

Supplementary Information

Polymorphic Janus ZrSC Monolayer: A First-Principles Study of Structural, Mechanical, Vibrational, and Electronic Properties

1. ZrSC_1H scf input file

```
&control
  calculation = 'scf',
  prefix = 'ZrSC_1H_0',
  outdir = './ZrSCh_0',
  tstress = .true.,
  tprnfor = .true.
/

&system
 ibrav = 4,
a = 3.73090000,
c = 24
nat = 3,
ntyp = 3,
ecutwfc = 50,
ecutrho = 400,
nspin = 2,
starting_magnetization(1) = 0.0, ! S
starting_magnetization(2) = 1.0, ! Zr
starting_magnetization(3) = 0.0, ! C
occupations = 'smearing',
smearing = 'gaussian',
degauss = 0.000735
vdw_corr = 'dft-d3'
/

&electrons
  mixing_beta = 0.7
  conv_thr = 1.0E-08
/

ATOMIC_SPECIES
S 32.06 S.pbe-n-kjpaw_psl.1.1.0.0.UPF
Zr 91.22 Zr.pbe-spn-kjpaw_psl.1.1.0.0.UPF
C 12.01 C.pbe-n-kjpaw_psl.1.1.0.0.UPF

ATOMIC_POSITIONS (crystal)
Zr 0.0000235209 -0.0000235209 0.4862878520
S 0.6666847126 0.3333152874 0.5466453062
C 0.6666917665 0.3333082335 0.4670668418

K_POINTS automatic
7 7 1 0 0 0
```

2. ZrSC_1T scf input file

```
&control
  calculation = 'scf',
  prefix = 'ZrSC_1T_0',
  outdir = './ZrSCt_0',
  tstress = .true.,
  tprnfor = .true.
/
&system
 ibrav = 4,
a = 3.6485,
c = 24.3169,
nat = 3,
ntyp = 3,
ecutwfc = 50,
ecutrho = 400,
nspin = 2,
starting_magnetization(1) = 0.0, ! S
starting_magnetization(2) = 1.0, ! Zr
starting_magnetization(3) = 0.0, ! C
occupations = 'smearing',
smearing = 'mp',
degauss = 0.001
/
&electrons
  mixing_beta = 0.7
  conv_thr = 1.0E-08
/

&ions
/

&cell
/

ATOMIC_SPECIES
S 32.06 S.pbe-n-kjpaw_psl.1.1.0.0.UPF
Zr 91.22 Zr.pbe-spn-kjpaw_psl.1.1.0.0.UPF
C 12.01 C.pbe-n-kjpaw_psl.1.1.0.0.UPF

ATOMIC_POSITIONS (crystal)
Zr -0.0000059093 0.0000059093 0.4861912358
S 0.6666688482 0.3333311518 0.5527618350
C 0.3333370611 0.6666629389 0.4610469289

K_POINTS automatic
8 8 1 0 0 0
```

3. ZrSC phonon input file

```
&inputph
  tr2_ph = 1.0d-14,
```

```
prefix = 'ZrSCh',
outdir = './tmp',
asr=.true.,
verbosity = 1,
ldisp = .true.,
fildyn = 'ZrSC.dyn',
nq1=4,
nq2=4,
nq3=1
/
```

4. ZrSC 1H phonon Statistics

```
 $\Gamma$ : x = 0.0000
Frequencies: B1: -0.2 B2: -0.2 B3: 0.0 B4: 256.7 B5: 257.6 B6: 330.9
K: x = 0.5774
Frequencies: B1: 106.2 B2: 106.6 B3: 223.4 B4: 242.3 B5: 288.6 B6: 294.5
M: x = 1.1547
Frequencies: B1: 106.3 B2: 107.6 B3: 222.5 B4: 242.8 B5: 289.1 B6: 295.5
K': x = 1.7321
Frequencies: B1: 106.2 B2: 106.6 B3: 223.4 B4: 242.3 B5: 288.6 B6: 294.5
 $\Gamma$ : x = 2.3094
Frequencies: B1: -0.2 B2: -0.2 B3: 0.0 B4: 256.7 B5: 257.6 B6: 330.9
M: x = 2.8868
Frequencies: B1: 96.1 B2: 190.5 B3: 218.9 B4: 264.6 B5: 269.2 B6: 276.0
 $\Gamma$ : x = 3.0000
Frequencies: B1: 96.8 B2: 192.7 B3: 218.0 B4: 265.5 B5: 269.2 B6: 274.7
```

```
Total data points: 101
Original frequency range: -5.4 to 643.2  $\text{cm}^{-1}$ 
Displayed frequency range: -20 to 400  $\text{cm}^{-1}$ 
```

Phonon DOS Statistics:

```
=====
Frequency range: 0.8 to 643.8  $\text{cm}^{-1}$ 
Total DOS maximum: 0.168366 at 96.8  $\text{cm}^{-1}$ 
PDOS 1 maximum: 0.121150 at 96.8  $\text{cm}^{-1}$ 
PDOS 2 maximum: 0.072221 at 247.8  $\text{cm}^{-1}$ 
PDOS 3 maximum: 0.117870 at 563.8  $\text{cm}^{-1}$ 
```

Prominent peaks found: 14

Peak positions (cm^{-1}):

```
96.8  $\text{cm}^{-1}$ 
107.8  $\text{cm}^{-1}$ 
220.8  $\text{cm}^{-1}$ 
247.8  $\text{cm}^{-1}$ 
262.8  $\text{cm}^{-1}$ 
272.8  $\text{cm}^{-1}$ 
282.8  $\text{cm}^{-1}$ 
304.8  $\text{cm}^{-1}$ 
518.8  $\text{cm}^{-1}$ 
563.8  $\text{cm}^{-1}$ 
```

5. ZrSC 1T phonon Statistics

Γ : x = 0.0000
Frequencies: B1: -0.0 B2: 0.0 B3: 0.0 B4: 156.0 B5: 156.0 B6: 266.9
K: x = 0.5774
Frequencies: B1:-155.0 B2: -79.8 B3: 25.0 B4: 168.4 B5: 190.8 B6: 237.1
M: x = 1.1547
Frequencies: B1:-155.0 B2: -79.8 B3: 25.0 B4: 168.4 B5: 190.8 B6: 237.1
K': x = 1.7321
Frequencies: B1:-155.0 B2: -79.8 B3: 25.0 B4: 168.4 B5: 190.8 B6: 237.1
 Γ : x = 2.3094
Frequencies: B1: -0.0 B2: 0.0 B3: 0.0 B4: 156.0 B5: 156.0 B6: 266.9
M: x = 2.8868
Frequencies: B1:-149.6 B2: -16.7 B3: 74.6 B4: 154.6 B5: 216.5 B6: 242.8
 Γ : x = 3.0000
Frequencies: B1:-151.0 B2: 21.0 B3: 71.4 B4: 157.0 B5: 219.0 B6: 241.9

Total data points: 101
Original frequency range: -155.0 to 570.3 cm^{-1}
Displayed frequency range: -20 to 400 cm^{-1}

Phonon DOS Statistics:

=====
Frequency range: 1.0 to 570.0 cm^{-1}
Total DOS maximum: 0.436422 at 154.0 cm^{-1}
PDOS 1 maximum: 0.106400 at 154.0 cm^{-1}
PDOS 2 maximum: 0.125660 at 506.0 cm^{-1}
PDOS 3 maximum: 0.319280 at 154.0 cm^{-1}

Prominent peaks found: 7

Peak positions (cm^{-1}):

24.0 cm^{-1}
154.0 cm^{-1}
191.0 cm^{-1}
237.0 cm^{-1}
311.0 cm^{-1}
506.0 cm^{-1}
563.0 cm^{-1}

6. Cohesive Energy Calculation Results

=== ATOMIC ENERGIES ===

Element	Energy (Ry)	Energy (eV)
C	-17.780645	-241.918092
S	-66.007146	-898.073299
Zr	-306.695950	-4172.812494

=== BULK STRUCTURES ===

Phase	File	nat	E (Ry)	E (eV)
1H	ZrSC_1H_scf.out	3	-392.023871	-5333.758430
1T	ZrSC_1T_scf.out	3	-391.875287	-5331.736837

```
=== COHESIVE ENERGY PER ATOM ===  
ZrSC 1H : -6.984849 eV/atom (nat = 3)  
ZrSC 1T : -6.310984 eV/atom (nat = 3)  
  
=== ENERGY DIFFERENCES ===  
 $\Delta E$  (1H-1T): -0.673864 eV/atom
```