756414349719710	0.6013379468846137
0.1069360549371459	0.3568702427498035	0.6256043545852704
0.5790810412854182	0.3294665084800523	0.5804396179508009
0.2013438447676071	0.3261478075857047	0.5990493546639588
0.7004570256908661	0.3253642137088729	0.6013627037052774
0.3600711006592589	0.1103626626313726	0.5822603623064952
0.8224284525789022	0.0731359595169292	0.6248814312008616
0.4547140924495389	0.0801340583221238	0.5626832228940594
0.9444499828105021	0.0814440044837677	0.6489431224020799
0.3601625578345397	0.3603019288212615	0.5821956476751179
0.8219721234341799	0.3218010831684957	0.6247846666743442
0.4549893523800639	0.3304446206516907	0.5626562195847797
0.9434121712107464	0.3219550141146299	0.6478071908554418
0.1064962355124938	0.6065645050143629	0.6261059750132617
0.5792232374496424	0.5794634566025031	0.5804585940088829
0.2014567962310789	0.5762751906110312	0.5996403857967986
0.7014451217358791	0.5761642241734719	0.6015013404551725
0.1069458501286612	0.8569963327634120	0.6255147069994260
0.5791367112611305	0.8292274216881450	0.5804690336761962
0.2014851651489939	0.8267026237195539	0.5995675781017503
0.7014848641936006	0.8267968202306236	0.6014950307087816
0.3600792608149664	0.6100853146280858	0.5823066426615068
0.8224676720763922	0.5713507552452262	0.6249355398454405
0.4550027370314250	0.5799490298485737	0.5626801657891859

0.9433934452799079 0.5644570925123991 0.6477784838593038
0.3599819304317137 0.8601223073203808 0.5823180708264292
0.8221938492726415 0.8219631930352318 0.6241546372881692
0.4547318475439007 0.8296737687070491 0.5626955046286690
0.9444903909918342 0.8068070340856095 0.6489131823227324
0.0353761885002424 0.1627369308967567 0.5650658272307788
0.5468629077669694 0.1722207075321232 0.4900988458709049
0.1619947158498452 0.1620000688339233 0.5136784603904292
0.6703064375660748 0.1704095155742780 0.5104137494004340
0.0356694701477693 0.4114371783570118 0.5658807007636681
0.5470768611875390 0.4224346478724842 0.4900320586561366
0.1617766003205260 0.4122725277927723 0.5145263860400355
0.6706649898944066 0.4209561342982304 0.5105896319976563
0.2899300596424216 0.1650752371855198 0.5154935098404253
0.7930461386912562 0.1680564134751911 0.5332977084079329
0.4195909394536054 0.1700735335707930 0.4760491870964808
0.9151639533824164 0.1666581996572009 0.5551696305107937
0.2898969135278811 0.4148900237832957 0.5155683604337933
0.7930323040950987 0.4177677781093110 0.5333383067153017
0.4196474666876095 0.4198738056163989 0.4759881869612415
0.9150456927312387 0.4147989308389347 0.5550011635406883
0.0356453031295262 0.6595430017649080 0.5658233469973473
0.5470925335294495 0.6722968198891680 0.4900618831054385
0.1617139236528418 0.6617285098663488 0.5150195503336322
0.6710205215916536 0.6710800341023462 0.5108561563615525
0.0353994561085223 0.9076099973673044 0.5649539451080035
0.5469016075834841 0.9220109217531410 0.4901321003192591
0.1618014329573845 0.9112881546482376 0.5144010042903349
0.6707030192765459 0.9205260859525163 0.5105777367065626
0.2898802585816661 0.6647853899806891 0.5158292824994557
0.7941918913028041 0.6686462751026908 0.5332158915912557
0.4195894766524474 0.6694810450920562 0.4760786208790915
0.9151417511691865 0.6630981335418499 0.5550933319002598
0.2899037468176964 0.9150654518977718 0.5157686842802653
0.7942129730740940 0.9193260683895941 0.5331601530065191
0.4195275111334529 0.9196974086124317 0.4761044790588376
0.9177487572724814 0.9173885562693977 0.5602208641341698
0.0152698532757785 0.0149767593979450 0.7010485974595866
0.0182492192890080 0.2708032557294380 0.7082006453086633
0.0177395531124338 0.5176271763346175 0.7087427449287912
0.0183542080492635 0.7653167645575332 0.7081889182312004
0.1443600507557504 0.0203520934538292 0.7099775399794693
0.1442475836587616 0.2681035787966879 0.7100403726545989
0.1452979614310277 0.5202285907466805 0.7106291699745640
0.1454008751744266 0.7704987874401148 0.7105750346451025
0.2700996231486040 0.0206205755483696 0.6631575124035410
0.2699804133348328 0.2700312409067835 0.6629231136767969
0.2700773720399872 0.5197753554205510 0.6632096188631810
0.2701694661136087 0.7703028761964694 0.6632994035098930
0.3927263907909190 0.0179259222033291 0.6694496686615137

0.3928493844704267 0.2680485222546509 0.6694525154319635
0.3928467313891698 0.5178565715487388 0.6694754253410571
0.3927557216823464 0.7678221491733049 0.6694679884083203
0.5287013811240218 0.1541594865409458 0.6573998854071471
0.6491180456168497 0.1491892601415151 0.6780576022249776
0.7691510806967310 0.1442961415670800 0.7002329412500218
0.8895148216410644 0.1440592443700714 0.7267070926214614
0.5289165054920202 0.4043581084865384 0.6574415311484006
0.6495155545985898 0.3999088221088304 0.6780163490545763
0.7691453281140181 0.3937462954580801 0.7002772676780810
0.8895121671184872 0.3892719603032864 0.7261700757997693
0.5289408470015940 0.6541063386899849 0.6574649981915146
0.6499274344364547 0.6500238109457049 0.6778196138153575
0.7704479965990955 0.6453757304550930 0.7004793905356835
0.8895829696043794 0.6345145041044565 0.7267833621742678
0.5287412900724930 0.9038916299043582 0.6574090281062667
0.6495934423619751 0.8993865232172960 0.6780230440384264
0.7704734757423664 0.8951941292036002 0.7004794406503650
0.8920187152645773 0.8916451647152204 0.7220705551249494