

First principles study of photocatalytic activity in ZnO-Janus van der Waals heterostructures

Supporting Information

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In the following sections, we report the optimized geometries of the considered monolayers and heterostructures in POSCAR format.

Monolayer

1) ZnO

ZnO

```
1.0000000000000000
 3.2873909235949093  0.0000000000000000  0.0000000000000000
-1.6436954617474941  2.8469640519483885  0.0000000000000000
 0.0000000000000000  0.0000000000000000  25.0000000000000000
```

```
Zn  0
  1  1
```

Direct

```
0.6666616512168062  0.3332983043009534  0.5000000000000000
0.3333283647831919  0.6666316896990452  0.5000000000000000
```

2) VBrSe

VBrSe

```
1.0000000000000000
```

3.3257136161056637	0.0000000000000000	0.0000000000000000
-1.6628568080528319	2.8801524773020297	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

V Br Se
1 1 1

Direct

0.9777769941599601	0.9888884970799765	0.5319645984386909
0.3111078566306418	0.6555538983153184	0.5987465201023454
0.3111151732093944	0.6555575566046983	0.4687889424589642

3) VBrTe

VBrTe

1.0000000000000000		
3.4584614553830213	0.0000000000000000	0.0000000000000000
-1.7292307276418202	2.9951154783601348	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Br V Te
1 1 1

Direct

0.6666646600000021	0.3333318230000017	0.3192125553210303
0.3333308400000021	0.6666652560000017	0.3729001313975786
0.6666634680000030	0.3333318829999996	0.4324013272813900

4) VClSe

VClSe

1.0000000000000000		
3.2258377479165077	0.0000000000000000	0.0000000000000000
-1.6129188739582538	2.7936574381830481	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

V Cl Se
1 1 1

Direct

0.3333308400000021	0.6666652560000017	0.3738854418515132
0.6666646600000021	0.3333318230000017	0.3228115574961521
0.6666634680000030	0.3333318829999996	0.4278170146523266

5) VCITe

VCITe

1.0000000000000000		
3.3687814618436374	0.0000000000000000	0.0000000000000000
-1.6843907309716419	2.9174503257725002	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

V Cl Te
1 1 1

Direct

0.3333308400000021	0.6666652560000017	0.3709559759908316
0.6666646600000021	0.3333318230000017	0.3218994540114508
0.6666634680000030	0.3333318829999996	0.4316585839977165

Heterostructures

1) ZnO-VBrSe (*m1*)

S1

ZnO-VBrSe

```
1.0000000000000000
 3.2823643802827078  0.0000000000000000  0.0000000000000000
-1.6411821901912773  2.8426109378690967  0.0000000000000000
 0.0000000000000000  0.0000000000000000  25.0000000000000000
```

```
Zn  O   V   Br  Se
 1   1   1   1   1
```

Direct

```
0.5796924780145218  0.1888606599644334  0.3341396953801805
0.9130128028222586  0.8555245735369610  0.3320556364326919
0.9098485445857847  0.8555699442044826  0.5166171274489884
0.2431544151028788  0.5222394188168025  0.5833789503638442
0.2431817724745500  0.5222364104773192  0.4533096373743035
```

S2

ZnO-VBrSe

```
1.0000000000000000
 3.2863179016722448  0.0000000000000000  0.0000000000000000
-1.6431589508861060  2.8460347878269219  0.0000000000000000
 0.0000000000000000  0.0000000000000000  25.0000000000000000
```

```
Zn  O   V   Br  Se
 1   1   1   1   1
```

Direct

```
0.1099611840071475  0.2553530021940773  0.3340016356986126
0.7766407263923796  0.5886813715845278  0.3314861498237391
0.7785344485149679  0.5890178525701870  0.5167945895353370
0.1118926065316330  0.2556954883614182  0.5835302500879180
0.1118610475538944  0.2556832922897811  0.4536884218544017
```

S3

ZnO-VBrSe

```
1.0000000000000000
 3.2847374713181758  0.0000000000000000  0.0000000000000000
-1.6423687357090477  2.8446660949913540  0.0000000000000000
 0.0000000000000000  0.0000000000000000  25.0000000000000000
```

```
Zn  O   V   Br  Se
 1   1   1   1   1
```

Direct

```
0.7765690157962339  0.5887475654780019  0.3353589917538073
0.4432424443035430  0.9220730430392834  0.3334440116066588
0.7785177989168020  0.5890014500396674  0.5157065902044380
0.1118670131938373  0.2556727229809681  0.5824889736626417
0.1118327727895831  0.2556682094620726  0.4525024797724626
```

S4

ZnO-VBrSe

1.0000000000000000
3.2883068699440754 0.0000000000000000 0.0000000000000000
-1.6441534350220515 2.8477572848776895 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Zn O V Br Se
1 1 1 1 1

Direct

0.1101698244017086 0.2544658296302273 0.3345806345340492
0.4435154092010691 0.9211501684730763 0.3322379779581581
0.7783357099417003 0.5896228659008784 0.5163077607168844
0.1116887364665260 0.2563086280394771 0.5830708591597684
0.1116573499889952 0.2562755099563532 0.4533038146311483

S5

ZnO-VBrSe

1.0000000000000000
3.2823687269181478 0.0000000000000000 0.0000000000000000
-1.6411843635089973 2.8426147021658084 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Zn O V Br Se
1 1 1 1 1

Direct

0.4429428337287646 0.9205534461173812 0.3341394511369771
0.7762828966534698 0.5872314475252622 0.3320558798277631
0.7787037343641146 0.5900033778712128 0.5166172147404211
0.1120625849272727 0.2566954842500877 0.5833789090981014
0.1120369953263918 0.2566702352360579 0.4533095921967316

S6

ZnO-VBrSe

1.0000000000000000
3.2847875504408388 0.0000000000000000 0.0000000000000000
-1.6423937752703799 2.8447094647837807 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Zn O V Br Se
1 1 1 1 1

Direct

0.0446655094711232 0.7228735062693588 0.3353807090250243
0.7113237288370229 0.0562043838794892 0.3334597212581301
0.0442396596944761 0.7217941524931177 0.5156939908817293
0.3775736844488762 0.3884543072241371 0.5824758532252616
0.3775774485485073 0.3884706341338955 0.4524907726098348

2) ZnO-VBrSe (m2)

S1

ZnO-VBrSe

1.0000000000000000

	3.2801657979987202	0.0000000000000000	0.0000000000000000
	-1.6400828990492502	2.8407069097588082	0.0000000000000000
	0.0000000000000000	0.0000000000000000	25.0000000000000000
Zn	0	V	Br
	1	1	1
Se			1

Direct

0.5803259534603313	0.1885869969805682	0.3297903915372586
0.9136459763874996	0.8552542643447794	0.3294417381888834
0.9094220941225402	0.8557512752408130	0.5211483998099879
0.2427579604412600	0.5224184680652328	0.4545129558846526
0.2427380285883629	0.5224200023685981	0.5846075615792188

S2

ZnO-VBrSe

1.0000000000000000		
3.2819862204436077	0.0000000000000000	0.0000000000000000
-1.6409931102717217	2.8422834418417384	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
Zn	0	V
	1	1
Se		1
Br		

Direct

0.1094515802304059	0.2557426973726677	0.3280740129243114
0.7761203756875616	0.5890593694110819	0.3278096216769057
0.7788795993047799	0.5887622248841708	0.5222230337341003
0.1122174267871046	0.2554273370922147	0.5856587239341522
0.1122210309901419	0.2554393782398563	0.4557356547305389

S3

ZnO-VBrSe

1.0000000000000000		
3.2814628009051257	0.0000000000000000	0.0000000000000000
-1.6407314005024729	2.8418301472245648	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
Zn	0	V
	1	1
Br		1
Se		

Direct

0.7758157950507325	0.5883813860871712	0.3301973134505261
0.4424872610746320	0.9217091051839290	0.3299334953522646
0.7790273538793429	0.5892476427561348	0.5208154312326343
0.1123222957348418	0.2559036117165547	0.4542875870431757
0.1123763392604573	0.2559212452561894	0.5842672199214149

S4

ZnO-VBrSe

1.0000000000000000		
3.2827430266326547	0.0000000000000000	0.0000000000000000
-1.6413715133662568	2.8429388552272092	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Br	Se
1	1	1	1	1

Direct

0.1113210023418176	0.2552279673331626	0.3281298452013601
0.4446343774363086	0.9218847658032914	0.3279466518777738
0.7775770966140456	0.5891233602789185	0.5221359328023070
0.1109259970156202	0.2557966229913902	0.4557146246200858
0.1109085565922356	0.2557902855932426	0.5855739924984817

S5

ZnO-VBrSe

1.0000000000000000		
3.2801673949768544	0.0000000000000000	0.0000000000000000
-1.6400836975383173	2.8407082927824421	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Br	Se
1	1	1	1	1

Direct

0.4416712904835620	0.9197509644532573	0.3297909465802462
0.7750171907742498	0.5864302499742493	0.3294419673484015
0.7795525019413887	0.5905416720666352	0.5211481901372892
0.1128839401891994	0.2572059484604523	0.4545127459908045
0.1129041216115994	0.2572251560454006	0.5846071969432529

S6

ZnO-VBrSe

1.0000000000000000		
3.2815099068031395	0.0000000000000000	0.0000000000000000
-1.6407549534514800	2.8418709421289132	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Br	Se
1	1	1	1	1

Direct

0.0446639908611388	0.7228136995491994	0.3302216669956763
0.7113250710156720	0.0561459092060943	0.3299511795309087
0.0442396517880610	0.7218324665228479	0.5208012331918823
0.3775796508588627	0.3885121203038722	0.4542747032700802
0.3775716664762712	0.3884927884179916	0.5842522640114538

3) ZnO-VBrTe (*m1*)

S1

ZnO-VBrTe

1.0000000000000000		
3.3414308170305245	0.0000000000000000	0.0000000000000000
-1.6702252177014167	2.8929149372261094	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Br	Te
1	1	1	1	1

Direct

0.1757453486071867	0.7872177821777768	0.3271921260663291
0.5092160100050052	0.4540139451274356	0.3256462281129942
0.5123855085348126	0.4565889969942418	0.5246552095436385
0.8457832379283872	0.1233130031418455	0.5897782326352043
0.8457599079246165	0.1232972795587060	0.4522292506418353

S2

ZnO-VBrTe

1.0000000000000000				
3.3449348263076262	0.0000000000000000	0.0000000000000000		
-1.6724674131538131	2.8967985335993016	0.0000000000000000		
0.0000000000000000	0.0000000000000000	25.0000000000000000		
Zn	O	V	Br	Te
1	1	1	1	1

Direct

0.1141439038954033	0.2574064664224380	0.3263438428174155
0.7807390552196836	0.5906987470463108	0.3246240901287436
0.7757876724326422	0.5876695694694831	0.5252116767654584
0.1090866997662232	0.2543129502363684	0.5903085012815410
0.1091326816860558	0.2543432738253912	0.4530129360068429

S3

ZnO-VBrTe

1.0000000000000000				
3.3432558181368286	0.0000000000000000	0.0000000000000000		
-1.6716279090684143	2.8953444698702229	0.0000000000000000		
0.0000000000000000	0.0000000000000000	25.0000000000000000		
Zn	O	V	Br	Te
1	1	1	1	1

Direct

0.7810048381516239	0.5909094528058674	0.3268363554594842
0.4476157891519961	0.9242111892777913	0.3255208616446552
0.7755724701717384	0.5875654926481033	0.5247610527911348
0.1088797403842534	0.2542137655746828	0.5899091219250465
0.1089562071404089	0.2542630906935415	0.4524736551796735

S4

ZnO-VBrTe

1.0000000000000000				
3.3468694639848291	0.0000000000000000	0.0000000000000000		
-1.6734347319924145	2.8984739789748857	0.0000000000000000		
0.0000000000000000	0.0000000000000000	25.0000000000000000		
Zn	O	V	Br	Te
1	1	1	1	1

Direct

0.1141603100861559	0.2576752860613496	0.3261736059468348
0.4474372090835885	0.9243061733476168	0.3246110501973405

0.7757001821212413 0.5875026728105013 0.5252294316803727
 0.1090071398347874 0.2541500926284428 0.5903506036262769
 0.1090621888742405 0.2541887771521019 0.4531363555491836

S5

ZnO-VBrTe

1.0000000000000000
 3.3409127338736679 0.0000000000000000 0.0000000000000000
 -1.6704563669368340 2.8933152993751081 0.0000000000000000
 0.0000000000000000 0.0000000000000000 25.0000000000000000

Zn O V Br Te
 1 1 1 1 1

Direct

0.4470108537805402 0.9243520192281309 0.3271873343842273
 0.7802907823834175 0.5909773023775600 0.3256407930798488
 0.7760305894830708 0.5875055534472438 0.5246587117275183
 0.1093277046719905 0.2541427544970247 0.5897820556506801
 0.1093691146809945 0.2541763614500425 0.4522321521577410

S6

ZnO-VBrTe

1.0000000000000000
 3.3432326728383206 0.0000000000000000 0.0000000000000000
 -1.6716163364191603 2.8953244254537363 0.0000000000000000
 0.0000000000000000 0.0000000000000000 25.0000000000000000

Zn O V Br Te
 1 1 1 1 1

Direct

0.6425693833152764 0.3213191469042371 0.3268302813591433
 0.3092652501925954 0.6546674471813034 0.3255147968474787
 0.6456323451908190 0.3228286824939630 0.5247649999960231
 0.9789751483111786 0.9895002375260731 0.5899138377991022
 0.9789379039901362 0.9894814698944288 0.4524771309982611

4) ZnO-VBrTe (*m2*)

S1

ZnO-VBrTe

1.0000000000000000
 3.3384971780265125 0.0000000000000000 0.0000000000000000
 -1.6692485890132562 2.8912233666472020 0.0000000000000000
 0.0000000000000000 0.0000000000000000 25.0000000000000000

Zn O V Br Te
 1 1 1 1 1

Direct

0.1752768312803070 0.7867673360049707 0.3295166409730896
 0.5086353393588894 0.4534549888859871 0.3290531749525698
 0.5127631413439957 0.4569530829439046 0.5177853651606696
 0.8461034385089334 0.1236230928302362 0.4528271419819916
 0.8461112625078755 0.1236325063349142 0.5903187239316594

S2

ZnO-VBrTe

```
1.0000000000000000
 3.3404331610690488  0.0000000000000000  0.0000000000000000
-1.6702165805345244  2.8928999771433421  0.0000000000000000
 0.0000000000000000  0.0000000000000000  25.0000000000000000
Zn  O   V   Te  Br
 1   1   1   1   1
```

Direct

```
0.1157425620375108  0.2572515737246093  0.3278370535512565
0.7823506963067359  0.5905692225313004  0.3274289239039518
0.7747116790752528  0.5877606218577967  0.5188343186282154
0.1080292795899496  0.2544261180824066  0.5913519452392393
0.1080557959905306  0.2544234708038857  0.4540488056773313
```

S3

ZnO-VBrTe

```
1.0000000000000000
 3.3413948298055085  0.0000000000000000  0.0000000000000000
-1.6706974149027543  2.8937328066991452  0.0000000000000000
 0.0000000000000000  0.0000000000000000  24.7589959576437337
Zn  O   V   Br  Te
 1   1   1   1   1
```

Direct

```
0.1154047562246703  0.2573604789125952  0.3270050008940544
0.4486885650940309  0.9240061052855353  0.3266854338996552
0.7748577065281523  0.5877045139359822  0.5193037958335651
0.1082429368649258  0.2543872667121150  0.4539750157606477
0.1081730652882413  0.2543646371537918  0.5925318006120790
```

S4

ZnO-VBrTe

```
1.0000000000000000
 3.3414003996456825  0.0000000000000000  0.0000000000000000
-1.6707001998228412  2.8937376303222311  0.0000000000000000
 0.0000000000000000  0.0000000000000000  25.0000000000000000
Zn  O   V   Br  Te
 1   1   1   1   1
```

Direct

```
0.1154150214130496  0.2572548779547930  0.3281565533111177
0.4486919009854020  0.9239045838454629  0.3278343815241413
0.7748520023430743  0.5877721288088296  0.5185618638239333
0.1082420757609981  0.2544591612601081  0.4538643393328812
0.1081660294974824  0.2544322501308045  0.5910839090079349
```

S5

ZnO-VBrTe

```
1.0000000000000000
```

3.3384581755317915	0.0000000000000000	0.0000000000000000
-1.6692290877658957	2.8911895894959621	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Te	Br
1	1	1	1	1

Direct

0.4478189453306385	0.9245370771877788	0.3295080466639533
0.7811164576246199	0.5911812047566798	0.3290430517578002
0.7754850287589647	0.5873742321918556	0.5177918217460515
0.1087970015637651	0.2540257671911021	0.5903259048532092
0.1088116117220324	0.2540357096725714	0.4528322219789942

S6

ZnO-VBrTe

1.0000000000000000		
3.3398910887269251	0.0000000000000000	0.0000000000000000
-1.6699455443634625	2.8924305287243719	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Br	Te
1	1	1	1	1

Direct

0.6425024053848389	0.3212716760826737	0.3302108110700814
0.3091930838107544	0.6546171907080236	0.3298567525277818
0.6456830266906763	0.3228634669788235	0.5172352310888115
0.9789739253258318	0.9895088578918632	0.4524200129620795
0.9790275897878971	0.9895357923386143	0.5897782393512472

5) ZnO-VClSe *m1*

S1

ZnO-VClSe

1.0000000000000000		
3.2451470394214770	0.0000000000000000	0.0000000000000000
-1.6225735196609143	2.8103797751762607	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Se	Cl
1	1	1	1	1

Direct

0.3760826713826404	0.3925063526634673	0.3342909137619969
0.7094403334544026	0.0591211073545637	0.3319646922281194
0.0455679077301454	0.7198189481618300	0.5188073202421108
0.3788821606298285	0.3865238978254979	0.4548414331924846
0.3789169398029983	0.3864607009946681	0.5795966875752754

S2

ZnO-VClSe

1.0000000000000000		
3.2434908864122529	0.0000000000000000	0.0000000000000000
-1.6217454431563278	2.8089455045977072	0.0000000000000000

```

0.0000000000000000 0.0000000000000000 25.0000000000000000
Zn  O   V   Se  Cl
 1   1   1   1   1
Direct
0.1072269009311526 0.2526682826376501 0.3339400518075166
0.7739505219156797 0.5860442158778909 0.3314244799203152
0.7803433108240583 0.5907916467310415 0.5191420546536349
0.1136531963518479 0.2574415159383676 0.4550899785098750
0.1137160829772697 0.2574853458150343 0.5799044821086667

```

S3

```

ZnO-VClSe
1.0000000000000000
 3.2419670048266882 0.0000000000000000 0.0000000000000000
-1.6209835023635693 2.8076257844322394 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Zn  O   V   Se  Cl
 1   1   1   1   1
Direct
0.7736386888542910 0.5857614182580093 0.3350767369354060
0.4403512959783598 0.9191309399103673 0.3331121505411758
0.7804692511688245 0.5909884472619424 0.5182116374908858
0.1137341084697709 0.2576027185517376 0.4540780194118952
0.1138357005287531 0.2576794670179154 0.5790225026206386

```

S4

```

ZnO-VClSe
1.0000000000000000
 3.2451666593142776 0.0000000000000000 0.0000000000000000
-1.6225833296073144 2.8103967665018450 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Zn  O   V   Cl  Se
 1   1   1   1   1
Direct
0.1070524146291874 0.2522783377726299 0.3343012263041487
0.4404414356159165 0.9189916640486899 0.3319717618040414
0.7804052893150484 0.5910765674625011 0.5188014518363175
0.1137730235833416 0.2577690649607831 0.5795902642242083
0.1136948668565267 0.2577073677554012 0.4548363428312925

```

S5

```

ZnO-VClSe
1.0000000000000000
 3.2401552841037051 0.0000000000000000 0.0000000000000000
-1.6200776420021052 2.8060567882615608 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
Zn  O   V   Se  Cl
 1   1   1   1   1

```

Direct

0.4398123657952979	0.9184515898475638	0.3342804739615843
0.7731897121042053	0.5851541400042990	0.3321146017341903
0.7807732721058969	0.5913954824836694	0.5188443156558407
0.1141020819471592	0.2580584383873159	0.4546271979184198
0.1141516130474258	0.2580943402771538	0.5796344577299806

S6

ZnO-VClSe

1.0000000000000000				
3.2420135180207295	0.0000000000000000	0.0000000000000000		
-1.6210067589605890	2.8076660660398902	0.0000000000000000		
0.0000000000000000	0.0000000000000000	25.0000000000000000		
Zn	O	V	Se	Cl
1	1	1	1	1

Direct

0.0433684957503218	0.7255397259768301	0.3351034281696954
0.7100482103202026	0.0588349019785710	0.3331331119240772
0.0451013293352958	0.7200203015566728	0.5181955513323473
0.3784159948320607	0.3867400956848286	0.4540630931455141
0.3784460007621462	0.3866619588031099	0.5790058624283674

6) ZnO-VClSe *m2*

S1

ZnO-VClSe

1.0000000000000000				
3.2385498632178189	0.0000000000000000	0.0000000000000000		
-1.6192749315591868	2.8046664529906065	0.0000000000000000		
0.0000000000000000	0.0000000000000000	25.0000000000000000		
Zn	O	V	Se	Cl
1	1	1	1	1

Direct

0.5811049450530419	0.1882699331585087	0.3336681778822381
0.9144203421731163	0.8549409206850243	0.3332772040696881
0.9089018715779176	0.8559617564602817	0.5162848009246233
0.2422189190607114	0.5226289415491223	0.5806137405466600
0.2422439351352352	0.5226294551470900	0.4556571235767848

S2

ZnO-VClSe

1.0000000000000000				
3.2399736037827092	0.0000000000000000	0.0000000000000000		
-1.6199868018416101	2.8058994484882089	0.0000000000000000		
0.0000000000000000	0.0000000000000000	25.0000000000000000		
Zn	O	V	Se	Cl
1	1	1	1	1

Direct

0.1052312186581972	0.2509060065971909	0.3319437095540252
--------------------	--------------------	--------------------

0.7719392036128383	0.5842715586158960	0.3316725533684703
0.7816863444616189	0.5919753152443477	0.5173608605173143
0.1150365632143746	0.2586552827232182	0.5816758193214540
0.1149966830529792	0.2586228438193388	0.4568481042387447

S3

ZnO-VClSe

1.0000000000000000		
3.2392598121903142	0.0000000000000000	0.0000000000000000
-1.6196299060454236	2.8052812868361827	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Se	Cl
1	1	1	1	1

Direct

0.7729792810549370	0.5852006761100839	0.3344444564013713
0.4396795190032634	0.9185612828848804	0.3341198837112955
0.7809276521569970	0.5913764701942554	0.5157160846310376
0.1142841556938308	0.2580631747141311	0.5800462441861924
0.1141584370909712	0.2579613870966284	0.4551743780701187

S4

ZnO-VClSe

1.0000000000000000		
3.2403438511737654	0.0000000000000000	0.0000000000000000
-1.6201719255371325	2.8062200921345513	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Se	Cl
1	1	1	1	1

Direct

0.1054633964599319	0.2510389111675764	0.3321301744983316
0.4388344251409038	0.9177371131181715	0.3319527523325831
0.7814835330242857	0.5919181413131724	0.5171882118045303
0.1148323961105149	0.2585983204964393	0.5815082211388969
0.1147532792643773	0.2585305159046598	0.4567216872256523

S5

ZnO-VClSe

1.0000000000000000		
3.2385511061919070	0.0000000000000000	0.0000000000000000
-1.6192755530462306	2.8046675294377432	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Se	Cl
1	1	1	1	1

Direct

0.4404879204636316	0.9188906756412436	0.3336629601774561
0.7738413175278893	0.5855748573056374	0.3332724558074176
0.7803411557883635	0.5911156719063584	0.5162880683821172
0.1136921853347062	0.2577988393192143	0.5806172174758260
0.1136664658854087	0.2577739468275482	0.4556603451571917

S6

ZnO-VClSe

```

1.0000000000000000
  3.2392606622903890    0.0000000000000000    0.0000000000000000
 -1.6196303310954610    2.8052820230444433    0.0000000000000000
  0.0000000000000000    0.0000000000000000    25.0000000000000000
Zn  O    V    Se    Cl
  1    1    1    1    1

```

Direct

```

0.0426465472216435    0.7267067875721835    0.3344444837203326
0.7093265938115962    0.0600074741862002    0.3341201709587125
0.0455877015212351    0.7192258251357373    0.5157159237867504
0.3789338708199921    0.3858654986096255    0.5800459925812191
0.3788853176255387    0.3859913984962304    0.4551744759530010

```

7) ZnO-VClTe ml
S1

ZnO-VClTe

```

1.0000000000000000
  3.3002729336267271    0.0000000000000000    0.0000000000000000
 -1.6501364667637810    2.8581201999302839    0.0000000000000000
  0.0000000000000000    0.0000000000000000    25.0000000000000000
Zn  O    V    Cl    Te
  1    1    1    1    1

```

Direct

```

0.1788112034538045    0.7901345856197111    0.3272422752912476
0.5121372454644941    0.4567844780086432    0.3257222917871871
0.5104261036556395    0.4547279658094325    0.5269101171397566
0.8437553151956294    0.1213879694796773    0.5860255948341404
0.8437601452304264    0.1213960080825345    0.4536007679476981

```

S2

ZnO-VClTe

```

1.0000000000000000
  3.3036711105836685    0.0000000000000000    0.0000000000000000
 -1.6518355552422008    2.8610631075015367    0.0000000000000000
  0.0000000000000000    0.0000000000000000    25.0000000000000000
Zn  O    V    Cl    Te
  1    1    1    1    1

```

Direct

```

0.1120456190371044    0.2567462791157880    0.3263288190583182
0.7786949691073772    0.5900545770434178    0.3246658337528388
0.7771631663837724    0.5881011231874993    0.5275112727734310
0.1104805498589059    0.2547516167722677    0.5865997220013597
0.1105057086128340    0.2547774108810188    0.4543953994140395

```

S3

ZnO-VClTe

1.0000000000000000
3.3021077894245829 0.0000000000000000 0.0000000000000000
-1.6510538946626816 2.8597092316635009 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Zn O V Te Cl
1 1 1 1 1

Direct

0.7776577062977310 0.5898491790363636 0.3266014204461314
0.4443209126245407 0.9231655698050290 0.3252935771933849
0.7777949195917273 0.5882686719587156 0.5272210790936427
0.1111340027199077 0.2549534758900833 0.4540304866886018
0.1111215037661140 0.2549260943097948 0.5863544835782619

S4

ZnO-VClTe

1.0000000000000000
3.3051050941430877 0.0000000000000000 0.0000000000000000
-1.6525525470218889 2.8623049736925972 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Zn O V Cl Te
1 1 1 1 1

Direct

0.1139550361888269 0.2570162403551919 0.3258386394694739
0.4472454516195228 0.9236641460794317 0.3243517831071827
0.7758311811681722 0.5879356378037528 0.5277438687455884
0.1091382635163427 0.2545856434957159 0.5868568536222867
0.1091970975071419 0.2546213342659058 0.4547099020554768

S5

ZnO-VClTe

1.0000000000000000
3.3002629290215162 0.0000000000000000 0.0000000000000000
-1.6501314644611762 2.8581115356880171 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000

Zn O V Cl Te
1 1 1 1 1

Direct

0.4454446539258967 0.9224960301850516 0.3272344581936864
0.7787522865164291 0.5891538951013899 0.3257168725418325
0.7770568068418982 0.5887235880352790 0.5269144582347067
0.1103770854685919 0.2553853662617129 0.5860305936575614
0.1103982122471763 0.2553951114165613 0.4536046643722145

S6

ZnO-VClTe

1.0000000000000000
3.3036492080261688 0.0000000000000000 0.0000000000000000

```

-1.6518246039634517    2.8610441393303345    0.0000000000000000
0.0000000000000000    0.0000000000000000    25.0000000000000000
Zn  O   V   Te  Cl
1   1   1   1   1
Direct
0.8434039093279750    0.1213791384365948    0.3263140981867139
0.5100900887671358    0.4547302630642491    0.3246541963033422
0.5117378097706293    0.4561166374071064    0.5275203927824776
0.8450614315626339    0.1227773189693551    0.4544032689132749
0.8450867915716387    0.1227936261227072    0.5866090908141999

```

8) ZnO-VClTe *m2*
S1

```

ZnO-VClTe
1.0000000000000000
3.2985186579526546    0.0000000000000000    0.0000000000000000
-1.6492593289267714    2.8566009526313030    0.0000000000000000
0.0000000000000000    0.0000000000000000    25.0000000000000000
Zn  O   V   Cl  Te
1   1   1   1   1
Direct
0.1774664393122833    0.7904791003817948    0.3331233028562082
0.5108027552005296    0.4571315524198312    0.3326389634794467
0.5113168585354515    0.4544981493174589    0.5130909205147276
0.8446598450006917    0.1211703584576398    0.4541798590676223
0.8446441149510449    0.1211518464232668    0.5864680010819825

```

S2

```

ZnO-VClTe
1.0000000000000000
3.3002621260165035    0.0000000000000000    0.0000000000000000
-1.6501310629586696    2.8581108402652764    0.0000000000000000
0.0000000000000000    0.0000000000000000    25.0000000000000000
Zn  O   V   Te  Cl
1   1   1   1   1
Direct
0.1112022538696920    0.2572523470571539    0.3317530262837209
0.7778678866895987    0.5905655837346657    0.3313136069295197
0.7777175772678362    0.5877592352878054    0.5139479536548137
0.1110589285956394    0.2544240590328428    0.5873086463088200
0.1110433665772206    0.2544297818875094    0.4551778138231484

```

S3

```

ZnO-VClTe
1.0000000000000000
3.2993017126626629    0.0000000000000000    0.0000000000000000
-1.6496508562817633    2.8572790979027198    0.0000000000000000
0.0000000000000000    0.0000000000000000    25.0000000000000000

```


Zn	O	V	Cl	Te
1	1	1	1	1

Direct

0.7778413305108458	0.5900170385385408	0.3342457904470493
0.4445042288818186	0.9233350187238258	0.3338136002258878
0.7776712170864784	0.5881526366788350	0.5122856995559530
0.1110005618604362	0.2548414683854148	0.4534866545188052
0.1110117066604204	0.2548168286733770	0.5856693022522990

S4

ZnO-VClTe

1.0000000000000000		
3.3007108423003344	0.0000000000000000	0.0000000000000000
-1.6503554211005789	2.8584994399661636	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Cl	Te
1	1	1	1	1

Direct

0.1128051327123174	0.2559286420745792	0.3321105865474010
0.4461224961307551	0.9225961307617112	0.3317633235768724
0.7765859605710830	0.5886542803428085	0.5136582725388479
0.1099350638159038	0.2553186364567779	0.4549425600603669
0.1099183767699543	0.2553253123641213	0.5870263042764989

S5

ZnO-VClTe

1.0000000000000000		
3.2985194267685189	0.0000000000000000	0.0000000000000000
-1.6492597133347038	2.8566016184453731	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Te	Cl
1	1	1	1	1

Direct

0.4475460250679006	0.9237514919374661	0.3331314627468771
0.7808502383195091	0.5904057967048715	0.3326469641966483
0.7756614257396919	0.5878909133978354	0.5130854050690488
0.1089848657410997	0.2545568212508442	0.5864620567950709
0.1089864901317981	0.2545489677089705	0.4541751581923563

S6

ZnO-VClTe

1.0000000000000000		
3.3002734751471259	0.0000000000000000	0.0000000000000000
-1.6501367375239808	2.8581206689007059	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

Zn	O	V	Cl	Te
1	1	1	1	1

Direct

0.8442075800852322	0.1209855685959695	0.3317450173065808
0.5108796157914526	0.4543320233771979	0.3313080625581719
0.5112083702226116	0.4563819025790750	0.5139524640319380
0.8445469435784858	0.1230457305782906	0.4551824048402864
0.8445375213222306	0.1230517588694653	0.5873130982630244

Here in the following, we report the optimised geometries of the configurations with the least binding energy without including van der Waals corrections.

ZnO-VBrSe *m1*

ZnO-VBrSe

1.0000000000000000				
3.3096157453812713	0.0000000000000000	0.0000000000000000		
-1.6548078727409739	2.8662113123328155	0.0000000000000000		
0.0000000000000000	0.0000000000000000	25.1690154779090491		
Zn	O	V	Br	Se
1	1	1	1	1

Direct

0.1143422806149843	0.2566461164608285	0.3256149205236341
0.4476460529218187	0.9233029415132989	0.3244753027138216
0.7755669543132981	0.5881775112315779	0.5219073252174056
0.1088859370463950	0.2548419092373777	0.5884307662247750
0.1089258051034889	0.2548545235569293	0.4590727323203510

ZnO-VBrSe *m2*

ZnO-VBrSe

1.0000000000000000				
3.3046163040775838	0.0000000000000000	0.0000000000000000		
-1.6523081520890537	2.8618816691589908	0.0000000000000000		
0.0000000000000000	0.0000000000000000	25.1309956516712099		
Zn	O	V	Br	Se
1	1	1	1	1

Direct

0.4378082705926403	0.9171236268422547	0.3086502790841124
0.7711429750738006	0.5837899046948039	0.3089593211831385
0.7821341219609010	0.5923006181298973	0.5351389924620804
0.1154749274220848	0.2589714880376448	0.4685160453893573
0.1154687499505798	0.2589683532954083	0.5982364088813057

ZnO-VBrTe *m1*

ZnO-VBrTe

1.0000000000000000				
3.3709537315992630	0.0000000000000000	0.0000000000000000		
-1.6854768657996315	2.9193315665606265	0.0000000000000000		
0.0000000000000000	0.0000000000000000	24.9780208760687614		
Zn	O	V	Br	Te
1	1	1	1	1

Direct

0.1090963710160295	0.2528123369293951	0.3175059224762578
--------------------	--------------------	--------------------

0.7757894737914057	0.5861820518154630	0.3166508323108559
0.7791118921002465	0.5906998542902500	0.5308188956601256
0.1124570312752198	0.2573833341875016	0.5961896690587238
0.1124352448171351	0.2573534297773961	0.4583357274940383

ZnO-VBrTe *m2*

ZnO-VBrTe

1.0000000000000000		
3.3669100881166765	0.0000000000000000	0.0000000000000000
-1.6834550440583382	2.9158296685808422	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.9480583730605936

Zn	O	V	Br	Te
1	1	1	1	1

Direct

0.1079054103490833	0.2510804293972626	0.3123552745390867
0.4412441793233910	0.9177555683427840	0.3124078323824619
0.7798535608672381	0.5918887862877256	0.5291282864316926
0.1131731455507108	0.2585372903420549	0.4637531708597109
0.1131907339096045	0.2585609276301781	0.6018564827870634

ZnO-VClSe *m1*

ZnO-VClSe

1.0000000000000000		
3.2637096686333269	0.0000000000000000	0.0000000000000000
-1.6318548342665546	2.8264554836348759	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0545026278471319

Zn	O	V	Se	Cl
1	1	1	1	1

Direct

0.1058965329122827	0.2514198154862228	0.3220014699960174
0.7725822111754752	0.5847673726530260	0.3211107610759640
0.7812454416419499	0.5916349031106947	0.5265599648561192
0.1145649871606977	0.2582911528803109	0.4624585993268795
0.1146008401095955	0.2583177628697300	0.5873702517450354

ZnO-VClSe *m2*

ZnO-VClSe

1.0000000000000000		
3.2610148334184741	0.0000000000000000	0.0000000000000000
-1.6305074166591695	2.8241216878797828	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0338152007083039

Zn	O	V	Se	Cl
1	1	1	1	1

Direct

0.7708697377008846	0.5833550867923805	0.3087058728746612
0.4375383267844484	0.9166895149022807	0.3089192692819935
0.7823193661116363	0.5925964196192268	0.5328363692382112
0.1156540796206400	0.2592638802848342	0.5970680710009333
0.1156475347824042	0.2592580894012784	0.4719714646041950

ZnO-VClTe *m1*

ZnO-VClTe

```
1.0000000000000000
 3.3279094429714022  0.0000000000000000  0.0000000000000000
-1.6639547214357036  2.8820541190945925  0.0000000000000000
 0.0000000000000000  0.0000000000000000  24.9987192620690593
Zn  O  V  Cl  Te
 1  1  1  1  1
```

Direct

```
0.1140092899172416  0.2580544557803606  0.3163860636531481
0.7806533877764750  0.5913689292180351  0.3157156959733882
0.7758550662615846  0.5872259836100540  0.5338213568872376
0.1091698540873907  0.2538771257893728  0.5930747379076209
0.1092024149573092  0.2539045126021691  0.4605031925786065
```

ZnO-VClTe *m2*

ZnO-VClTe

```
1.0000000000000000
 3.3241454280889196  0.0000000000000000  0.0000000000000000
-1.6620727139945191  2.8787943865861552  0.0000000000000000
 0.0000000000000000  0.0000000000000000  24.9704445890474851
Zn  O  V  Cl  Te
 1  1  1  1  1
```

Direct

```
0.7849570450026917  0.5911361882474822  0.3110634294305044
0.4516208876126981  0.9244693296765902  0.3110482033478732
0.7729256389713086  0.5874079883126626  0.5277302478893446
0.1062689486116284  0.2540746308101873  0.4684134473891888
0.1062565248016796  0.2540748539530711  0.6012457189430975
```