

SUPPLEMENTARY INFORMATION

Theoretical study of electronic and transport thermoelectric properties of unconventional bulk and 2D γ -SnSe and γ -SnS

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Structure data in CIF format for 2D and bulk SnS and SnSe phases

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#=====
#
# CRYSTAL DATA
#-----
-
data_SnSe_3D_alpha

  _chemical_name_common          'SnSe'
  _cell_length_a                 4.211737
  _cell_length_b                 4.557569
  _cell_length_c                 11.782299
  _cell_angle_alpha              90.000000
  _cell_angle_beta               90.000000
  _cell_angle_gamma              90.000000
  _cell_volume                   226.164562
  _space_group_name_H-M_alt      'P 1'
  _space_group_IT_number         1

loop_
  _space_group_symop_operation_xyz
    'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  Sn1          1.0          0.249999          0.383412          0.621252          Uiso    ? Sn
```

Sn2	1.0	0.249999	0.116589	0.121252	Uiso	? Sn
Sn3	1.0	0.750000	0.616587	0.378748	Uiso	? Sn
Sn4	1.0	0.750000	0.883413	0.878748	Uiso	? Sn
Se1	1.0	0.249999	0.025452	0.355290	Uiso	? Se
Se2	1.0	0.249999	0.474549	0.855290	Uiso	? Se
Se3	1.0	0.750000	0.974547	0.644710	Uiso	? Se
Se4	1.0	0.750000	0.525453	0.144710	Uiso	? Se

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# CRYSTAL DATA
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```
data_SnSe_2D_alpha
```

```
_chemical_name_common      'SnSe'
_cell_length_a              4.283233
_cell_length_b              4.410285
_cell_length_c              25.585487
_cell_angle_alpha           90.000000
_cell_angle_beta            90.000000
_cell_angle_gamma           90.000000
_cell_volume                483.316994
_space_group_name_H-M_alt    'P 1'
_space_group_IT_number       1
```

```
loop_
_space_group_symop_operation_xyz
  'x, y, z'
```

```
loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  Sn1      1.0      0.750000      0.600613      0.160825      Uiso      ? Sn
  Sn2      1.0      0.250000      0.101418      0.053099      Uiso      ? Sn
  Se1      1.0      0.250000      0.045498      0.159362      Uiso      ? Se
  Se2      1.0      0.750000      0.545867      0.054547      Uiso      ? Se
```

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# CRYSTAL DATA
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```

```
data_SnSe_3D_gamma
```

```

_chemical_name_common      'SnSe'
_cell_length_a             4.192973
_cell_length_b             8.557502
_cell_length_c             6.232721
_cell_angle_alpha          90.029701
_cell_angle_beta           90.012184
_cell_angle_gamma          89.986389
_cell_volume               223.638554
_space_group_name_H-M_alt  'P 1'
_space_group_IT_number     1

```

```

loop_
_space_group_symop_operation_xyz
  'x, y, z'

```

```

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  Sn1      1.0      0.627416      0.603214      0.700032      Uiso  ?  Sn
  Sn2      1.0      0.126418      0.874972      0.199680      Uiso  ?  Sn
  Sn3      1.0      0.628084      0.103166      0.822760      Uiso  ?  Sn
  Sn4      1.0      0.126022      0.375046      0.323304      Uiso  ?  Sn
  Se1      1.0      0.127396      0.823296      0.643752      Uiso  ?  Se
  Se2      1.0      0.626024      0.654786      0.143914      Uiso  ?  Se
  Se3      1.0      0.626784      0.154854      0.378654      Uiso  ?  Se
  Se4      1.0      0.127348      0.323350      0.879080      Uiso  ?  Se

```

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#=====
#
# CRYSTAL DATA
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-
data_SnSe_2D_gamma

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```

_chemical_name_common      'SnSe'
_cell_length_a             3.937749
_cell_length_b             6.186510
_cell_length_c            23.581026
_cell_angle_alpha          90.000000
_cell_angle_beta           90.000000
_cell_angle_gamma          90.000000
_cell_volume               574.455569

```

```
_space_group_name_H-M_alt      'P 1'
_space_group_IT_number          1
```

```
loop_
_space_group_symop_operation_xyz
  'x, y, z'
```

```
loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  Sn1      1.0      0.500000      0.172354      0.048531      Uiso      ? Sn
  Sn2      1.0      0.000000      0.672516      0.133419      Uiso      ? Sn
  Se1      1.0      0.000000      0.147411      0.128777      Uiso      ? Se
  Se2      1.0      0.500000      0.647450      0.053168      Uiso      ? Se
```

```
#=====
#
# CRYSTAL DATA
#-----
-
data_SnS_3D_alpha
```

```
_chemical_name_common          'SnSe'
_cell_length_a                  11.258350
_cell_length_b                  4.020000
_cell_length_c                  4.318500
_cell_angle_alpha               90.000000
_cell_angle_beta               90.000000
_cell_angle_gamma               90.000000
_cell_volume                    195.449129
_space_group_name_H-M_alt       'P n m a'
_space_group_IT_number          62
```

```
loop_
_space_group_symop_operation_xyz
  'x, y, z'
  '-x, -y, -z'
  '-x+1/2, -y, z+1/2'
  'x+1/2, y, -z+1/2'
  '-x, y+1/2, -z'
  'x, -y+1/2, z'
```

```

'x+1/2, -y+1/2, -z+1/2'
'-x+1/2, y+1/2, z+1/2'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  Sn1      1.0      0.619470      0.250000      0.380870      Biso
1.000000 Sn
  S1      1.0      0.352700      0.250000      0.027510      Biso
1.000000 S

#=====
#
# CRYSTAL DATA
#-----
-
data_SnS_2D_alpha

  _chemical_name_common      'SnS'
  _cell_length_a      4.078460
  _cell_length_b      4.310366
  _cell_length_c      25.585487
  _cell_angle_alpha      90.000000
  _cell_angle_beta      90.000000
  _cell_angle_gamma      90.000000
  _cell_volume      449.784089
  _space_group_name_H-M_alt      'P 1'
  _space_group_IT_number      1

loop_
  _space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  Sn1      1.0      0.750000      0.613005      0.162589      Uiso  ? Sn

```

Sn2	1.0	0.249999	0.113157	0.051357	Uiso	? Sn
S1	1.0	0.249999	0.033921	0.151908	Uiso	? S
S2	1.0	0.750000	0.533310	0.061979	Uiso	? S

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#=====
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```

```
# CRYSTAL DATA
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#-----
-
```

```
data_SnS_3D_gamma
```

```
_chemical_name_common      'SnS'
_cell_length_a              4.018080
_cell_length_b              8.471977
_cell_length_c              5.977116
_cell_angle_alpha           90.000000
_cell_angle_beta            90.000000
_cell_angle_gamma           90.000000
_cell_volume                203.467513
_space_group_name_H-M_alt   'P 1'
_space_group_IT_number      1
```

```
loop_
_space_group_symop_operation_xyz
  'x, y, z'
```

```
loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  Sn1      1.0      0.500010      0.380760      0.187344      Biso
1.000000 Sn
  Sn2      1.0      0.000010      0.619240      0.812654      Biso
1.000000 Sn
  Sn3      1.0      0.999990      0.119240      0.687346      Biso
1.000000 Sn
  Sn4      1.0      0.499990      0.880760      0.312656      Biso
1.000000 Sn
  S1       1.0      0.000002      0.672224      0.371972      Biso
1.000000 S
  S2       1.0      0.500002      0.327776      0.628028      Biso
1.000000 S
  S3       1.0      0.499998      0.827776      0.871972      Biso
1.000000 S
```

```

      S4      1.0      0.999998      0.172224      0.128028      Biso
1.000000 S

```

```

#=====
#
# CRYSTAL DATA
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-

```

```

data_SnS_2D_gamma

```

```

_chemical_name_common      'SnS'
_cell_length_a              3.803752
_cell_length_b              5.866401
_cell_length_c              23.581026
_cell_angle_alpha           90.000000
_cell_angle_beta            90.000000
_cell_angle_gamma           90.000000
_cell_volume                526.194915
_space_group_name_H-M_alt   'P 1'
_space_group_IT_number      1

```

```

loop_
_space_group_symop_operation_xyz
  'x, y, z'

```

```

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
Sn1      1.0      0.500001      0.177075      0.044359      Uiso ? Sn
Sn2      1.0      0.000000      0.677037      0.137590      Uiso ? Sn
S1       1.0      0.000000      0.142821      0.119766      Uiso ? S
S2       1.0      0.500001      0.642798      0.062180      Uiso ? S

```