Quantum Espresso
System: WSe_2

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1 The lattice parameter and the position of the unit cell atoms after the geometry optimization

1.1 $2H-WSe_2$

Spacegroup: $P6_3/mmc$, **hexagonal**

Reference: doi 10.17188/1192989

Atom positions in cartesian coordinate (Å)

Element	x	y	z
W	1.6599664600	0.9583820825	10.302890475
W	0.0000000000	1.9167641651	3.4342968250
Se	0.0000000000	1.9167641651	11.962021105
Se	1.6599664600	0.9583820825	5.0934274550
Se	0.0000000000	1.9167641651	8.6437598450
Se	1.6599664600	0.9583820825	1.7751661950

Optimized cell parameters

v	x	y	z
v1	3.3199329200	0.0000000000	0.0000000000
v2	-1.6599664600	2.8751462476	0.0000000000
v3	0.0000000000	0.0000000000	13.7371873000

1.2 $1T-WSe_2$

Spacegroup: $P\bar{3}m1$, **trigonal**

Reference: doi 10.17188/1405335

Atom positions in cartesian coordinate (Å)

Element	x	y	z
W	1.6589266350	0.9577817393	3.2774093905
W	0.0000000000	1.9155634786	20.7911098800
Se	0.0000000000	1.9155634786	4.9342978364
Se	1.6589266350	0.9577817393	22.4502658760
Se	0.0000000000	1.9155634786	1.6182533940
Se	1.6589266350	0.9577817393	19.1342214340

Optimized cell parameters

v	x	y	z
v1	3.3178532700	0.0000000000	0.0000000000
v2	-1.6589266350	2.8733452178	0.0000000000
v3	0.0000000000	0.0000000000	24.0685192700

2 The density of states

2.1 $2H - WSe_2$

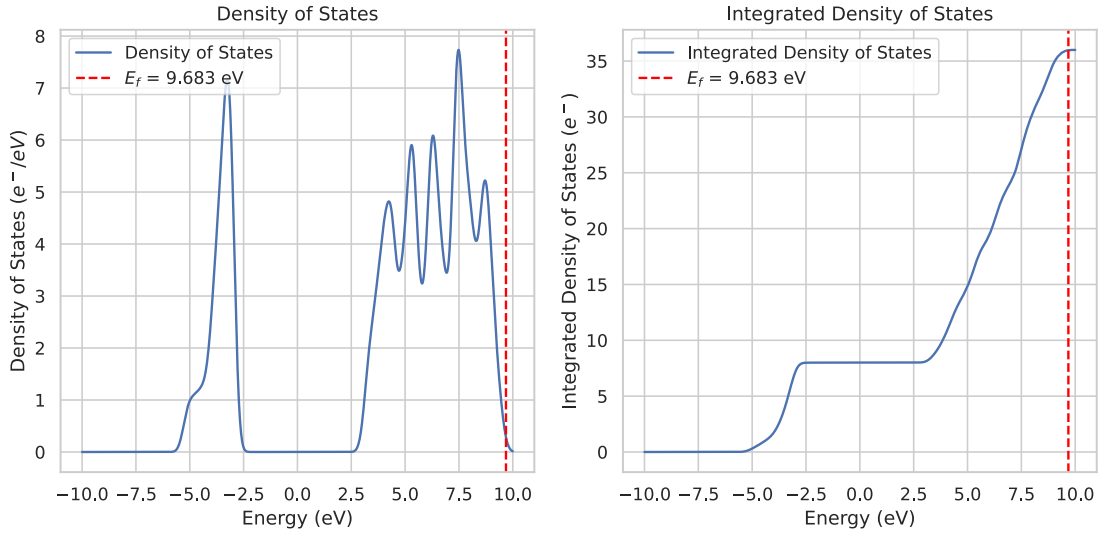

Figure 1: The density of states and integrated density of state $2H - WSe_2$

The Fermi level (E_f) is shown as a red dashed line at 9.683 eV (fig. 1). Since semiconductor Fermi levels are usually near the top of the valence band, this value is unusually high for DOS plots.There are no states at the Fermi level, which implies that the material is not metallic. Given a relatively large band gap, it seems to be an insulator or a poor semiconductor, since originally the 2H phase of WSe_2 is known to be a semiconductor with a direct band gap, which is the flat region observed in the DOS plot. The significant peaks in the DOS plot before the Fermi level are where electrons occupy the energy states at zero temperature. These are the valence bands filled with electrons.

2.2 $1T - WSe_2$

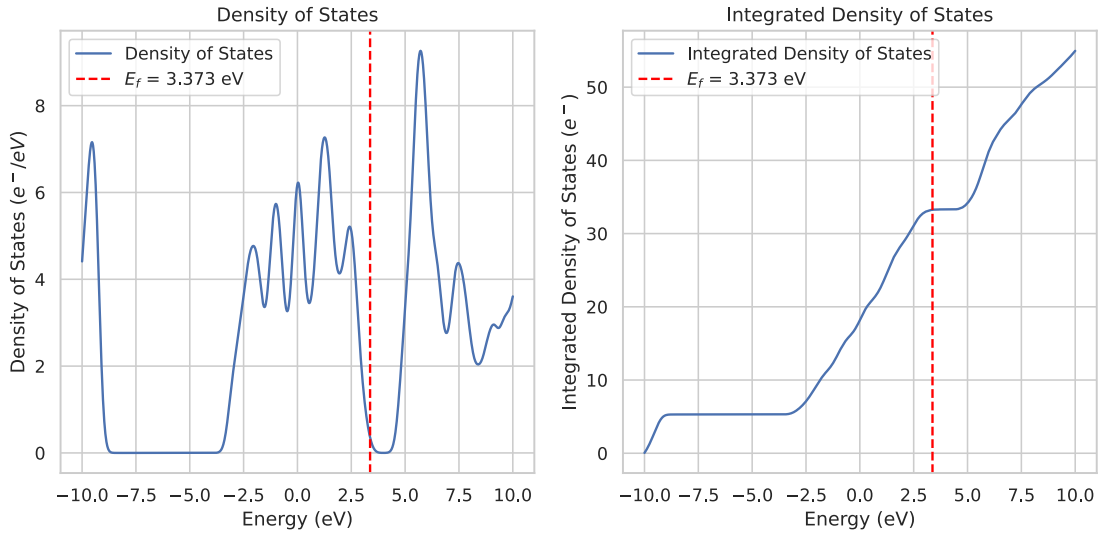

Figure 2: The density of states and integrated density of state $1T - WSe_2$

In the plot 2, we can notice the value of the Fermi level is significantly lower in comparison to the 2H phase and equal to 3.373 eV. Apart from that, the band gap is also smaller (from 2.5 to 5.0 eV). The 1T phase has semiconductive characteristics. This phase conducts electricity better compared to 2H.

3 Band structure

3.1 $2H - WSe_2$

In the fig. 3, the conduction band minimum and the valence band maximum are both at the K point, confirming the direct band gap nature of the material. The bands are not symmetric around the Γ point, which is expected due to the breaking of inversion symmetry in the 2H phase.

3.2 $1T - WSe_2$

The band structure fig.4 shows multiple bands crossing the Fermi level, indicating that the 1T phase of WSe2 is a conductor, which aligns with the known properties of the 1T phase of transition metal dichalcogenides being metallic/semi-metallic. The absence of a band gap near the Fermi level further confirms the semimetallic nature of this phase. The high density of states at the Fermi level implies decent electrical conductivity. However, the presence of the band gap itself means that this phase cannot be a pure conductor.

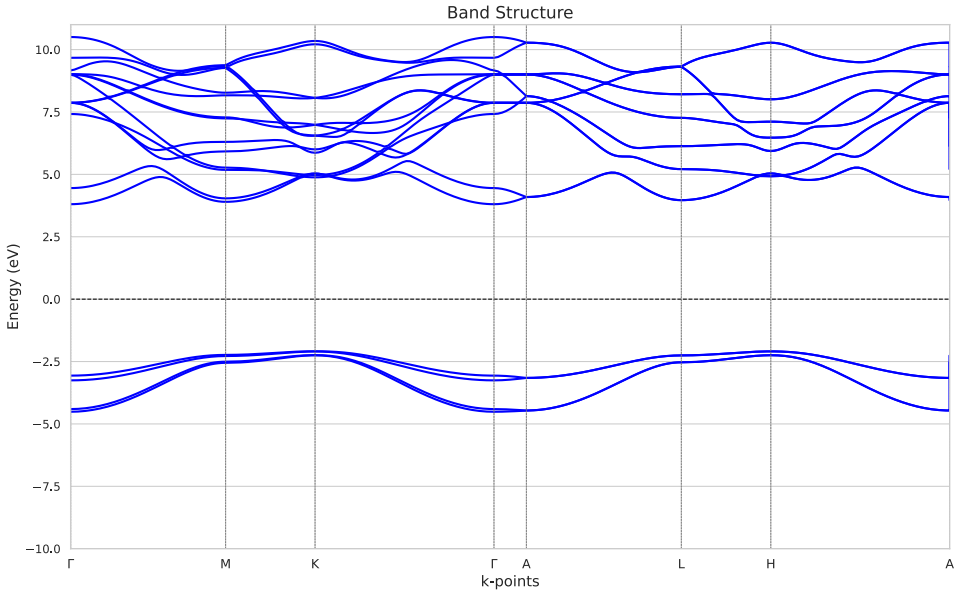

Figure 3: The electronic band structure $2H - WSe_2$

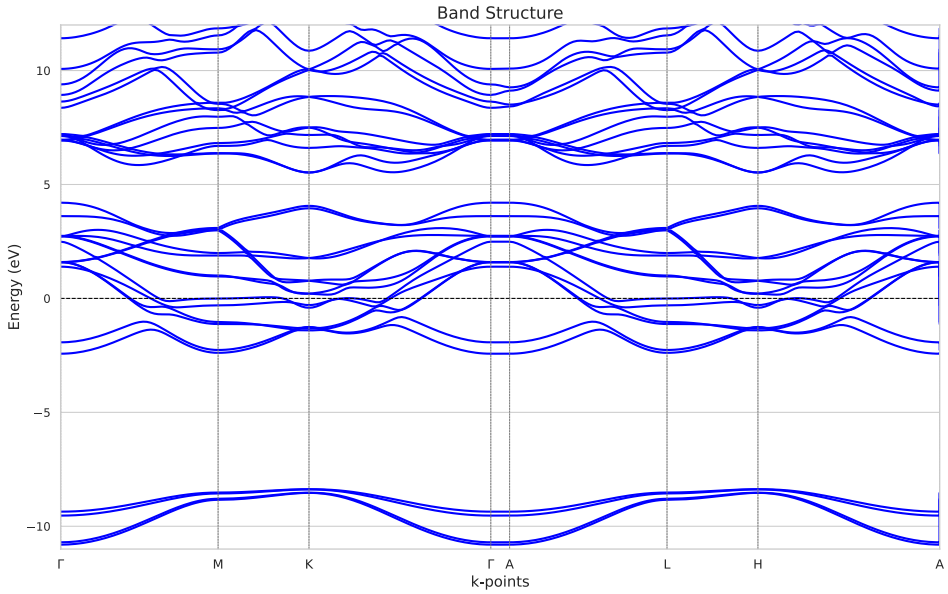

Figure 4: The electronic band structure $1T - WSe_2$

To sum up, the DOS and band structure plots for the WSe_2 1T phase proves semiconductor characteristics, given a high density of states at the Fermi level. However, according to papers, this state is less stable than 2H and could be obtained by, for example, irradiation of the 2H phase (doi.org/10.1021/acssuschemeng.1c07179).
NB! The bulk calculations were performed.

Appendix: input files

$2H - WSe_2$

Optimization

```
&CONTROL
  calculation = 'relax'
  etot_conv_thr =   6.0000000000d-05
  forc_conv_thr =   1.0000000000d-04
  outdir = './'
  prefix = 'WSe2-2H'
  pseudo_dir = './'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
  degauss =   1.4699723600d-02
  ecutrho =   2.4000000000d+02
  ecutwfc =   3.0000000000d+01
  ibrav = 0
  nat = 6
  nosym = .false.
  ntyp = 2
  occupations = 'smearing'
  smearing = 'cold'
/
&ELECTRONS
  conv_thr =   1.2000000000d-09
  electron_maxstep = 80
  mixing_beta =   4.0000000000d-01
/
&IONS
ion_dynamics='bfgs'
/
ATOMIC_SPECIES
Se     78.96 Se.upf
W      183.84 W.upf
ATOMIC_POSITIONS crystal
W             0.6666666700       0.3333333300       0.7500000000
W             0.3333333300       0.6666666700       0.2500000000
Se            0.3333333300       0.6666666700       0.8710007900
Se            0.6666666700       0.3333333300       0.3710007900
Se            0.3333333300       0.6666666700       0.6289992100
Se            0.6666666700       0.3333333300       0.1289992100
K_POINTS automatic
11 11 3 0 0 0
CELL_PARAMETERS angstrom
      3.3199329200       0.0000000000       0.0000000000
     -1.6599664600       2.8751462476       0.0000000000
      0.0000000000       0.0000000000      13.7371873000
```

SCF

```
&CONTROL
  calculation = 'scf'
  title = 'WSe2-2H-SCF'
  prefix = 'WSe2-2H'
  outdir = './out/'
  pseudo_dir = './'
  verbosity = 'high'
/
&SYSTEM
  ibrav = 0
  nat = 6
  ntyp = 2
  ecutwfc = 50.0
  ecutrho = 400.0
  nbnd = 30
/
&ELECTRONS
  conv_thr = 1.0D-8
  mixing_beta = 0.4
/
ATOMIC_SPECIES
Se     78.96 Se.upf
W      183.84 W.upf
ATOMIC_POSITIONS crystal
W             0.6666666700        0.3333333300        0.7500000000
W             0.3333333300        0.6666666700        0.2500000000
Se            0.3333333300        0.6666666700        0.8707765894
Se            0.6666666700        0.3333333300        0.3707765894
Se            0.3333333300        0.6666666700        0.6292234106
Se            0.6666666700        0.3333333300        0.1292234106
K_POINTS automatic
11 11 3 0 0 0
CELL_PARAMETERS angstrom
      3.3199329200       0.0000000000       0.0000000000
     -1.6599664600       2.8751462476       0.0000000000
      0.0000000000       0.0000000000      13.7371873000
```

NSCF

```
&CONTROL
  calculation = 'nscf'
  title = 'WSe2-2H-NSCF'
  prefix = 'WSe2-2H'
  outdir = './out/'
  pseudo_dir = './'
  verbosity = 'high'
/
&SYSTEM
  ibrav = 0
  nat = 6
  ntyp = 2
  ecutwfc = 50.0
  ecutrho = 400.0
  nbnd = 40
```

```
/
&ELECTRONS
  conv_thr = 1.0D-8
  mixing_beta = 0.4
/
ATOMIC_SPECIES
Se     78.96 Se.upf
W      183.84 W.upf
ATOMIC_POSITIONS crystal
W             0.6666666700        0.3333333300        0.7500000000
W             0.3333333300        0.6666666700        0.2500000000
Se            0.3333333300        0.6666666700        0.8707765894
Se            0.6666666700        0.3333333300        0.3707765894
Se            0.3333333300        0.6666666700        0.6292234106
Se            0.6666666700        0.3333333300        0.1292234106
K_POINTS automatic
18 18 6 0 0 0
CELL_PARAMETERS angstrom
      3.3199329200       0.0000000000       0.0000000000
     -1.6599664600       2.8751462476       0.0000000000
      0.0000000000       0.0000000000      13.7371873000
```

DOS

```
&DOS
    prefix='WSe2-2H',
    outdir='./out/',
    fildos='WSe2-2H.dos',
    Emin=-10.0,
    Emax=10.0,
    DeltaE=0.01,
    degauss=0.02
/
```

Band structure

```
&CONTROL
    calculation = 'bands'
    prefix = 'WSe2-2H'
    verbosity ='high'
    disk_io = 'low'
    outdir = './'
    pseudo_dir = './'
    wf_collect = .true.
    etot_conv_thr = 1.0D-4
    forc_conv_thr = 1.0D-3
    nstep = 200
/
&SYSTEM
    ibrav = 0
    nat = 6
    ntyp = 2
    ecutwfc = 50.0
    ecutrho = 400.0
```

```
    nbnd = 40
/
&ELECTRONS
  conv_thr = 1.0D-8  ! SCF convergence threshold is typically fine for NSCF
  electron_maxstep = 200,
  mixing_mode = 'plain'
  mixing_beta = 0.1
/
&IONS
ion_dynamics = 'bfgs'
/
ATOMIC_SPECIES
Se     78.96 Se.upf
W      183.84 W.upf
ATOMIC_POSITIONS crystal
W             0.6666666700        0.3333333300        0.7500000000
W             0.3333333300        0.6666666700        0.2500000000
Se            0.3333333300        0.6666666700        0.8707765894
Se            0.6666666700        0.3333333300        0.3707765894
Se            0.3333333300        0.6666666700        0.6292234106
Se            0.6666666700        0.3333333300        0.1292234106
K_POINTS crystal
257
<...>
CELL_PARAMETERS angstrom
    3.3199329200     0.0000000000     0.0000000000
   -1.6599664600     2.8751462476     0.0000000000
    0.0000000000     0.0000000000    13.7371873000
```

```
&BANDS
prefix='WSe2-2H'
outdir='./'
filband='WSe2-2H-b'
/
```

$1T - WSe_2$

Optimization

```
&CONTROL
  calculation = 'relax'
  etot_conv_thr =   6.0000000000d-05
  forc_conv_thr =   1.0000000000d-04
  outdir = './out/'
  prefix = 'WSe2-1T'
  pseudo_dir = './'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
  degauss =   1.4699723600d-02
  ecutrho =   2.4000000000d+02
  ecutwfc =   3.0000000000d+01
  ibrav = 0
  nat = 6
```

```
  nosym = .false.
  ntyp = 2
  occupations = 'smearing'
  smearing = 'cold'
/
&ELECTRONS
  conv_thr =   1.2000000000d-09
  electron_maxstep = 80
  mixing_beta =   4.0000000000d-01
/
&IONS
ion_dynamics='bfgs'
/
ATOMIC_SPECIES
Se     78.96 Se.upf
W      183.84 W.upf
ATOMIC_POSITIONS crystal
W            0.6666666700       0.3333333300       0.1415375200
W            0.3333333300       0.6666666700       0.8584624800
Se           0.3333333300       0.6666666700       0.2105944900
Se           0.6666666700       0.3333333300       0.9275621000
Se           0.3333333300       0.6666666700       0.0724379000
Se           0.6666666700       0.3333333300       0.7894055100
K_POINTS automatic
11 11 2 0 0 0
CELL_PARAMETERS angstrom
      3.3178532700       0.0000000000       0.0000000000
     -1.6589266350       2.8733452178       0.0000000000
      0.0000000000       0.0000000000      24.0685192700
```

SCF

```
&CONTROL
  calculation = 'scf'
  title = 'WSe2-1T-SCF'
  prefix = 'WSe2-1T'
  outdir = './out/'
  pseudo_dir = './'
  verbosity = 'high'
/
&SYSTEM
  ibrav = 0
  nat = 6
  ntyp = 2
  ecutwfc = 50.0
  ecutrho = 400.0
  nbnd = 30
/
&ELECTRONS
  conv_thr = 1.0D-8
  mixing_beta = 0.4
/
ATOMIC_SPECIES
Se     78.96 Se.upf
W      183.84 W.upf
ATOMIC_POSITIONS crystal
```

```
W              0.6666666700         0.3333333300         0.1361699635
W              0.3333333300         0.6666666700         0.8638300365
Se             0.3333333300         0.6666666700         0.2050104446
Se             0.6666666700         0.3333333300         0.9327647299
Se             0.3333333300         0.6666666700         0.0672352701
Se             0.6666666700         0.3333333300         0.7949895554
K_POINTS automatic
11 11 2 0 0 0
CELL_PARAMETERS angstrom
      3.3178532700        0.0000000000        0.0000000000
     -1.6589266350        2.8733452178        0.0000000000
      0.0000000000        0.0000000000       24.0685192700
```

NSCF

```
&CONTROL
  calculation = 'nscf'
  title = 'WSe2-1T-NSCF'
  prefix = 'WSe2-1T'
  outdir = './out/'
  pseudo_dir = './'
  verbosity = 'high'
/
&SYSTEM
  ibrav = 0
  nat = 6
  ntyp = 2
  ecutwfc = 50.0
  ecutrho = 400.0
  nbnd = 40
/
&ELECTRONS
  conv_thr = 1.0D-8
  mixing_beta = 0.4
/
ATOMIC_SPECIES
Se     78.96 Se.upf
W      183.84 W.upf
ATOMIC_POSITIONS crystal
W              0.6666666700         0.3333333300         0.1361699635
W              0.3333333300         0.6666666700         0.8638300365
Se             0.3333333300         0.6666666700         0.2050104446
Se             0.6666666700         0.3333333300         0.9327647299
Se             0.3333333300         0.6666666700         0.0672352701
Se             0.6666666700         0.3333333300         0.7949895554
K_POINTS automatic
18 18 6 0 0 0
CELL_PARAMETERS angstrom
      3.3178532700        0.0000000000        0.0000000000
     -1.6589266350        2.8733452178        0.0000000000
      0.0000000000        0.0000000000       24.0685192700
```

DOS

```
&DOS
    prefix='WSe2-1T',
    outdir='./out/',
    fildos='WSe2-1T.dos',
    Emin=-10.0,
    Emax=10.0,
    DeltaE=0.01,
    degauss=0.02
/
```

Band structure

```
&CONTROL
    calculation = 'bands'
    prefix = 'WSe2-1T'
    verbosity ='high'
    disk_io = 'low'
    outdir = './'
    pseudo_dir = './'
    wf_collect = .true.
    etot_conv_thr = 1.0D-4
    forc_conv_thr = 1.0D-3
    nstep = 200
/
&SYSTEM
    ibrav = 0
    nat = 6
    ntyp = 2
    ecutwfc = 50.0
    ecutrho = 400.0
    nbnd = 40
/
&ELECTRONS
  conv_thr = 1.0D-8  ! SCF convergence threshold is typically fine for NSCF
  electron_maxstep = 200,
  mixing_mode = 'plain'
  mixing_beta = 0.1
/
&IONS
ion_dynamics = 'bfgs'
/
ATOMIC_SPECIES
Se     78.96 Se.upf
W      183.84 W.upf
ATOMIC_POSITIONS crystal
W             0.6666666700        0.3333333300        0.1361699635
W             0.3333333300        0.6666666700        0.8638300365
Se            0.3333333300        0.6666666700        0.2050104446
Se            0.6666666700        0.3333333300        0.9327647299
Se            0.3333333300        0.6666666700        0.0672352701
Se            0.6666666700        0.3333333300        0.7949895554
K_POINTS crystal
245
    <...>
```

```
CELL_PARAMETERS angstrom
    3.3178532700      0.0000000000      0.0000000000
   -1.6589266350      2.8733452178      0.0000000000
    0.0000000000      0.0000000000     24.0685192700
```

```
&BANDS
prefix='WSe2-1T'
outdir='./'
filband='WSe2-1T-b'
/
```