



Supporting Information

for

Theoretical understanding of electronic and mechanical properties of 1T' transition metal dichalcogenide crystals

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The elastic constants, lattice constants, and fractional coordinates of 1T' MoS₂, MoSe₂, WS₂, and WSe₂

Table S1: Elastic constants of 1T' TMDs.

TMD	C_{11} (GPa)	C_{22} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{66} (GPa)
MoS ₂ -1T'	184	184	34	26	30	17	72
MoSe ₂ -1T'	140	140	48	18	28	12	63
WS ₂ -1T'	179	179	29	27	35	15	74
WSe ₂ -1T'	161	161	43	18	30	10	66

Lattice constants and the corresponding fractional coordinates of MoS₂

1T'

6.3896450466670984	0.00000000000000008	-0.00000000000000001
-3.1948225233335488	5.7334302035443461	-0.0046169662032723
0.00000000000000001	-0.0025832378751777	5.8533210182003934

Mo S

4 8

Direct

0.0249100683464292	0.5498201366928583	0.9903531575298317
0.9750899316535708	0.9501798633071417	0.0096468424701683
0.5249100683464292	0.5498201366928583	0.9903531575298317
0.4750899316535708	0.9501798633071417	0.0096468424701683
0.3312301382877720	0.6624602766755601	0.7115900311713190
0.6687698617122280	0.8375397233244399	0.2884099688286810
0.8312301382877720	0.6624602766755601	0.7115900311713190
0.1687698617122280	0.8375397233244399	0.2884099688286810
0.1642746424836190	0.3285492848672362	0.2270530292419650
0.8357253575163810	0.1714507151327638	0.7729469707580350
0.6642746424836190	0.3285492848672362	0.2270530292419650
0.3357253575163810	0.1714507151327638	0.7729469707580350

Lattice vectors and the corresponding fractional coordinate of MoSe₂

1T'

6.5355606848268772	0.0000000000000005	-0.0000000000000001
-3.2677803424134391	5.9605312743774821	-0.0906926502774131
0.0000000000000001	-0.0849343856189682	6.5006933161539138

Mo Se

4 8

Direct

0.0290750595021705	0.5581501190043200	0.9896230404994407
0.9709249404978295	0.9418498809956800	0.0103769595005595
0.5290750595021705	0.5581501190043200	0.9896230404994407
0.4709249404978293	0.9418498809956800	0.0103769595005595
0.3272601685119871	0.6545203371239902	0.7146140989348233
0.6727398314880129	0.8454796628760098	0.2853859010651766
0.8272601685119871	0.6545203371239902	0.7146140989348233
0.1727398314880129	0.8454796628760098	0.2853859010651766
0.1647887744037275	0.3295775487074461	0.2176471467585184
0.8352112255962725	0.1704224512925542	0.7823528532414888
0.6647887744037275	0.3295775487074461	0.2176471467585184
0.3352112255962728	0.1704224512925542	0.7823528532414888

Lattice vectors and the corresponding fractional coordinate of WS₂

1T'

1.0000000000000000
6.4504160368482530 0.00000000000000008 -0.00000000000000001
-3.2252080184241261 5.7129809797774760 0.0036739357926529
0.00000000000000001 0.0062438259686736 5.7724584614076333

W S
4 8

Direct

0.0250259519529066 0.5500519039058204 0.9913466733250006
0.9749740480470933 0.9499480960941796 0.0086533266749994
0.5250259519529067 0.5500519039058204 0.9913466733250006
0.4749740480470934 0.9499480960941796 0.0086533266749994
0.3293408884560970 0.6586817770122171 0.7072539760472207
0.6706591115439030 0.8413182229877829 0.2927460239527793
0.8293408884560970 0.6586817770122171 0.7072539760472207
0.1706591115439030 0.8413182229877829 0.2927460239527793
0.1653080018332155 0.3306160035664292 0.2294794234771181
0.8346919981667845 0.1693839964335707 0.7705205765228819
0.6653080018332155 0.3306160035664292 0.2294794234771181
0.3346919981667845 0.1693839964335707 0.7705205765228819

Lattice vectors and the corresponding fractional coordinate of WSe₂

1T'

6.5713076526683087 0.0000000000000009 -0.0000000000000001
-3.2856538263341535 5.9401005272150673 -0.0755272029720784
0.0000000000000001 -0.0742183519869420 6.2779127348156480

W Se

4 8

Direct

0.0293193584847273 0.5586387169694547 0.9890611518402181
0.9706806415152656 0.9413612830305453 0.0109388481597819
0.5293193584847344 0.5586387169694547 0.9890611518402181
0.4706806415152656 0.9413612830305453 0.0109388481597819
0.3266491310919974 0.6532982622839967 0.7029118506403123
0.6733508689080026 0.8467017377160033 0.2970881493596877
0.8266491310919974 0.6532982622839967 0.7029118506403123
0.1733508689080026 0.8467017377160033 0.2970881493596877
0.1647839415961130 0.3295678830922171 0.2250558405099312
0.8352160584038870 0.1704321169077829 0.7749441594900688
0.6647839415961130 0.3295678830922171 0.2250558405099312
0.3352160584038870 0.1704321169077829 0.7749441594900688