Supplementary Information

Prediction of Band Inversion in Janus In_2XYZ (X, Y, and Z= S, Se, Te) monolayers

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A Atomic structures

The lattice constant and atomic positions are reported in the format of quantum espresso. All values are in the unit of Å.

A.1 In_2X_2Y monolayers

In_2SeSS
a= 7.520155727;
Atomic positions
Se -1.989758007 -1.148787321 0.005849094
In 0.000000000 0.000000000 1.309281614
S 0.000000000 0.000000000 3.725821555
In 1.989758007 1.148787321 5.333606796
S -1.989758007 -1.148787321 6.525440941
In_2SSeS
a= 7.484026347,
Atomic positions
S -1.980198534 -1.143268157 0.013543562
In -0.000000000 -0.000000000 1.145732337
Se 0.000000000 0.000000000 3.691748632
In 1.980198534 1.143268157 5.421394376
S -1.980198534 -1.143268157 6.627581094
In_2SSSe
a= 7.523293957,
Atomic positions
S -1.990588350 -1.149266720 0.119505629
In -0.000000000 -0.000000000 1.233415139
S -0.000000000 -0.000000000 3.656479593
In 1.990588350 1.149266720 5.261435620
Se -1.990588350 -1.149266720 6.629164019
In_2SSeSe
a= 7.591012008,
S -2.008505870 -1.159611405 0.009199481
In -0.000000000 -0.000000000 1.113641546
Se -0.000000000 -0.000000000 3.664458209
In 2.008505870 1.159611405 5.374211111
Se -2.008505870 -1.159611405 6.738489652
In_2SeSSe
a= 7.630499662,
Se -2.018953909 -1.165643583 0.002065167
In 0.000000000 0.000000000 1.278487771
S 0.000000000 0.000000000 3.701963004
In 2.018953909 1.165643583 5.287361240
Se -2.018953909 -1.165643583 6.630122818

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$In_2SeSSeS$
a= 7.586740258,
Se -2.007375608 -1.158958848 -0.104791048
In 0.000000000 0.000000000 1.189981601
Se -0.000000000 -0.000000000 3.735485796
In 2.007375608 1.158958848 5.447096077
S -2.007375608 -1.158958848 6.632227574
In_2TeSS
a= 7.74227109,
Atomic positions
Te -2.048527511 -1.182717910 -0.137259107
In -0.000000000 -0.000000000 1.375346197
S 0.000000000 0.000000000 3.794965434
In 2.048527511 1.182717910 5.362833033
S -2.048527511 -1.182717910 6.504114443
In_2STeS
a= 7.642249801,
Atomic positions
S -2.022062878 -1.167438548 -0.155789023
In 0.000000000 0.000000000 0.918216570
Te 0.000000000 0.000000000 3.687952461
In 2.022062878 1.167438548 5.639599021
S -2.022062878 -1.167438548 6.810020970
In_2SSTe
a= 7.727642128,
Atomic positions
S -2.044656833 -1.180483173 0.148738869
In -0.000000000 -0.000000000 1.174557193
S 0.000000000 0.000000000 3.625229077
In 2.044656833 1.180483173 5.161747879
Te -2.044656833 -1.180483173 6.789726982
In_2STeTe
a= 7.945985397,
Atomic positions
S -2.102428278 -1.213837533 -0.125463320
In -0.000000000 -0.000000000 0.844302810
Te -0.000000000 -0.000000000 3.637989011
In 2.102428278 1.213837533 5.483155495
Te -2.102428278 -1.213837533 7.060016004
In_2TeSTe
a= 8.082346043,
Atomic positions
Te -2.138507943 -1.234668137 -0.117741660
In -0.000000000 -0.000000000 1.294929195
S 0.000000000 0.000000000 3.723267299
In 2.138507943 1.234668137 5.247133532
Te -2.138507943 -1.234668137 6.752411635
In_2TeTeS
a= 7.928635543,
Atomic positions
Te -2.103183230 -1.214273404 -0.411123999
In 0.000000000 0.000000000 1.053130703
Te 0.000000000 0.000000000 3.802400270
In 2.103183230 1.214273404 5.667243236
S -2.103183230 -1.214273404 6.788349789
$In_2TeSeSe$
a= 7.948838682,
Atomic positions
Te -2.097837680 -1.211187150 -0.240597961
In 0.000000000 0.000000000 1.223220039
Se 0.000000000 0.000000000 3.776692787
In 2.097837680 1.211187150 5.426461190

Se -2.097837680 -1.211187150 6.714223944
$In_2SeTeSe$
a= 7.852551126,
Atomic positions
Se -2.077706505 -1.199564410 -0.268267930
In 0.000000000 0.000000000 0.953433096
Te -0.000000000 -0.000000000 3.713511340
In 2.077706505 1.199564410 5.593404952
Se -2.077706505 -1.199564410 6.907918543
$In_2SeSeTe$
a= 7.919389422,
Atomic positions
Se -2.095391250 -1.209774703 -0.079185615
In 0.000000000 0.000000000 1.111041747
Se -0.000000000 -0.000000000 3.673566542
In 2.095391250 1.209774703 5.318145833
Te -2.095391250 -1.209774703 6.876431492
$In_2SeTeTe$
a= 8.061860553,
Atomic positions
Se -2.133087687 -1.231538751 -0.251888567
In 0.000000000 0.000000000 0.907910937
Te 0.000000000 0.000000000 3.683572576
In 2.133087687 1.231538751 5.512998778
Te -2.133087687 -1.231538751 7.047406276
$In_2TeSeTe$
a= 8.14148823,
Atomic positions
Te -2.154156373 -1.243702762 -0.228278049
In -0.000000000 -0.000000000 1.178722587
Se -0.000000000 -0.000000000 3.740285065
In 2.154156373 1.243702762 5.356175779
Te -2.154156373 -1.243702762 6.853094617
$In_2TeTeSe$
a= 8.064904127,
Atomic positions
Te -2.133892985 -1.232003690 -0.410085597
In -0.000000000 -0.000000000 1.023043035
Te 0.000000000 0.000000000 3.779607712
In 2.133892985 1.232003690 5.615232246
Se -2.133892985 -1.232003690 6.892202604

B In_2XYZ monolayers

In_2SSeTe
a= 7.793275669,
Atomic positions
S -2.062022811 -1.190509426 0.036089941
In 0.000000000 0.000000000 1.052170076
Se -0.000000000 -0.000000000 3.634282433
In 2.062022811 1.190509426 5.280127453
Te -2.062022811 -1.190509426 6.897330097
In_2STeSe
a= 7.747239103,
Atomic positions
S -2.049841996 -1.183476829 -0.151943499
In 0.000000000 0.000000000 0.891247912
Te -0.000000000 -0.000000000 3.664756325
In 2.049841996 1.183476829 5.582957685
Se -2.049841996 -1.183476829 6.912981577
In_2SeSTe
a= 7.850112639,

Atomic positions
Se -2.077061306 -1.199191905 0.022971081
In -0.000000000 -0.000000000 1.230796137
S -0.000000000 -0.000000000 3.663412473
In 2.077061306 1.199191905 5.206965848
Te -2.077061306 -1.199191905 6.775854461

In_2SeTeS

a= 7.74229853,
Atomic positions
Se -2.048534771 -1.182722102 -0.268125564
In -0.000000000 -0.000000000 0.981128277
Te 0.000000000 0.000000000 3.732719277
In 2.048534771 1.182722102 5.649174116
S -2.048534771 -1.182722102 6.805103894

In_2TeSSe

a= 7.858468305,
Atomic positions
Te -2.079272132 -1.200468325 -0.136345653
In 0.000000000 0.000000000 1.343525312
S 0.000000000 0.000000000 3.767366430
In 2.079272132 1.200468325 5.315421524
Se -2.079272132 -1.200468325 6.610032388

In_2TeSeS

a= 7.800944817,
Atomic positions
Te -2.064051992 -1.191680974 -0.249317497
In 0.000000000 0.000000000 1.252955346
Se 0.000000000 0.000000000 3.802393226
In 2.064051992 1.191680974 5.475560905
S -2.064051992 -1.191680974 6.618408020
