hands-on IR2PW

Web:
https://tm.iphy.ac.cn/UnconvMat.html
https://tm.iphy.ac.cn/TopMat_1651msg.html

Source code:
https://github.com/zjwang11/IR2PW/

Ref:

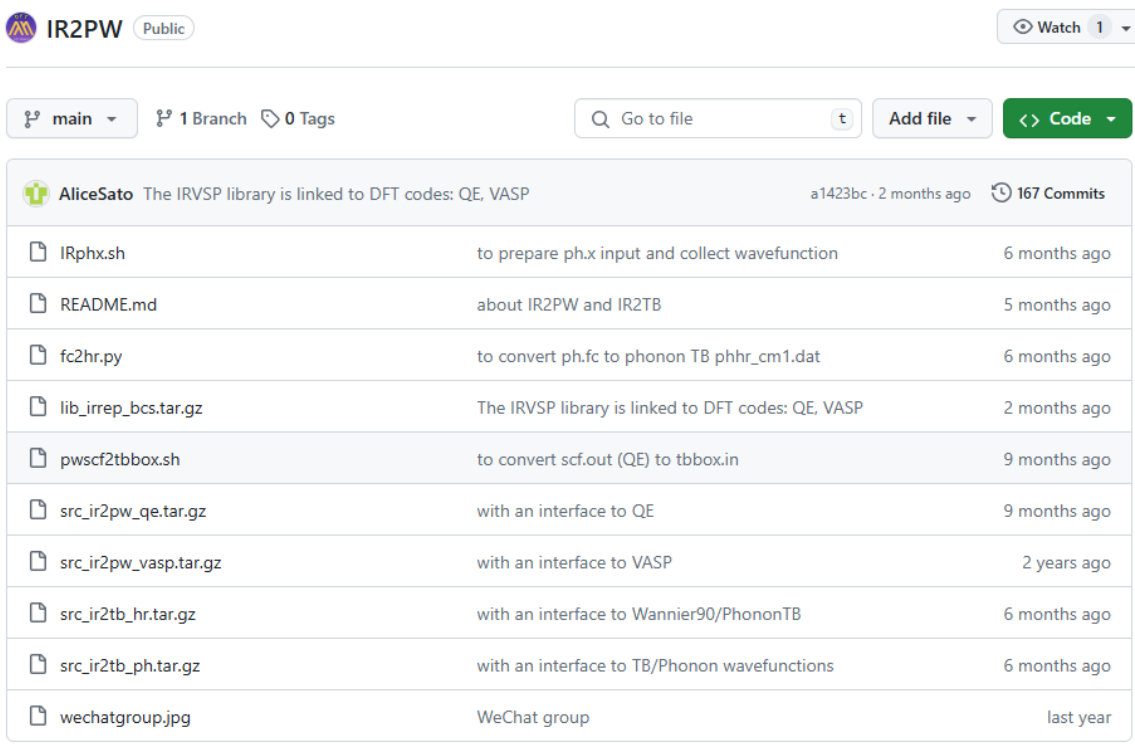
Gao, J. et al. "IRVSP: to obtain irreducible representations in the VASP", Comput. Phys. Comm. 261, 107760 (2021).
Zhang, R. et al. "Large shift current, π Zak phase and unconventional nature of Se and Te", Phys. Rev. Research 5, 023142 (2023).

Ruihan Zhang 2024/6/5

Outline

- 0 Installation
- 1 Find band-crossing (or gap)　—IRVSP
- 2 Solve the EBR/ABR decompostion and CR　—IRVSP
- 3 Solve the CR and calculate SI　—IRVSP
- 4 Calculate the phonon BRs by Quantum Espresso (QE)　—IR2PH
- 5 Solve CR and calculate SI by IR2TB　—IR2TB

0 Installation



1)
```
$ tar -zxvf lib_irrep_bcs.tar.gz
$ cd lib_irrep_bcs
$ ./configure.sh
$ make
$ cd ../
```

2)
```
$ tar -zxvf src_ir2pw_qe.tar.gz
$ cd src_ir2pw_qe
$ make
$ cd ../
```

3)
```
$ tar -zxvf src_ir2pw_vasp.tar.gz
$ cd src_ir2pw_vasp
$ make
$ cd ../
```

4)
```
$ tar -zxvf src_ir2tb_hr.tar.gz
$ cd src_ir2tb_hr
$ make
$ cd ../
```

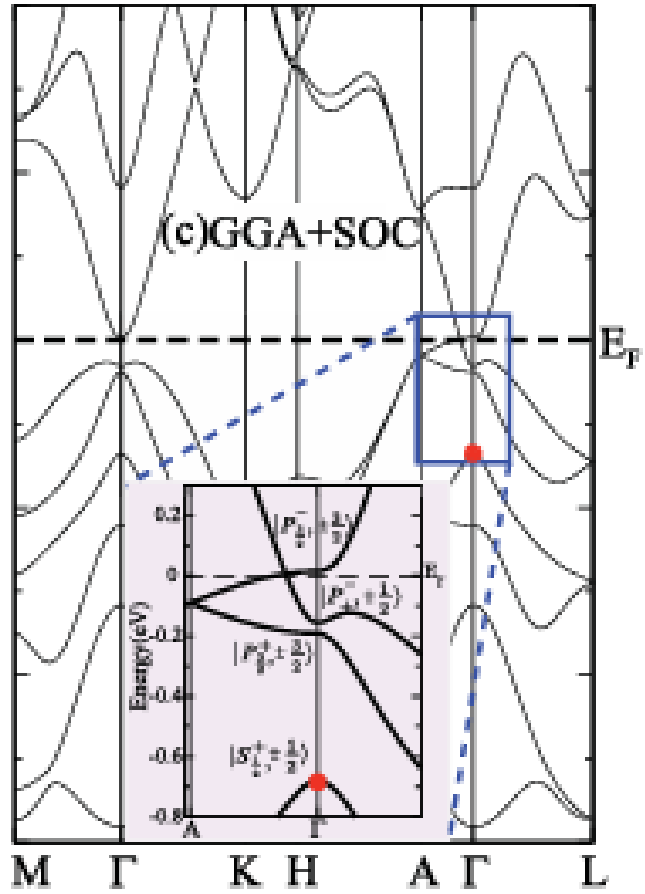
5)
```
$ tar -zxvf src_ir2tb_ph.tar.gz
$ cd src_ir2tb_ph
$ make
$ cd ../
```

https://github.com/zjwang11/ir2pw

1 Find band-crossing (or gap)

- In first-principles calculations, we often need to find band-crossing (or gap). If the k-points are not given enough, it may be difficult.
- Here we take the Na_3Bi as an example to introduce how to calculate the band representations (BRs) of different k-points to find band-crossing (or gap) by using IRVSP.

band structures with spin-orbit coupling



PHYSICAL REVIEW B 85,195320 (2012)

Step 1

1) Prepare the original POSCAR file. (Na_3Bi as an example)
2) $ phonopy --tolerance 0.01 --symmetry -c POSCAR
   $ vim PPOSCAR

"POSCAR"

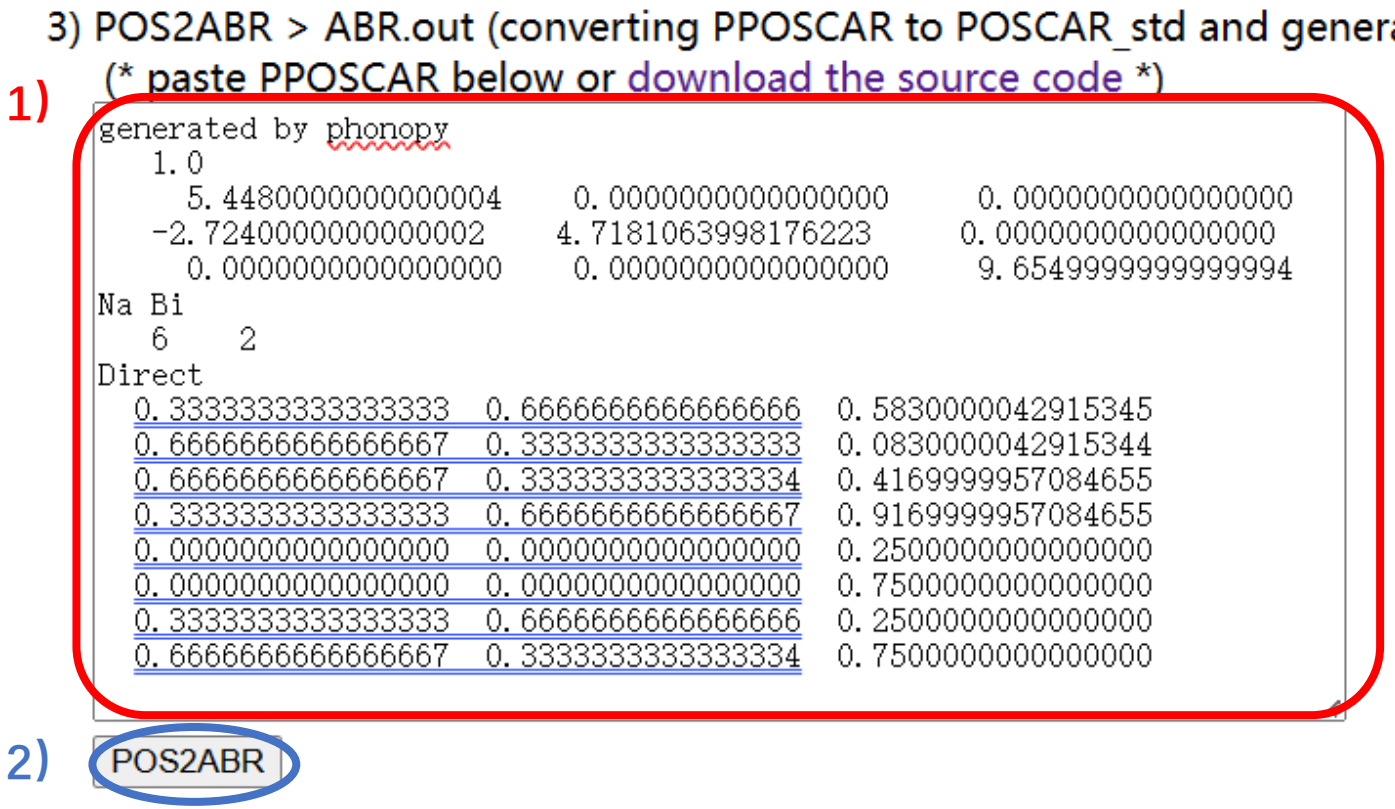
```
Na3Bi
   1.0
      4.718106399817621    -2.724000000000002     0.000000000000000
      0.000000000000000     5.448000000000000     0.000000000000000
      0.000000000000000     0.000000000000000     9.654999999999999
   Na Bi
   6  2
Direc
  0.3333333333333334   0.6666666666666666   0.5830000042915345
 -0.3333333333333334  -0.6666666666666666   1.0830000042915344
  0.6666666666666666   0.3333333333333334  -0.5830000042915344
 -0.6666666666666666  -0.3333333333333334  -0.0830000042915344
  0.0000000000000000   0.0000000000000000   0.2500000000000000
  0.0000000000000000   0.0000000000000000   0.7500000000000000
  0.3333333333333334   0.6666666666666666   0.2500000000000000
 -0.3333333333333334  -0.6666666666666666   0.7500000000000000
```

"PPOSCAR"

```
generated by phonopy
   1.0
     5.4480000000000004   0.0000000000000000   0.0000000000000000
    -2.7240000000000002   4.7181063998176223   0.0000000000000000
     0.0000000000000000   0.0000000000000000   9.6549999999999994
Na Bi
   6    2
Direct
  0.3333333333333333  0.6666666666666666  0.5830000042915345
  0.6666666666666667  0.3333333333333333  0.0830000042915344
  0.6666666666666667  0.3333333333333334  0.4169999957084655
  0.3333333333333333  0.6666666666666667  0.9169999957084655
  0.0000000000000000  0.0000000000000000  0.2500000000000000
  0.0000000000000000  0.0000000000000000  0.7500000000000000
  0.3333333333333333  0.6666666666666666  0.2500000000000000
  0.6666666666666667  0.3333333333333334  0.7500000000000000
```

Step 2

Open the web: https://tm.iphy.ac.cn/UnconvMat.html



1) Paste PPOSCAR into this box.

2) Press POS2ABR button.

Step 3

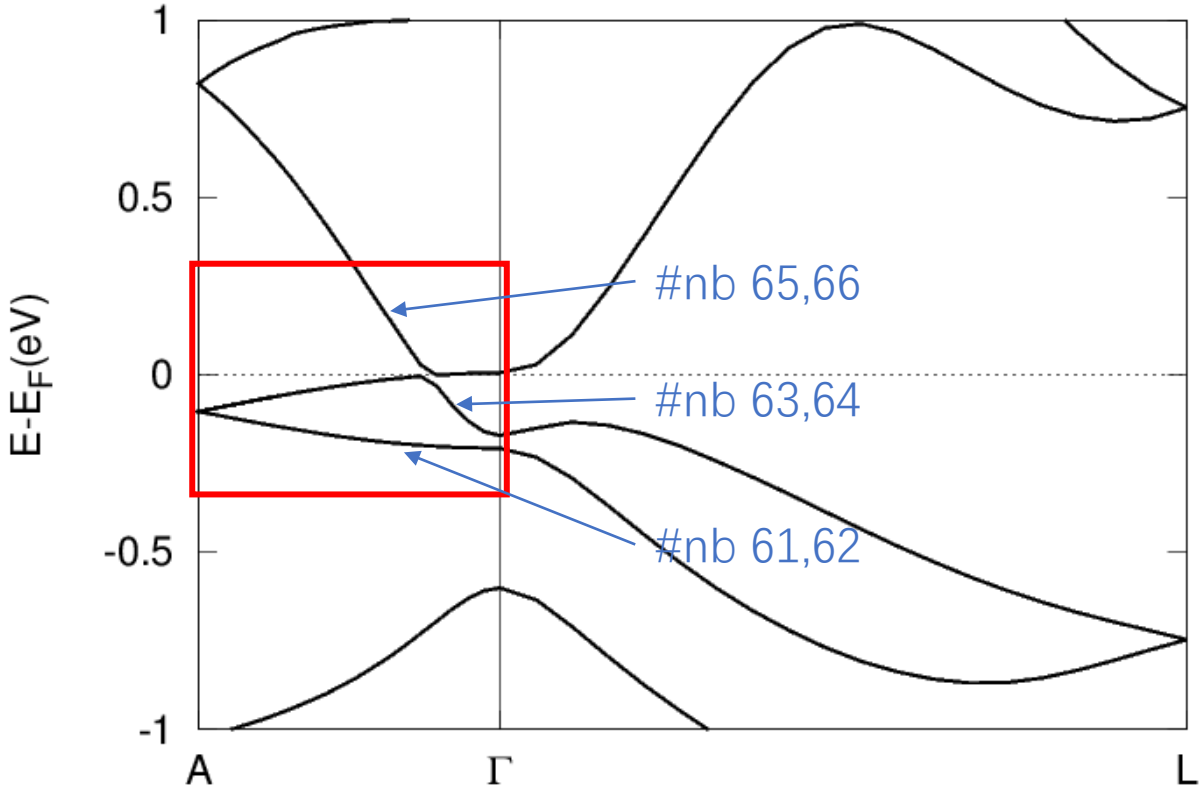
We can get the standard POSCAR (POSCAR_std) and the space group number of Na_3Bi is 194.

Copy the content in the red box to POSCAR, and then do VASP calculations.

```
POSCAR std :
SG 194   0.000   0.000   0.000 :Generated by pos2aBR for irvsp!
     1.0
       5.4480000000000004      0.0000000000000000      0.0000000000000000
      -2.7240000000000002      4.7181063998176223      0.0000000000000000
       0.0000000000000000      0.0000000000000000      9.6549999999999994
 Na   Bi
    6    2
Direct
  0.3333333333333333  0.6666666666666666  0.5830000042915345
  0.6666666666666667  0.3333333333333333  0.0830000042915344
  0.6666666666666667  0.3333333333333334  0.4169999957084655
  0.3333333333333333  0.6666666666666667  0.9169999957084655
  0.0000000000000000  0.0000000000000000  0.2500000000000000
  0.0000000000000000  0.0000000000000000  0.7500000000000000
  0.3333333333333333  0.6666666666666666  0.2500000000000000
  0.6666666666666667  0.3333333333333334  0.7500000000000000
```

Step 4

Through the analysis of the band structure, we find that there may be a band-crossing in the $A - \Gamma$ path near the Fermi energy.



Step 5

-nb #nmin #nmax : Minimum and maximum target band numbers

```
$ irvsp -sg 194 -nb 61 66 > outir
$ vim outir
```

IRVSP will read the wave function from WAVECAR and calculate the BRs at each k point.

outir:

```
knum = 15    kname=
k = 0.000000 0.000000 0.131579
...
bnd ndg eigval     E              ...    24
 61  2  1.991043 2.00+0.00i    ...  0.00+0.00i =DT7
 63  2  2.185607 2.00+0.00i    ...  0.00+0.00i =DT7
 65  2  2.218277 2.00+0.00i    ...  0.00+0.00i =DT8
```

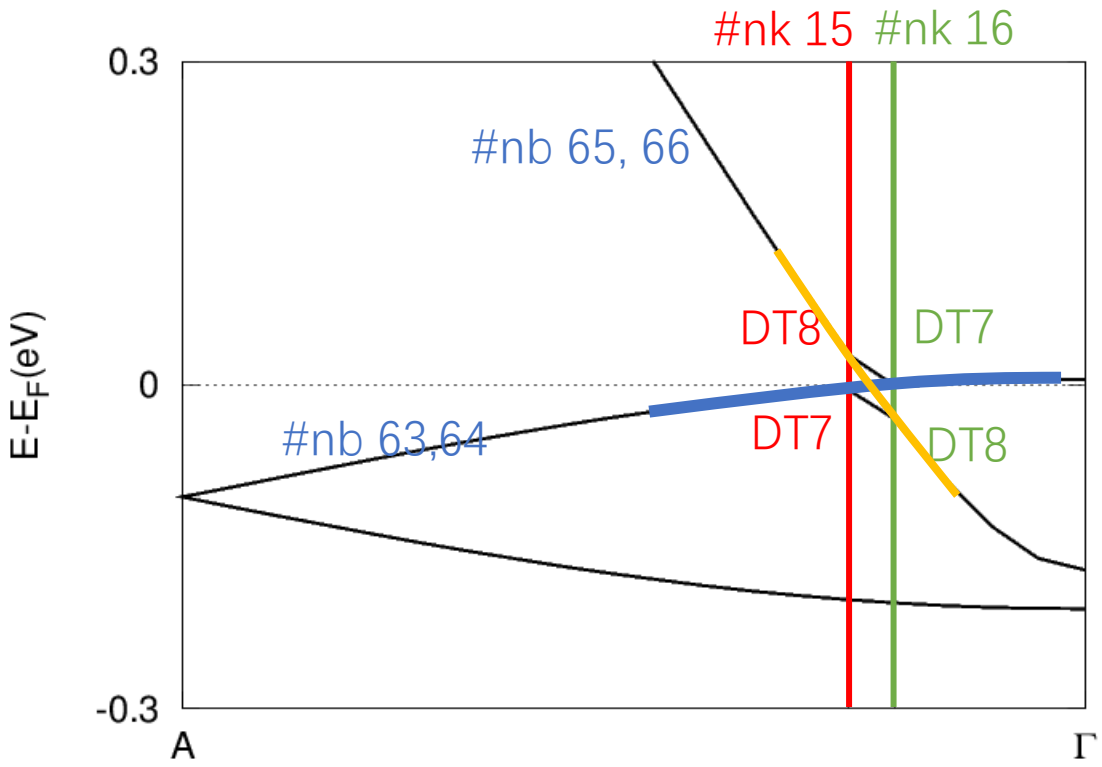
...

```
knum = 16    kname=
k = 0.000000 0.000000 0.105263
...
bnd ndg  eigval     E              ...    24
 61  2  1.987986 2.00+0.00i    ...  0.00+0.00i =DT7
 63  2  2.158086 2.00+0.00i    ...  0.00+0.00i =DT8
 65  2  2.188929 2.00+0.00i    ...  0.00+0.00i =DT7
```

Step 6

We can see that the orders of BRs at No. 15 k-point and No. 16 k-point are different, so there is a symmetry-protected band-crossing in the $A - \Gamma$ path near the Fermi energy.

There is a Dirac point between #nk 15 and #nk 16.



2 Solve the EBR/ABR decompostion and CR

- Based on topological quantum chemistry theory, we can calculate the irreducible representations (irreps) at several high-symmetry k-points (HSKPs) to diagnose whether the band structure of a material is topological.
- If the irreps of all occupied bands cannot be decomposed as a sum of elementary BRs (EBRs), this material is topological.
- If the irreps of all occupied bands can be decomposed as a sum of EBRs but cannot be decomposed as a sum of atomic valence-electron BRs (ABRs), this material is topologically trivial but has unconventional properties.

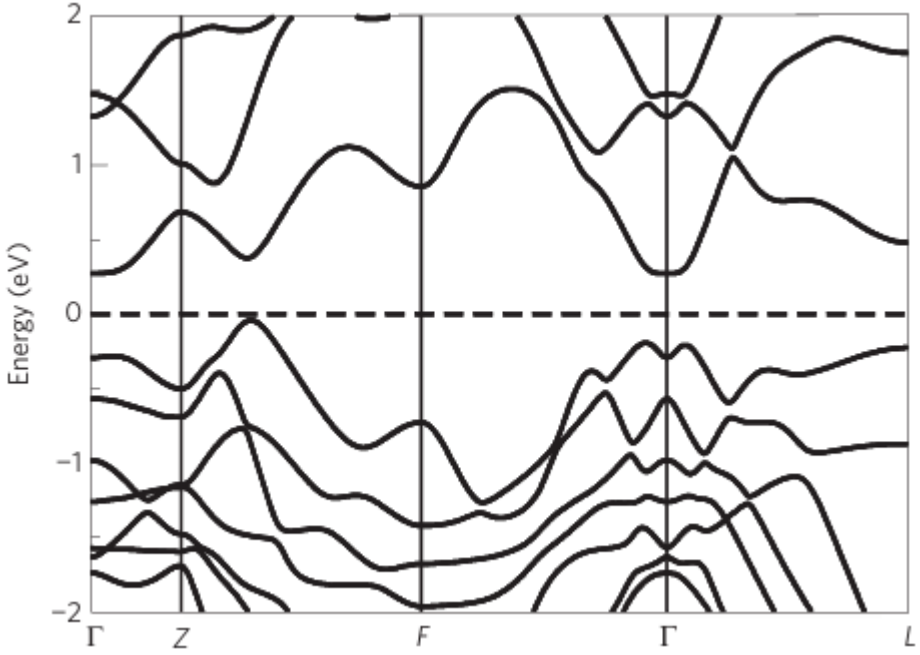
2 Solve the EBR/ABR decompostion and CR and calculate SI

- Here we take the topological material Bi_2Se_3 and unconventional material $NbSe_2$ as examples to introduce how to calculate irreps to solve EBR/ABR decompositions and the compatibility relationship (CR) and symmetry indicators (SIs) to diagnose topological or unconventional materials.

2.1 Bi_2Se_3

- Here we take the topological material Bi_2Se_3 as an examples to introduce how to calculate irreps to solve the CR and SIs to diagnose topological materials.

Band structure for Bi_2Se_3 with SOC



Nature Physics volume 5, pages438–442 (2009)

Step 1

1) Prepare the original POSCAR file. (Bi_2Se_3 as an example)
2) $ phonopy --tolerance 0.01 --symmetry -c POSCAR
   $ vim PPOSCAR

phonopy_version: '2.20.0'
space_group_type: 'R-3m'
space_group_number: 166
point_group_type: '-3m'

"POSCAR"

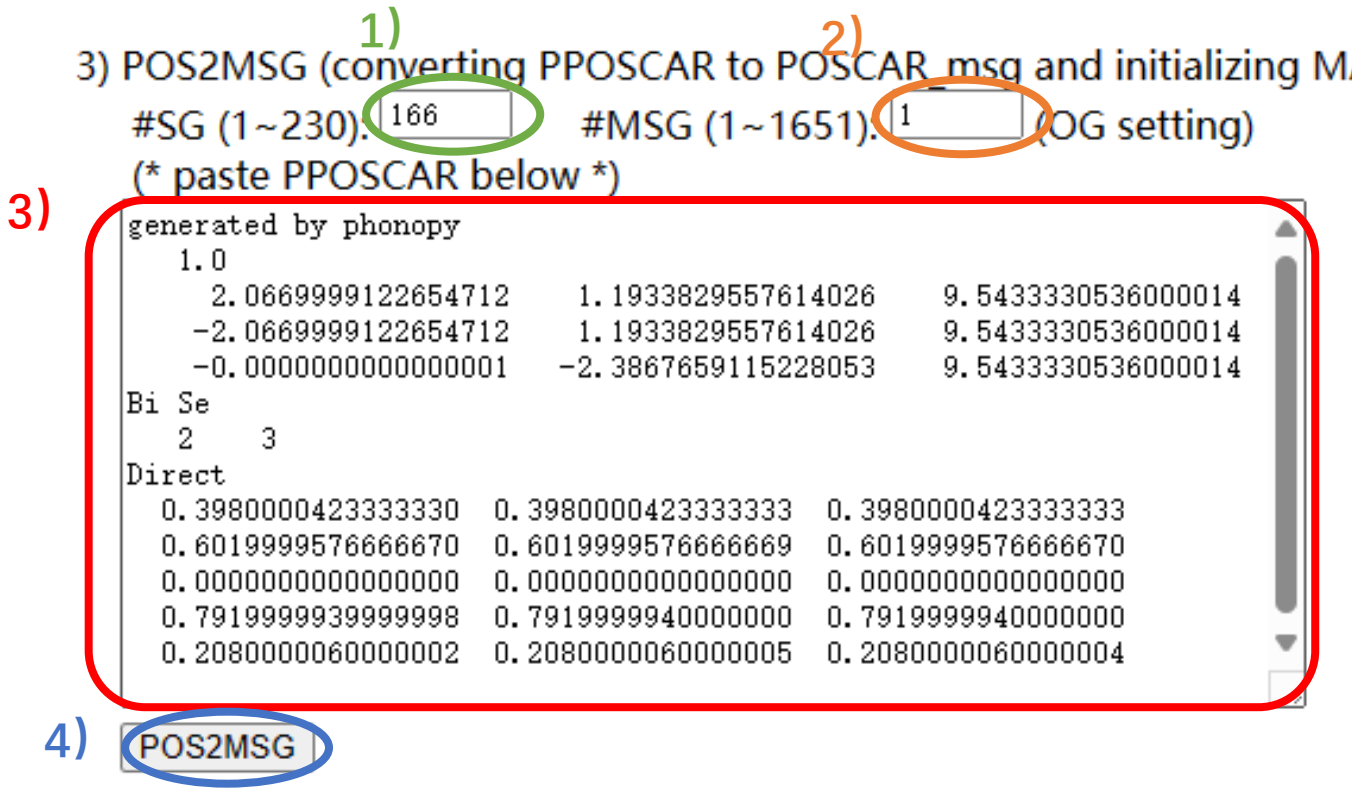
```
Bi2 Se3
1.0
    2.0669999122654712   1.1933829557614029   9.5433330536000032
   -2.0669999122654712   1.1933829557614029   9.5433330536000032
    0.0000000000000000  -2.3867659115228057   9.5433330536000032
Bi Se
2  3
Direct
  0.3980000423333330  0.3980000423333330  0.3980000423333331
  0.6019999576666670  0.6019999576666670  0.6019999576666668
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.7919999939999998  0.7919999939999998  0.7919999939999998
  0.2080000060000003  0.2080000060000003  0.2080000060000003
```

"PPOSCAR"

```
generated by phonopy
   1.0
    2.0669999122654712   1.1933829557614026   9.5433330536000014
   -2.0669999122654712   1.1933829557614026   9.5433330536000014
   -0.0000000000000001  -2.3867659115228053   9.5433330536000014
Bi Se
   2    3
Direct
  0.3980000423333330  0.3980000423333333  0.3980000423333333
  0.6019999576666670  0.6019999576666669  0.6019999576666670
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.7919999939999998  0.7919999940000000  0.7919999940000000
  0.2080000060000002  0.2080000060000005  0.2080000060000004
```

Step 2

Open the web:https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Give the group number(SG) from phonopy: 166.

2) Give any reasonable magnetic space group (MSG) number, such as 1.

3) Paste PPOSCAR into this box.

4) Press POS2MSG button.

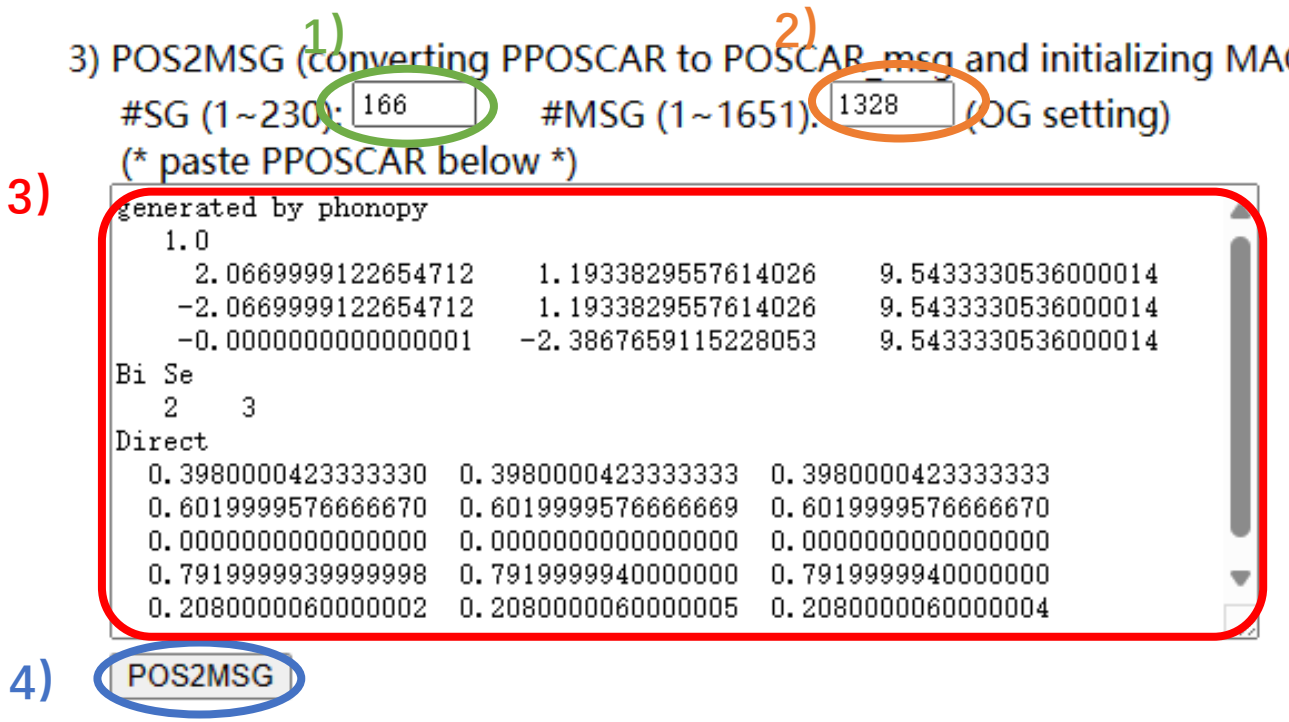
Step 3

```
The OG magnetic space group number do not match with the given space group number.
Possible OG magnetic space group numbers are given below:
1327, type 1
1328, type 2
1329, type 3
1330, type 3
1331, type 3
1332, type 4
1333, type 4
```

Nonmagnetic materials are the type-2 MSGs, which include time inversion operation.

Step 4

Back to the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Give the correct space group (SG) number: 166.

2) Give the correct magnetic space group(MSG) number: 1328.

3) Paste PPOSCAR into this box.

4) Press POS2MSG button.

Step 5

```
POSCAR_msg:
SG#B 166    OG (  166.2.1328)    BNS (      166.98)
  1.0
    2.06699991226547     1.19338295576140     9.54333305360000
   -2.06699991226547     1.19338295576140     9.54333305360000
   -0.00000000000000    -2.38676591152281     9.54333305360000
    Bi    Se
     2     3
Direct
     0.39800004233333     0.39800004233333     0.39800004233333
     0.60199995766667     0.60199995766667     0.60199995766667
     0.00000000000000     0.00000000000000     0.00000000000000
     0.79199999400000     0.79199999400000     0.79199999400000
     0.20800000600000     0.20800000600000     0.20800000600000

INCAR:
LSORBIT = T
LNONCOLLINEAR = T
SAXIS = 0 0 1
MAGMOM=300*0.0

KPOINTS:
MKPOINTS used for magnetic space group
  4
rec
     0.00000000     0.00000000     0.00000000     1.0     ! GM
     0.50000000     0.50000000     0.50000000     1.0     ! T
     0.50000000     0.50000000     0.00000000     1.0     ! F
     0.00000000     0.50000000     0.00000000     1.0     ! L
```

We can get the standard POSCAR (POSCAR_msg) and some setting parameters of INCAR and KPOINTS.

All space groups' HSKPs can be found on: https://github.com/zjwang11/IR2PW/lib_irrep_bcs/max_KPOINTS_VASP/

Then we do VASP calculations.

Step 6

The number of valence electrons in Bi_2Se_3 is 48

```
$ irvsp -sg 166 -nb 1 48 > outir
$ vim tqc.data
```

After IRVSP calculating the wave function of HSKPs, file tqc.data will be generated.

"tqc.data"

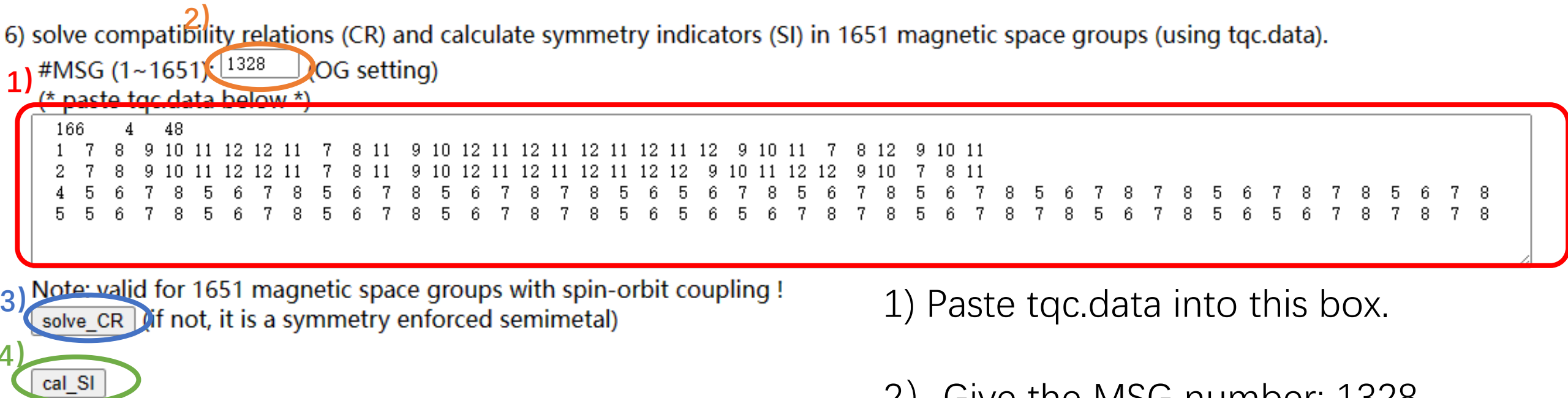
```
166    4   48
 1  7  8  9 10 11 12 12 11  7  8 11  9 10 12 11 12 11 12 11 12 11 12  9 10 11  7  8 12  9 10 11
 2  7  8  9 10 11 12 12 11  7  8 11  9 10 12 11 12 11 12 11 12 12  9 10 11 12 12  9 10  7  8 11
 4  5  6  7  8  5  6  7  8  5  6  7  8  5  6  7  8  7  8  5  6  5  6  7  8  5  6  7  8  5  6  7  8  7  8  5  6  7  8  7  8  5  6  7  8
 5  5  6  7  8  5  6  7  8  5  6  7  8  5  6  7  8  7  8  5  6  5  6  5  6  7  8  7  8  5  6  7  8  7  8  5  6  7  8  5  6  5  6  7  8  7  8  7  8
```

Format of tqc.data

```
#SG (space group number)   #nk (number of HSKPs)   #nb (number of bands)
 HSKP#1  irrep(HSKP#1)#1  irrep(HSKP#1)#2  ···
 HSKP#2  irrep(HSKP#2)#1  irrep(HSKP#2)#2  ···
 ...
```

Step 7

Back to the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Paste tqc.data into this box.

2) Give the MSG number: 1328.

3) Press solve_CR button.

4) Press cal_SI button.

Step 8

solve_CR :

```
The input data is calculated with spin-orbit coupling.
Satisfy CR
```

cal_SI :

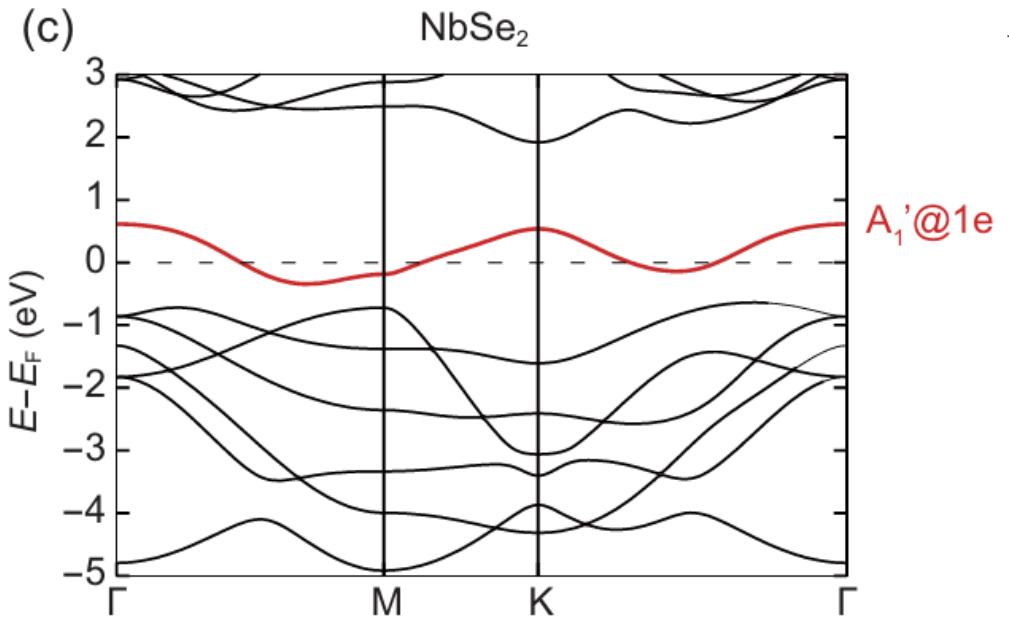
```
The input data is calculated with spin-orbit coupling.
Z2=0,Z4=1,
```

We can see that Bi_2Se_3 satisfies the CR, and its SI is Z4=1,
so we can diagnose that this is a topological material.

2.2 $NbSe_2$

- Here we take the unconventional material 1H-$NbSe_2$ as an examples to introduce how to calculate irreps to solve ABR decompositions to diagnose unconventional materials.

Band structure for
$NbSe_2$ without SOC



Sci. China-Phys. Mech. Astron. 67, 246811 (2024)

Step 1

1) Prepare the original POSCAR file. ($NbSe_2$ as an example)
2) $ phonopy --tolerance 0.01 --symmetry -c POSCAR
   $ vim PPOSCAR

"POSCAR"

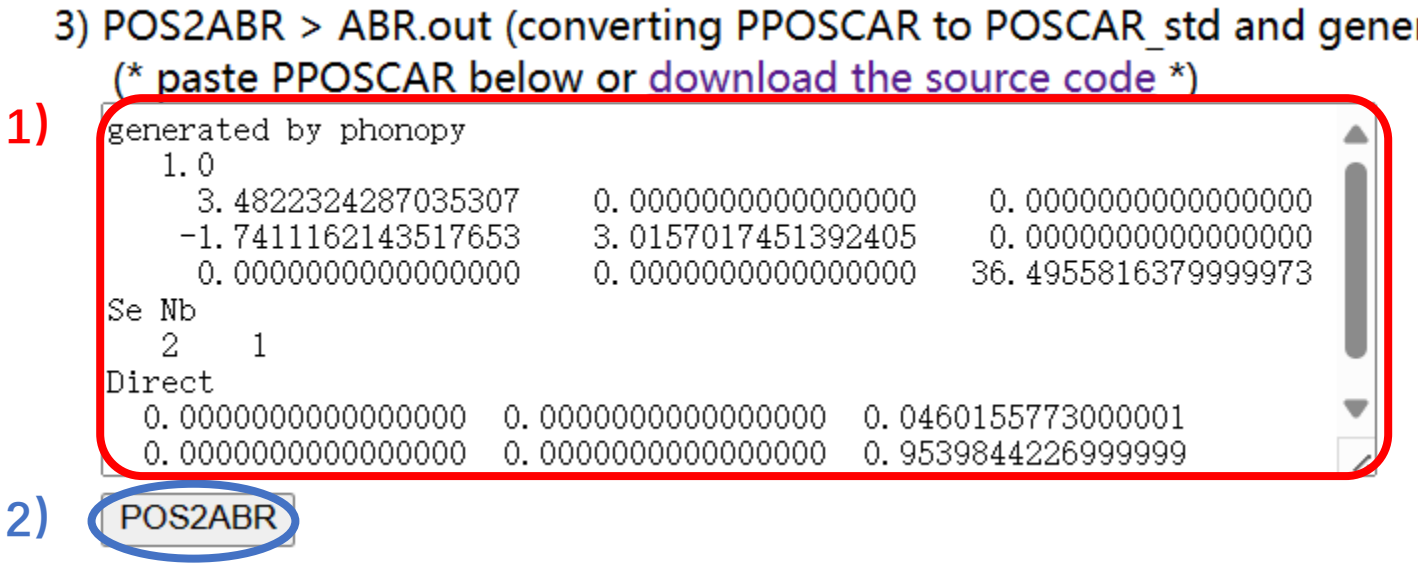
```
qe relaxed
1.0
   3.482232429  -0.000000000   0.000000000
  -1.741116214   3.015701745   0.000000000
  -0.000000000  -0.000000000  36.495581638
Se Nb
2 1
Direct
 0.333332986   0.666666985  0.0460155773000000
 0.333332986   0.666666985  0.9539844227000000
 0.666666985   0.333332986  0.0000000000000000
```

"PPOSCAR"

```
generated by phonopy
   1.0
     3.4822324287035307    0.0000000000000000    0.0000000000000000
    -1.7411162143517653    3.0157017451392405    0.0000000000000000
     0.0000000000000000    0.0000000000000000   36.4955816379999973
Se Nb
   2    1
Direct
  0.0000000000000000  0.0000000000000000  0.0460155773000001
  0.0000000000000000  0.0000000000000000  0.9539844226999999
  0.3333333333333334  0.6666666666666667  0.0000000000000000
```

Step 2

Open the web: https://tm.iphy.ac.cn/UnconvMat.html



1) Paste PPOSCAR into this box.

2) Press POS2ABR button.

Step 3

We can get the standard POSCAR (POSCAR_std) and the space group number of $NbSe_2$ is 187.

Copy the content in the red box to POSCAR.

```
POSCAR_std :
SG 187   0.000   0.000   0.000 :Generated by pos2aBR for irvsp!
    1.0
     3.4822324287035307     0.0000000000000000     0.0000000000000000
    -1.7411162143517653     3.0157017451392405     0.0000000000000000
     0.0000000000000000     0.0000000000000000    36.495581637999973
 Se   Nb
   2    1
Direct
  0.0000000000000000  0.0000000000000000  0.046015577300001
  0.0000000000000000  0.0000000000000000  0.953984422699999
  0.3333333333333334  0.6666666666666667  0.0000000000000000
```

Step 4

Note: When we diagnose whether the band structure of a material is unconventional , we only need to calculate irreps at several maximal HSKPs.

All space groups' HSKPs can be found on:
https://github.com/zjwang11/IR2PW/lib_irrep_bcs/max_KPOINTS_VASP/

First, do scf VASP calculations.
Second, paste KPOINTS_187.txt into KPOINTS and do nscf VASP calculations.

"KPOINTS_187.txt"

```
k-points
  6
rec
    0.00000000    0.00000000    0.50000000    1.0
    0.00000000    0.00000000    0.00000000    1.0
    0.33333300    0.33333300    0.50000000    1.0
    0.33333300    0.33333300    0.00000000    1.0
    0.50000000    0.00000000    0.50000000    1.0
    0.50000000    0.00000000    0.00000000    1.0
```

Step 5

The number of valence electrons in $NbSe_2$ is 25, we only focus on the half-filled band #13. (without SOC)

```
$ irvsp -sg 187 -nb 13 13 > outir
$ vim tqc.data
```

After IRVSP calculating the wave function of HSKPs, file tqc.data will be generated.

"tqc.data"

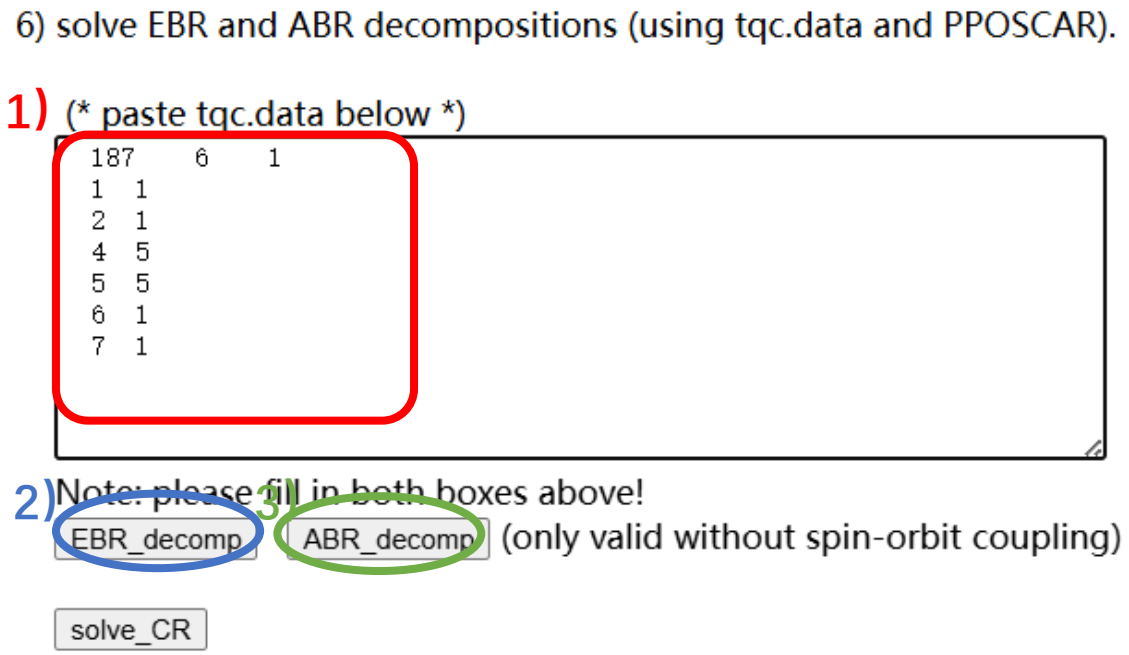
```
 187   6   1
 1  1
 2  1
 4  5
 5  5
 6  1
 7  1
```

Format of tqc.data

```
#SG (space group number)   #nk (number of HSKPs)   #nb (number of bands)
 HSKP#1  irrep(HSKP#1)#1  irrep(HSKP#1)#2  ···
 HSKP#2  irrep(HSKP#2)#1  irrep(HSKP#2)#2  ···
 ...
```

Step 6

Open the web: https://tm.iphy.ac.cn/UnconvMat.html



1) Paste tqc.data into this box.

2) Press EBR_decomp button.

3) Press ABR_decomp button.

Step 7

2) Press EBR_decomp button.

```
There are 1 solutions for eBR decomposition.
      1
   1   1@10    A1'@1f    (  1) :  0;
   2   2@10    A2'@1f    (  1) :  0;
   3   3@10   A2''@1f    (  1) :  0;
   4   4@10   A1''@1f    (  1) :  0;
   5   5@10     E'@1f    (  1) :  0;
   6   6@10    E''@1f    (  1) :  0;
   7   1@11    A1'@1e    (  1) :  1;
   8   2@11    A2'@1e    (  1) :  0;
   9   3@11   A2''@1e    (  1) :  0;
  10   4@11   A1''@1e    (  1) :  0;
  11   5@11     E'@1e    (  1) :  0;
  12   6@11    E''@1e    (  1) :  0;
  13   1@12    A1'@1d    (  1) :  0;
  14   2@12    A2'@1d    (  1) :  0;
  15   3@12   A2''@1d    (  1) :  0;
  16   4@12   A1''@1d    (  1) :  0;
  17   5@12     E'@1d    (  1) :  0;
  18   6@12    E''@1d    (  1) :  0;
  19   1@13    A1'@1c    (  1) :  0;
  20   2@13    A2'@1c    (  1) :  0;
  21   3@13   A2''@1c    (  1) :  0;
  22   4@13   A1''@1c    (  1) :  0;
  23   5@13     E'@1c    (  1) :  0;
  24   6@13    E''@1c    (  1) :  0;
  25   1@14    A1'@1b    (  1) :  0;
  26   2@14    A2'@1b    (  1) :  0;
  27   3@14   A2''@1b    (  1) :  0;
  28   4@14   A1''@1b    (  1) :  0;
  29   5@14     E'@1b    (  1) :  0;
  30   6@14    E''@1b    (  1) :  0;
  31   1@15    A1'@1a    (  1) :  0;
  32   2@15    A2'@1a    (  1) :  0;
  33   3@15   A2''@1a    (  1) :  0;
  34   4@15   A1''@1a    (  1) :  0;
  35   5@15     E'@1a    (  1) :  0;
  36   6@15    E''@1a    (  1) :  0;
```

topologically trivial

Step 8

3) Press ABR_decomp button

The irreps induced by atomic-orbital

```
        187 P-6m2
 \\
  SN  Mult. Wyck. Atom   s    p    d  Wyck. Name
    1    2    9   34    2    4    0    2g   Se
    2    1   13   41    1    6    4    1c   Nb
 \\
  SN  Orb. @ Site      Symm.          BCS  CJB  MUL
   1  Se-s @ 2g( 9)    3m(19) >>>    (1)  (2)  (3)       Basis
                                  1  GM1 ;GM1 ; A1 ;      z;x2+y2;z2
   1  Se-p @ 2g( 9)    3m(19) >>>    (1)  (2)  (3)       Basis
                                  1  GM1 ;GM1 ; A1 ;      z;x2+y2;z2
                                  3  GM3 ;GM3 ; E  ;      x,y;xz,yz;x2-y2,xy;Jx,Jy
   2  Nb-s @ 1c(13)  -62m(26) >>>   (1)  (2)  (3)       Basis
                                  1  GM1 ;GM1 ; A1';      x2+y2;z2
   2  Nb-p @ 1c(13)  -62m(26) >>>   (1)  (2)  (3)       Basis
                                  3  GM3 ;GM4 ;A2'';      z
                                  5  GM5 ;GM6 ; E' ;      x,y;x2-y2,xy
   2  Nb-d @ 1c(13)  -62m(26) >>>   (1)  (2)  (3)       Basis
                                  1  GM1 ;GM1 ; A1';      x2+y2;z2
                                  5  GM5 ;GM6 ; E' ;      x,y;x2-y2,xy
                                  6  GM6 ;GM5 ; E'';      xz,yz;Jx,Jy
There are 1 solutions for eBR decomposition.

There are 0 solutions for aBR decomposition.
It is unconventional with charge mismatch.

A1'@1e : the essential BR
+aBRs :
       1
   1   1@9      A1@2g    (  2) :  0;
   2   3@9       E@2g    (  1) :  0;
   3   1@13    A1'@1c    (  2) :  0;
   4   3@13   A2''@1c    (  1) :  0;
   5   5@13     E'@1c    (  2) :  0;
   6   6@13    E''@1c    (  1) :  0;
```

unconventional material

3 Solve the CR and calculate SI

- Using the CRs and magnetic BRs (MBRs), we reproduce the symmetry-based classifications for MSGs, and we obtain a set of Fu-Kane-like formulas of symmetry indicators (SIs) in both spinless (bosonic) and spinful (fermionic) systems, which are implemented in an automatic code—TOPMAT—to diagnose topological magnetic materials.
- Here we take the magnetic material $Eu_3In_2As_4$ and nonmagnetic material SnTe as examples to introduce how to solve the CR and calculate SI to magnetic topological materials.

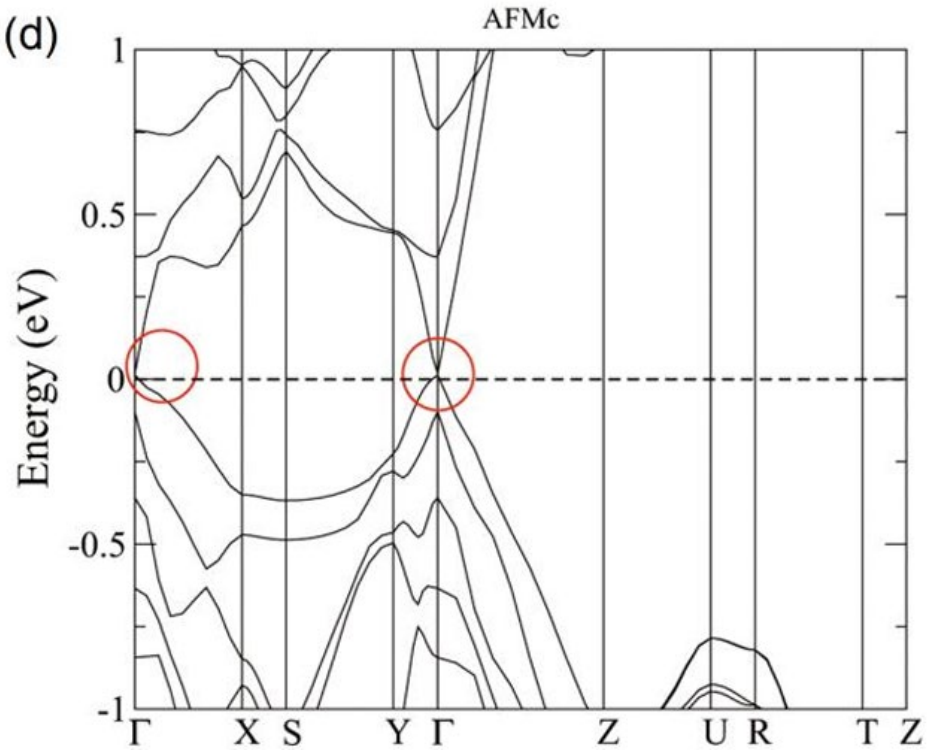
https://tm.iphy.ac.cn/TopMat_1651msg.html

PHYSICAL REVIEW B 106, 035150 (2022)

3.1.1 $Eu_3In_2As_4$-AFMc

- Here we take the magnetic material $Eu_3In_2As_4$ (AFMc) as an examples to introduce how to calculate irreps to solve the CR and Sis to diagnose topological magnetic materials.

The band structures of Eu3In2As4 for the magnetic configuration AFMc



arXiv:2403.07637(2024)

Step 1

1) Prepare the original POSCAR file. ($Eu_3In_2As_4$ as an example)
2) $ phonopy --tolerance 0.01 --symmetry -c POSCAR
   $ vim PPOSCAR

"POSCAR"

```
EuInAs
  1.0
    6.82999992370000    0.00000000000000    0.00000000000000
    0.00000000000000   16.50670051570000    0.00000000000000
    0.00000000000000    0.00000000000000    4.41020011900000
   Eu   In   As
    6    4    8
Direct
    0.00000000000000    0.50000000000000    0.00000000000000
    0.50000000000000    0.00000000000000    0.50000000000000
    0.70820999100000    0.69827002300000    0.00000000000000
    0.29179000900000    0.30172997700000    0.00000000000000
    0.79179000900000    0.19827002300000    0.50000000000000
    0.20820999100000    0.80172997700000    0.50000000000000
    0.36037999400000    0.58630001500000    0.50000000000000
    0.63962000600000    0.41369998500000    0.50000000000000
    0.13962000600000    0.08630001500000    0.00000000000000
    0.86037999400000    0.91369998500000    0.00000000000000
    0.74603998700000    0.56970000300000    0.50000000000000
    0.25396001300000    0.43029999700000    0.50000000000000
    0.75396001300000    0.06970000300000    0.00000000000000
    0.24603998700000    0.93029999700000    0.00000000000000
    0.23329000200000    0.66851002000000    0.00000000000000
    0.76670999800000    0.33148998000000    0.00000000000000
    0.26670999800000    0.16851002000000    0.50000000000000
    0.73329000200000    0.83148998000000    0.50000000000000
```

```
phonopy_version: '2.20.0'
space_group_type: 'Pnnm'
space_group_number: 58
point_group_type: 'mmm'
```

"PPOSCAR"

```
generated by phonopy
  1.0
    6.8299999237000000    0.0000000000000000    0.0000000000000000
    0.0000000000000000   16.5067005156999969    0.0000000000000000
    0.0000000000000000    0.0000000000000000    4.4102001189999980
Eu In As
  6   4   8
Direct
  0.0000000000000000  0.5000000000000001  0.0000000000000000
  0.5000000000000000  0.0000000000000000  0.5000000000000001
  0.7082099910000000  0.6982700230000001  0.0000000000000000
  0.2917900090000000  0.3017299770000001  0.0000000000000000
  0.7917900090000000  0.1982700230000001  0.5000000000000001
  0.2082099909999999  0.8017299770000003  0.5000000000000001
  0.3603799940000000  0.5863000150000001  0.5000000000000001
  0.6396200060000000  0.4136999850000002  0.5000000000000001
  0.1396200060000000  0.0863000150000000  0.0000000000000000
  0.8603799940000000  0.9136999850000003  0.0000000000000000
  0.7460399870000000  0.5697000030000001  0.5000000000000001
  0.2539600130000000  0.4302999970000001  0.5000000000000001
  0.7539600130000000  0.0697000029999999  0.0000000000000000
  0.2460399870000001  0.9302999970000002  0.0000000000000000
  0.2332900020000000  0.6685100200000001  0.0000000000000000
  0.7667099980000001  0.3314899800000000  0.0000000000000000
  0.2667099980000000  0.1685100200000001  0.5000000000000001
  0.7332900019999999  0.8314899800000002  0.5000000000000001
```

Step 2

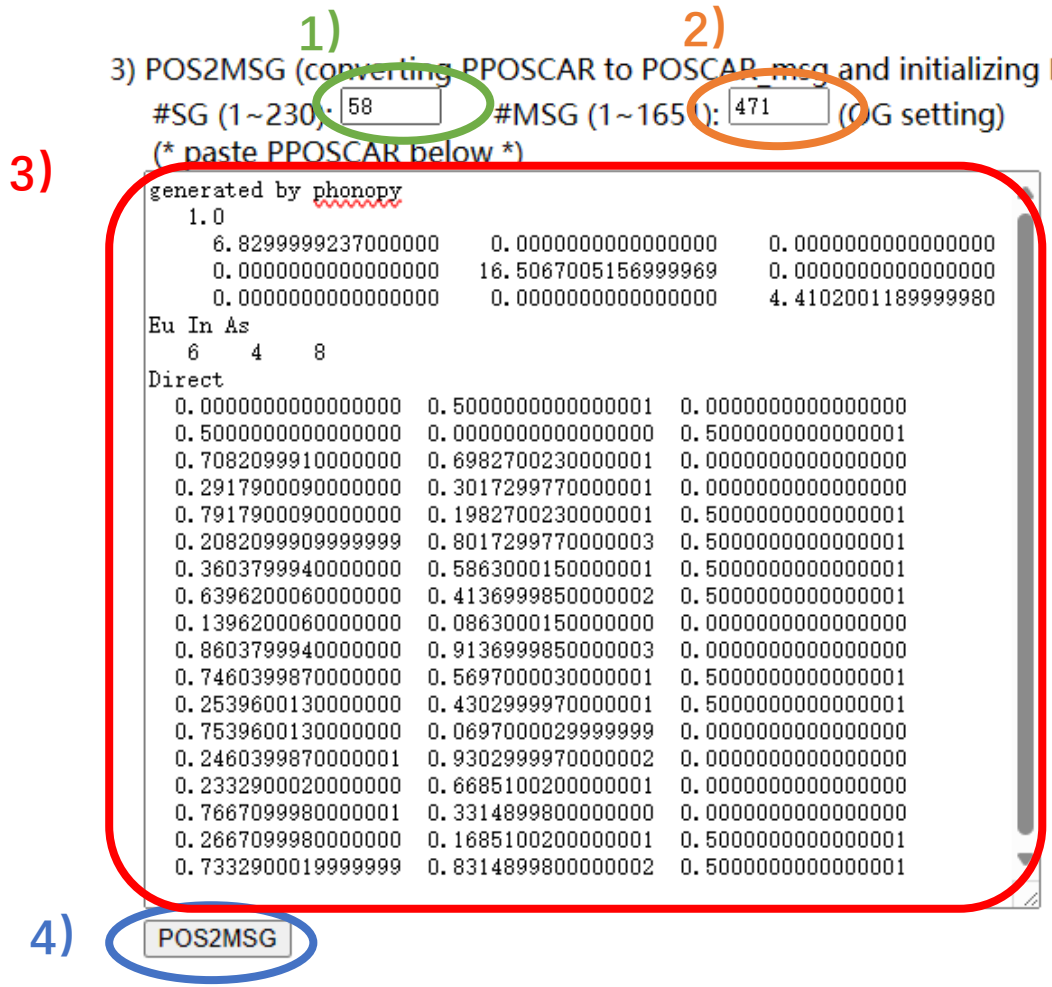
The crystalline space group is what the crystal has if the magnetic order is neglected. Once condidering magnetic order, the MSGs, magnetic type, and the symmetry-indicator classfications are given below. For each MSG, the detailed information is given in the corresponding MSG table.

OG setting		BNS setting		MSG type	Detailed Inf.	integer spin	half-integer spin
58.1.471	$Pnnm$	$Pnnm$	#58.393	I	Table MSG471	Z_2	Z_2
58.2.472	$Pnnm1'$	$Pnnm1'$	#58.394	II	Table MSG472	Z_2	Z_4
58.3.473	$Pn'nm$	$Pn'nm$	#58.395	III	Table MSG473	∅	∅
58.4.474	$Pnnm'$	$Pnnm'$	#58.396	III	Table MSG474	∅	∅
58.5.475	$Pn'n'm$	$Pn'n'm$	#58.397	III	Table MSG475	$Z_2\times Z_2$	$Z_2\times Z_2$
58.6.476	$Pnn'm'$	$Pnn'm'$	#58.398	III	Table MSG476	Z_2	Z_2
58.7.477	$Pn'n'm'$	$Pn'n'm'$	#58.399	III	Table MSG477	∅	∅
		P_annm	#58.400	IV	OG 53.12.426		
		P_cnnm	#58.401	IV	OG 55.10.450		
		P_Bnnm	#58.402	IV	OG 63.15.525		
		P_Cnnm	#58.403	IV	OG 66.11.574		
		P_Innm	#58.404	IV	OG 71.8.628		

PHYSICAL REVIEW B 106, 035150 (2022)

Step 3

Open the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Give the correct space group (SG) number: 58.

2) Give the MSG number: 471.

3) Paste PPOSCAR into this box.

4) Press POS2MSG button.

Step 4

```
POSCAR_msg:
SG#B  58   OG (    58.1.471)   BNS (      58.393)
  1.0
    6.82999992370000    0.00000000000000    0.00000000000000
    0.00000000000000   16.50670051570000    0.00000000000000
    0.00000000000000    0.00000000000000    4.41020011900000
   Eu   In   As
    6    4    8
Direct
    0.00000000000000    0.50000000000000    0.00000000000000
    0.50000000000000    0.00000000000000    0.50000000000000
    0.70820999100000    0.69827002300000    0.00000000000000
    0.29179000900000    0.30172997700000    0.00000000000000
    0.79179000900000    0.19827002300000    0.50000000000000
    0.20820999100000    0.80172997700000    0.50000000000000
    0.36037999400000    0.58630001500000    0.50000000000000
    0.63962000600000    0.41369998500000    0.50000000000000
    0.13962000600000    0.08630001500000    0.00000000000000
    0.86037999400000    0.91369998500000    0.00000000000000
    0.74603998700000    0.56970000300000    0.50000000000000
    0.25396001300000    0.43029999700000    0.50000000000000
    0.75396001300000    0.06970000300000    0.00000000000000
    0.24603998700000    0.93029999700000    0.00000000000000
    0.23329000200000    0.66851002000000    0.00000000000000
    0.76670999800000    0.33148998000000    0.00000000000000
    0.26670999800000    0.16851002000000    0.50000000000000
    0.73329000200000    0.83148998000000    0.50000000000000

INCAR:
LSORBIT = T
LNONCOLLINEAR = T
SAXIS = 0 0 1
MAGMOM= 0  0  7  0  0 -7  0  0  7  0  0  7  0  0 -7  0  0 -7 300*0.0

KPOINTS:
MKPOINTS used for magnetic space group
  8
rec
    0.00000000    0.00000000    0.00000000    1.0    ! GM
    0.50000000    0.50000000    0.50000000    1.0    ! R
    0.50000000    0.50000000    0.00000000    1.0    ! S
    0.00000000    0.50000000    0.50000000    1.0    ! T
    0.50000000    0.00000000    0.50000000    1.0    ! U
    0.50000000    0.00000000    0.00000000    1.0    ! X
    0.00000000    0.50000000    0.00000000    1.0    ! Y
    0.00000000    0.00000000    0.50000000    1.0    ! Z
```

We can get the standard POSCAR (POSCAR_msg) and some setting parameters of INCAR and KPOINTS.

Then we do VASP calculations.

Step 5

There is a big gap in the bottom 48 occupied band

$ irvsp -sg 58 -nb 49 154
$ vim tqc.data

"tqc.data"

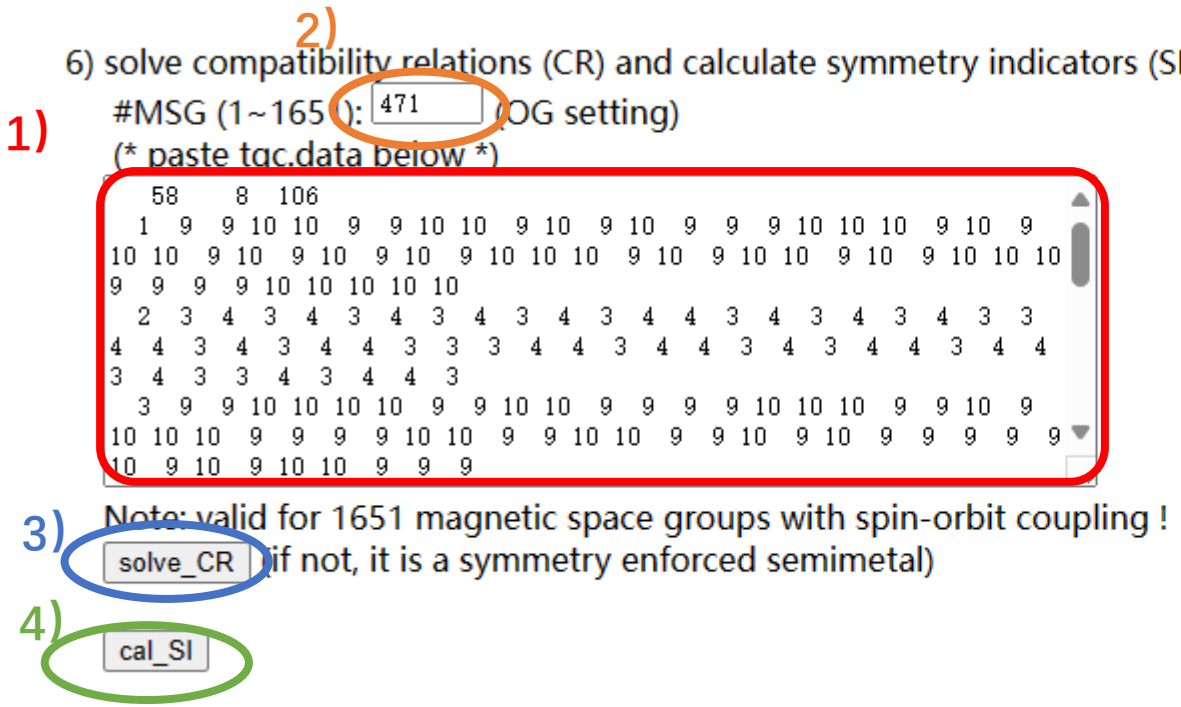
```
 58   8  106
  1  9  9 10 10  9  9 10 10  9 10  9 10  9  9  9 10 10 10  9 10  9 10 10  9 10  9 10  9 10  9 10  9 10 10 10  9 10  9 10 10  9 10 10 10 10 10
  2  3  4  3  4  3  4  3  4  3  4  3  4  4  3  4  3  4  3  3  4  4  3  4  3  4  4  3  3  3  4  4  3  4  4  3  4  3  4  4  3  4  3  4  4  3  4  4  3  4  3  3  4  3  4  4  3
  3  9  9 10 10 10 10  9  9 10 10  9  9  9  9 10 10 10  9  9 10  9 10 10 10  9  9  9 10 10  9  9 10 10  9  9 10  9 10  9  9  9  9  9 10  9 10  9 10 10  9  9  9
  4  5  3  4  6 10  7  8  9  5  3  4  6  8 10  7  9  8  9  7 10  5  3  4  6  3  9  5  7  6  4  8 10  3  5  6  4  8 10  4  9  6  7  9  3  7  5  8 10  6  4  7  9  3  6  4  5  8 10  3  7  5  4  9  6 10  7  8  6  4 10  9  8  3  5  7  9  3  5  4  6  6  4  3  5  6  4  9  4  6  3  5  7 10  8  7  9  4  5  3  6  8 10  5
 4  3  6
  5  5  3  4  6  5  3  6  4  7  8  9 10 10  8  9  7 10  9  8  7  3  4  5  6  7  9  6  8  5  4 10  3  6  4  5  3  3  5  4  6  8 10  4  7  9  3  6  5  6  4  8 10  3  5  7  9  4  6  7  9  3  5  8 10  7  9  8 10  7  6  9  4  3  8  5 10  7  9  4  7  6  9  8 10  7  9 10  4  6  7  9  8  3  5  8  7  9 10 10  9  8  7
 7  9  8 10
  6  3  4  3  4  4  3  3  4  4  3  3  4  3  4  4  3  4  3  3  4  3  4  3  3  4  4  3  4  3  3  4  4  3  4  3  4  4  3  4  3  3  4  3  4  3  4  3  3  4
  7  3  4  3  4  4  3  4  3  3  4  4  3  3  4  4  3  4  3  4  4  3  3  3  4  4  3  4  3  4  3  4  3  4  3  4  4  3  4  3  4  3  3  4  3  4  3  4  3  4  4  3  3  4
  8  3  4  3  4  4  3  3  4  3  4  3  4  4  3  4  3  3  4  3  4  4  4  3  4  3  3  4  4  3  3  4  4  4  3  3  4  4  3  4  4  3  3  4  3  4  3  4  4  3  4  3  3  4
```

Format of tqc.data

#SG (space group number) #nk (number of HSKPs) #nb (number of bands)
HSKP#1 irrep(HSKP#1)#1 irrep(HSKP#1)#2 …
HSKP#2 irrep(HSKP#2)#1 irrep(HSKP#2)#2 …
…

Step 6

Back to the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Paste tqc.data into this box.

2) Give the MSG number: 471.

3) Press solve_CR button.

4) Press cal_SI button.

Step 7

solve_CR :

```
The input data is calculated with spin-orbit coupling.
Satisfy CR
```

cal_SI : trivial

```
The input data is calculated with spin-orbit coupling.
Z2=0,
```

The gap at point Γ is only 4 meV, so it is very easy to achieve band inversion. We can simulate the band inversion at Γ by exchanging the 2 highest occupied states and 2 lowest empty bands.

After band inversion:

solve_CR :

```
The input data is calculated with spin-orbit coupling.
Satisfy CR
```

cal_SI : topological

```
The input data is calculated with spin-orbit coupling.
Z2=1,
```

3.1.2 $Eu_3In_2As_4$-AFMb

- Here we take the magnetic material $Eu_3In_2As_4$ (AFMb) as an examples to introduce how to calculate irreps to solve the CR and Sis to diagnose magnetic materials.
- We will use **mom2msg** to find $Eu_3In_2As_4$ (AFMb) MSG.

The list of results of SG 58 $Eu_3In_2As_4$ given by TopMat

	MSG(#OG)	Type	Configuration	Energy(eV/atom)	SIs
$Eu_3In_2As_4$ SG58	471	I	AFMc	-6.9430	Z_2=0
	472	II	NM	∅	∅
	473	III	ZM	∅	∅
	474	III	ZM	∅	∅
	475	III	FMc	-6.9427	Nodal line
	476	III	Canted-FM	-6.9428	Weyl points
			FMa	-6.9428	
			FMb	-6.9428	
	477	III	ZM	∅	∅

https://github.com/zjwang11/TopMat/

arXiv:2403.07637(2024)

Step 1

1) Prepare the original POSCAR file. ($Eu_3In_2As_4$ as an example)
2) Add the magnetic configuration (Cart. coord.) in POSCAR as follows.

"POSCAR"

```
AFMb
 1.0
    6.82999992370000    0.00000000000000    0.00000000000000
    0.00000000000000   16.50670051570000    0.00000000000000
    0.00000000000000    0.00000000000000    4.41020011900000
   Eu   In   As
    6    4    8
Direct
    0.00000000000000    0.50000000000000    0.00000000000000
    0.50000000000000    0.00000000000000    0.50000000000000
    0.70820999100000    0.69827002300000    0.00000000000000
    0.29179000900000    0.30172997700000    0.00000000000000
    0.79179000900000    0.19827002300000    0.50000000000000
    0.20820999100000    0.80172997700000    0.50000000000000
    0.36037999400000    0.58630001500000    0.50000000000000
    0.63962000600000    0.41369998500000    0.50000000000000
    0.13962000600000    0.08630001500000    0.00000000000000
    0.86037999400000    0.91369998500000    0.00000000000000
    0.74603998700000    0.56970000300000    0.50000000000000
    0.25396001300000    0.43029999700000    0.50000000000000
    0.75396001300000    0.06970000300000    0.00000000000000
    0.24603998700000    0.93029999700000    0.00000000000000
    0.23329000200000    0.66851002000000    0.00000000000000
    0.76670999800000    0.33148998000000    0.00000000000000
    0.26670999800000    0.16851002000000    0.50000000000000
    0.73329000200000    0.83148998000000    0.50000000000000
```

"POSCAR-add magnetic config"

```
AFMb
 1.0
    6.82999992370000    0.00000000000000    0.00000000000000
    0.00000000000000   16.50670051570000    0.00000000000000
    0.00000000000000    0.00000000000000    4.41020011900000
   Eu   In   As
    6    4    8
Direct
    0.00000000000000    0.50000000000000    0.00000000000000  0  1  0
    0.50000000000000    0.00000000000000    0.50000000000000  0 -1  0
    0.70820999100000    0.69827002300000    0.00000000000000  0  1  0
    0.29179000900000    0.30172997700000    0.00000000000000  0  1  0
    0.79179000900000    0.19827002300000    0.50000000000000  0 -1  0
    0.20820999100000    0.80172997700000    0.50000000000000  0 -1  0
    0.36037999400000    0.58630001500000    0.50000000000000
    0.63962000600000    0.41369998500000    0.50000000000000
    0.13962000600000    0.08630001500000    0.00000000000000
    0.86037999400000    0.91369998500000    0.00000000000000
    0.74603998700000    0.56970000300000    0.50000000000000
    0.25396001300000    0.43029999700000    0.50000000000000
    0.75396001300000    0.06970000300000    0.00000000000000
    0.24603998700000    0.93029999700000    0.00000000000000
    0.23329000200000    0.66851002000000    0.00000000000000
    0.76670999800000    0.33148998000000    0.00000000000000
    0.26670999800000    0.16851002000000    0.50000000000000
    0.73329000200000    0.83148998000000    0.50000000000000
```

Step 2

1) $ mom2msg > outdir

We give the MSG classification, number and all operations

```
                          Int.       Sch.    #SG    #symm
Crystalline SG(org.):     Pnnm     D2h^12     58       8
unitary  part (only):    P2_1/c     C2h^5     14       4
unitary +antiunitary:     Pnnm     D2h^12     58       8

Magnetic SG type : Type III (translationgleiche)
Magnetic SG number (OG) :   476
 SG#B 14   OG( 58. 6. 476 )
He:
  0.11000000  0.12000000  0.15000001
 -0.11000000 -0.12000000 -0.15000001
  0.61000000  0.38000000  0.34999999
  0.39000000  0.62000000  0.65000001
 -0.11000000 -0.12000000  0.15000001
  0.11000000  0.12000000 -0.15000001
  0.39000000  0.62000000  0.34999999
  0.61000000  0.38000000  0.65000001
```

“msgout.txt”

```
###M ≡ G + AG, where M is a magnetic space group, G is its unitary part, and A is an antiunitary symmetry###

#spg_symm :     8
#  1    unit
   1  0  0    0.000000
   0  1  0    0.000000
   0  0  1    0.000000
#  2    unit
  -1  0  0    0.000000
   0 -1  0    0.000000
   0  0 -1    0.000000
#  3   anti-unit
  -1  0  0    0.000000
   0 -1  0    0.000000
   0  0  1    0.000000
#  4   anti-unit
   1  0  0    0.000000
   0  1  0    0.000000
   0  0 -1    0.000000
#  5    unit
   1  0  0    0.500000
   0 -1  0    0.500000
   0  0 -1    0.500000
#  6    unit
  -1  0  0    0.500000
   0  1  0    0.500000
   0  0  1    0.500000
#  7   anti-unit
  -1  0  0    0.500000
   0  1  0    0.500000
   0  0 -1    0.500000
#  8   anti-unit
   1  0  0    0.500000
   0 -1  0    0.500000
   0  0  1    0.500000

#symm_mag,  #symm:     8     8

Magnetic SG type : Type III (translationgleiche)
```

Step 3

The crystalline space group is what the crystal has if the magnetic order is neglected. Once condidering magnetic order, the MSGs, magnetic type, and the symmetry-indicator classfications are given below. For each MSG, the detailed information is given in the corresponding MSG table.

OG setting		BNS setting		MSG type	Detailed Inf.	integer spin	half-integer spin
58.1.471	$Pnnm$	$Pnnm$	#58.393	I	Table MSG471	Z_2	Z_2
58.2.472	$Pnnm1'$	$Pnnm1'$	#58.394	II	Table MSG472	Z_2	Z_4
58.3.473	$Pn'nm$	$Pn'nm$	#58.395	III	Table MSG473	∅	∅
58.4.474	$Pnnm'$	$Pnnm'$	#58.396	III	Table MSG474	∅	∅
58.5.475	$Pn'n'm$	$Pn'n'm$	#58.397	III	Table MSG475	$Z_2\times Z_2$	$Z_2\times Z_2$
58.6.476	$Pnn'm'$	$Pnn'm'$	#58.398	III	Table MSG476	Z_2	Z_2
58.7.477	$Pn'n'm'$	$Pn'n'm'$	#58.399	III	Table MSG477	∅	∅
		P_annm	#58.400	IV	OG 53.12.426		
		P_cnnm	#58.401	IV	OG 55.10.450		
		P_Bnnm	#58.402	IV	OG 63.15.525		
		P_Cnnm	#58.403	IV	OG 66.11.574		
		P_Innm	#58.404	IV	OG 71.8.628		

PHYSICAL REVIEW B 106, 035150 (2022)

Step 4

Open the web: https://tm.iphy.ac.cn/TopMat_1651msg.html

1) Give the unitary +antiunitary (SG) number: 58.

2) Give the MSG number: 476.

3) Paste POSCAR and additional He atoms into this box.

4) Press POS2MSG button.

```
POSCAR_msg:
SG#B  14   OG (    58.6.476)   BNS (      58.398)
  1.0
    0.00000000000000  -16.50670051570000    0.00000000000000
    6.82999992370000    0.00000000000000    0.00000000000000
    0.00000000000000   16.50670051570000    4.41020011900000
   Eu   In   As   He
    6    4    8    8
Direct
    0.50000000000000    0.00000000000000    0.00000000000000
    0.50000000000000    0.50000000000000    0.50000000000000
    0.30172997700000    0.70820999100000    0.00000000000000
    0.69827002300000    0.29179000900000    0.00000000000000
    0.30172997700000    0.79179000900000    0.50000000000000
    0.69827002300000    0.20820999100000    0.50000000000000
    0.91369998500000    0.36037999400000    0.50000000000000
    0.08630001500000    0.63962000600000    0.50000000000000
    0.91369998500000    0.13962000600000    0.00000000000000
    0.08630001500000    0.86037999400000    0.00000000000000
    0.93029999700000    0.74603998700000    0.50000000000000
    0.06970000300000    0.25396001300000    0.50000000000000
    0.93029999700000    0.75396001300000    0.00000000000000
    0.06970000300000    0.24603998700000    0.00000000000000
    0.33148998000000    0.23329000200000    0.00000000000000
    0.66851002000000    0.76670999800000    0.00000000000000
    0.33148998000000    0.26670999800000    0.50000000000000
    0.66851002000000    0.73329000200000    0.50000000000000
    0.03000001000000    0.11000000000000    0.15000001000000
    0.96999999000000    0.89000000000000    0.84999999000000
    0.96999999000000    0.61000000000000    0.34999999000000
    0.03000001000000    0.39000000000000    0.65000001000000
    0.27000001000000    0.89000000000000    0.15000001000000
    0.72999999000000    0.11000000000000    0.84999999000000
    0.72999999000000    0.39000000000000    0.34999999000000
    0.27000001000000    0.61000000000000    0.65000001000000

INCAR:
LSORBIT = T
LNONCOLLINEAR = T
SAXIS = 0 0 1
MAGMOM= 7  7  0  7 -7  0  7  7  0  7  7  0  7 -7  0  7 -7  0 300*0.0

KPOINTS:
MKPOINTS used for magnetic space group
  8
rec
    0.50000000    0.00000000    0.50000000    1.0    ! A
    0.00000000    0.00000000    0.50000000    1.0    ! B
    0.50000000    0.50000000    0.00000000    1.0    ! C
    0.00000000    0.50000000    0.50000000    1.0    ! D
    0.50000000    0.50000000    0.50000000    1.0    ! E
    0.00000000    0.00000000    0.00000000    1.0    ! GM
    0.50000000    0.00000000    0.00000000    1.0    ! Y
    0.00000000    0.50000000    0.00000000    1.0    ! Z
```

Step 5

Note that the He atom is only to find the correct MSG.

The magnetic moment given by the website is a possible configuration. Our initial magnetic moment also satisfies this possible configuration.

```
INCAR:
LSORBIT = T
LNONCOLLINEAR = T
SAXIS = 0 0 1
MAGMOM= 0  7  0  0 -7  0  0  7  0  0  7  0  0 -7  0  0 -7  0 300*0.0 ···
```

```
POSCAR_msg:
SG#B  14   OG (    58.6.476)   BNS (      58.398)
  1.0
    0.00000000000000  -16.50670051570000    0.00000000000000
    6.82999992370000    0.00000000000000    0.00000000000000
    0.00000000000000   16.50670051570000    4.41020011900000
   Eu   In   As
    6    4    8
Direct
    0.50000000000000    0.00000000000000    0.00000000000000
    0.50000000000000    0.50000000000000    0.50000000000000
    0.30172997700000    0.70820999100000    0.00000000000000
    0.69827002300000    0.29179000900000    0.00000000000000
    0.30172997700000    0.79179000900000    0.50000000000000
    0.69827002300000    0.20820999100000    0.50000000000000
    0.91369998500000    0.36037999400000    0.50000000000000
    0.08630001500000    0.63962000600000    0.50000000000000
    0.91369998500000    0.13962000600000    0.00000000000000
    0.08630001500000    0.86037999400000    0.00000000000000
    0.93029999700000    0.74603998700000    0.50000000000000
    0.06970000300000    0.25396001300000    0.50000000000000
    0.93029999700000    0.75396001300000    0.00000000000000
    0.06970000300000    0.24603998700000    0.00000000000000
    0.33148998000000    0.23329000200000    0.00000000000000
    0.66851002000000    0.76670999800000    0.00000000000000
    0.33148998000000    0.26670999800000    0.50000000000000
    0.66851002000000    0.73329000200000    0.50000000000000
```

Step 6

We can get the standard POSCAR (POSCAR_msg) and some setting parameters of INCAR and KPOINTS.

Then we do VASP calculations (REMOVING He atoms).

```
INCAR:
LSORBIT = T
LNONCOLLINEAR = T
SAXIS = 0 0 1
MAGMOM= 0  7  0  0 -7  0  0  7  0  0  7  0  0 -7  0  0 -7  0 300*0.0 ···
```

```
KPOINTS:
MKPOINTS used for magnetic space group
  8
rec
    0.50000000    0.00000000    0.50000000    1.0    ! A
    0.00000000    0.00000000    0.50000000    1.0    ! B
    0.50000000    0.50000000    0.00000000    1.0    ! C
    0.00000000    0.50000000    0.50000000    1.0    ! D
    0.50000000    0.50000000    0.50000000    1.0    ! E
    0.00000000    0.00000000    0.00000000    1.0    ! GM
    0.50000000    0.00000000    0.00000000    1.0    ! Y
    0.00000000    0.50000000    0.00000000    1.0    ! Z
```

Step 7

We use unitary part (SG#B) to calculate the representation

$ irvsp -sg 14 -nb 49 154
$ vim tqc.data

"tqc.data"

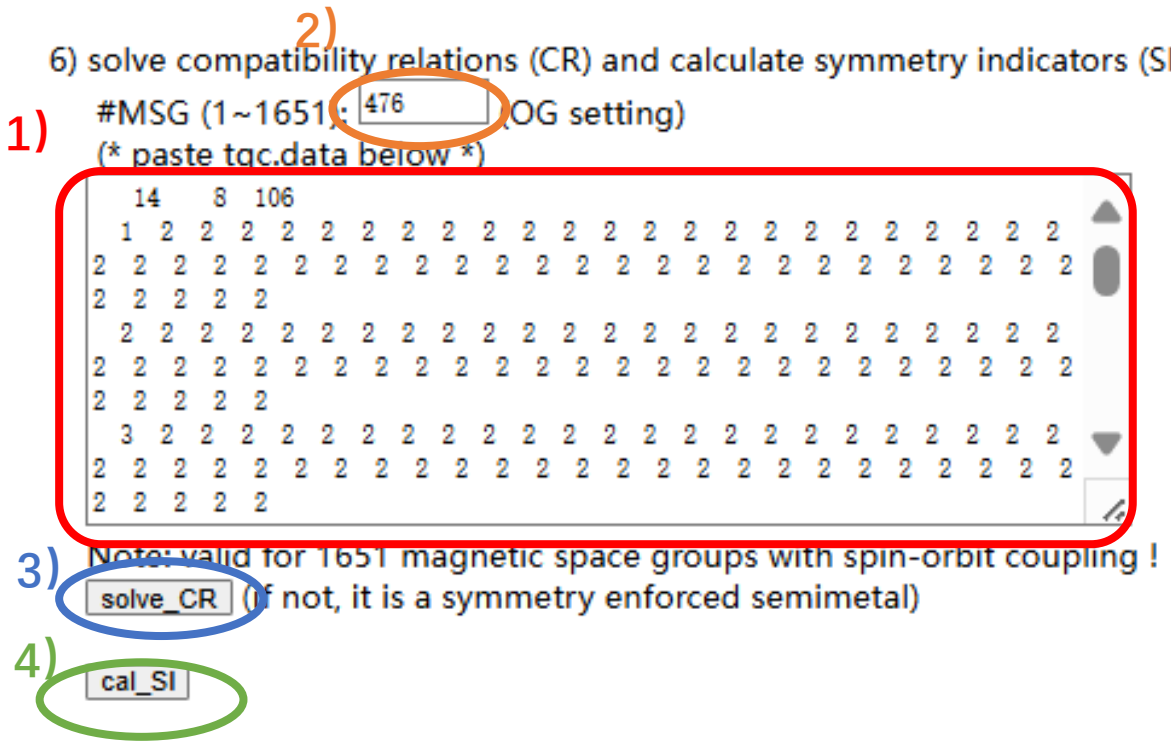
```
 14   8  106
 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 4 6 5 5 6 6 5 6 5 7 7 8 8 8 7 8 7 8 7 8 7 5 5 6 6 7 8 6 7 6 5 8 5 6 5 6 5 5 6 5 7 8 6 5 6 5 6 7 8 5 6 7 8 5 7 6 8 5 7 6 8 8 7 5 6 7 8 7 8 7 5 6 8 7 8 5 6 7 8 7 8 5 6 7 8 8 7 5 6 8 7 7 5 8 6 7 7 8 8 8 8 7 7 7 8 7
8
 5 5 6 5 6 7 8 7 8 7 8 7 8 5 6 5 6 7 8 7 8 5 6 5 6 5 6 5 6 7 8 7 8 7 8 5 6 7 8 5 6 5 6 7 8 7 8 5 6 7 8 5 6 7 8 5 6 5 6 5 6 7 8 7 8 5 6 7 8 5 6 7 8 5 6 5 6 7 8 5 6 5 6 5 6 5 6 5 6 7 8 7 8 5 6 5 6 7 8 7 8 5 6 5 6 5
6
 6 5 6 5 6 7 8 7 8 5 6 6 5 7 8 8 7 5 6 7 8 5 6 7 8 5 6 5 6 5 6 8 7 7 8 8 5 7 6 7 8 7 8 6 5 7 8 6 5 7 8 5 6 5 6 8 7 7 8 7 8 7 8 5 6 5 6 7 8 8 7 6 5 7 8 7 8 5 6 8 7 6 5 8 7 7 8 7 8 5 6 5 6 6 5 5 6 8 7 8 7 7 8 8 7 7
8
 7 5 6 5 6 7 8 7 8 5 6 5 6 7 8 7 8 7 8 7 8 5 6 5 6 5 6 7 8 5 6 7 8 5 6 5 6 7 8 7 8 5 6 7 8 5 6 5 6 7 8 5 6 7 8 5 6 7 8 5 6 7 8 7 8 5 6 5 6 7 8 5 6 7 8 5 6 7 8 5 6 5 6 5 6 5 6 7 8 5 6 7 8 5 6 7 8 5 6 5 6 7 8 5 6 5
6
 8 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

Format of tqc.data

#SG (space group number)   #nk (number of HSKPs)   #nb (number of bands)
HSKP#1 irrep(HSKP#1)#1 irrep(HSKP#1)#2 …
HSKP#2 irrep(HSKP#2)#1 irrep(HSKP#2)#2 …
…

Step 8

Back to the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Paste tqc.data into this box.

2) Give the MSG number: 476.

3) Press solve_CR button.

4) Press cal_SI button.

Step 9

solve_CR :

```
The input data is calculated with spin-orbit coupling.
Satisfy CR
```

cal_SI :

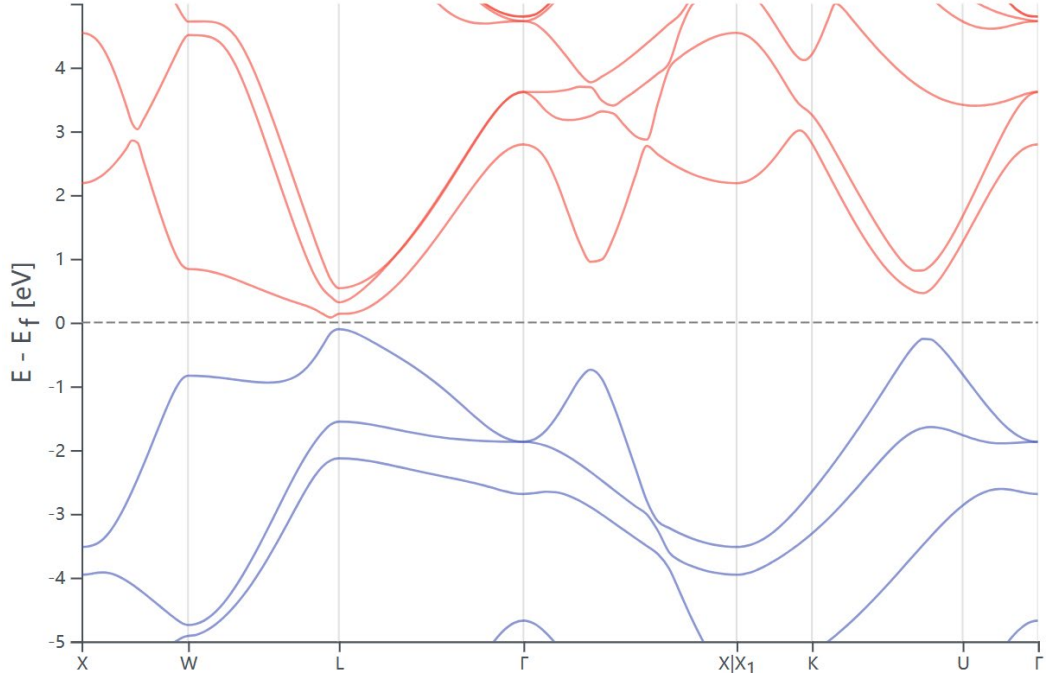
```
The input data is calculated with spin-orbit coupling.
Z2=0,
```

trivial

3.2 SnTe

Compound:	Symmetry Group:	Topological Status (Type):	Topological indices:
Sn1 Te1	225 (*Fm*-3*m*)	TI (SEBR)	$Z_{2w,1} = 0, Z_{2w,2} = 0, Z_{2w,3} = 0, Z_4 = 0, Z_2 = 0, Z_8 = 4$

- Here we take the nonmagnetic material SnTe as an examples to introduce how to calculate irreps to solve the CR and Sis to diagnose topological nonmagnetic materials.



www.topologicalquantumchemistry.com/#/detail/601065y.com

Step 1

1) Prepare the original POSCAR file. (SnTe as an example)
2) $ phonopy --tolerance 0.01 --symmetry -c POSCAR
   $ vim PPOSCAR

“POSCAR”

```
Sn Te
 1.0000000000000000
    6.3010000000000002    0.0000000000000000    0.0000000000000000
    0.0000000000000000    6.3010000000000002    0.0000000000000000
    0.0000000000000000    0.0000000000000000    6.3010000000000002
 Sn  Te
   4   4
Cartesian
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.0000000000000000  3.1505000000000001  3.1505000000000001
  3.1505000000000001  0.0000000000000000  3.1505000000000001
  3.1505000000000001  3.1505000000000001  0.0000000000000000
  3.1505000000000001  3.1505000000000001  3.1505000000000001
  3.1505000000000001  0.0000000000000000  0.0000000000000000
  0.0000000000000000  3.1505000000000001  0.0000000000000000
  0.0000000000000000  0.0000000000000000  3.1505000000000001
```

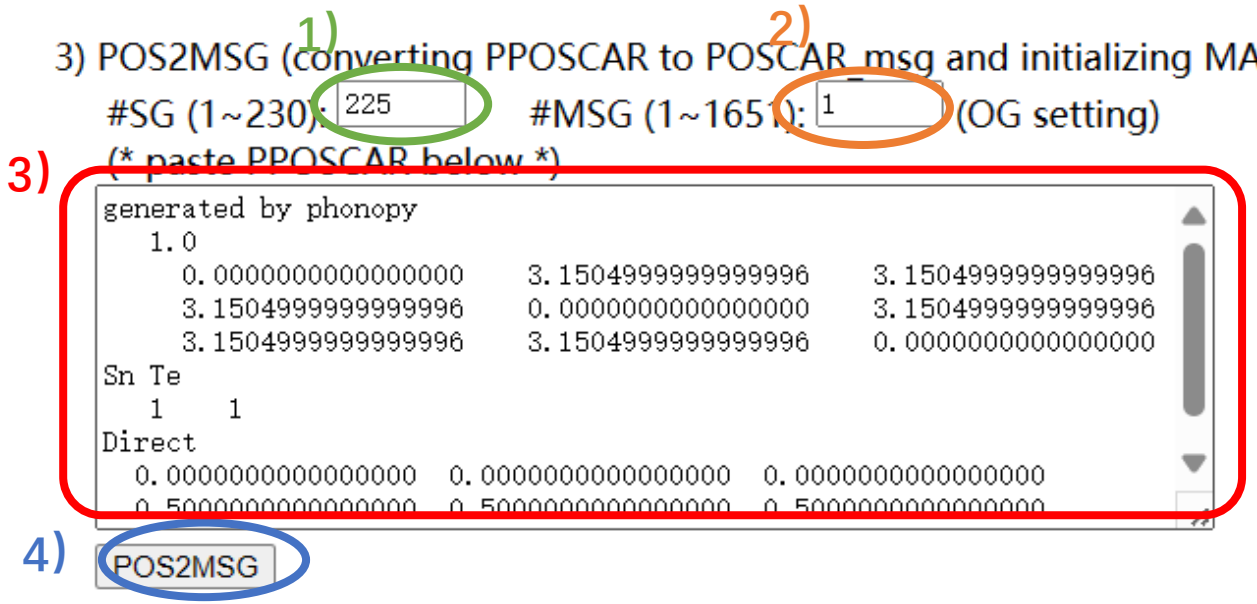
```
phonopy_version: '2.20.0'
space_group_type: 'Fm-3m'
space_group_number: 225
point_group_type: 'm-3m'
```

“PPOSCAR”

```
generated by phonopy
   1.0
     0.0000000000000000    3.1504999999999996    3.1504999999999996
     3.1504999999999996    0.0000000000000000    3.1504999999999996
     3.1504999999999996    3.1504999999999996    0.0000000000000000
Sn Te
   1    1
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.5000000000000000  0.5000000000000000  0.5000000000000000
```

Step 2

Open the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Give the correct space group (SG) number: 58.

2) Give any reasonable magnetic space group (MSG) number, such as 1.

3) Paste PPOSCAR into this box.

4) Press POS2MSG button.

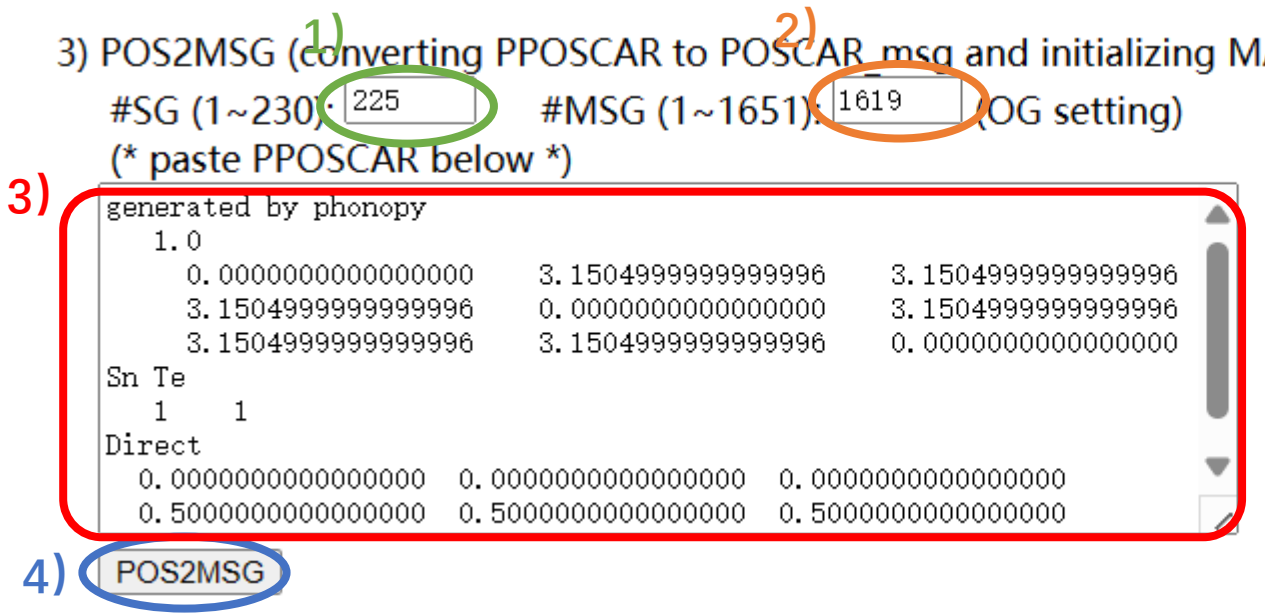
Step 3

```
The OG magnetic space group number do not match with the given space group number.
Possible OG magnetic space group numbers are given below:
1618, type 1
1619, type 2
1620, type 3
1621, type 3
1622, type 3
```

Nonmagnetic materials are the type-2 MSG.

Step 4

Back to the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Give the correct space group (SG) number: 58.

2) Give the correct magnetic space group (MSG) number: 1619.

3) Paste PPOSCAR into this box.

4) Press POS2MSG button.

Step 5

```
POSCAR_msg:
SG#B 225    OG (  225.2.1619)    BNS (     225.117)
  1.0
    0.00000000000000    3.15050000000000    3.15050000000000
    3.15050000000000    0.00000000000000    3.15050000000000
    3.15050000000000    3.15050000000000    0.00000000000000
   Sn   Te
    1    1
Direct
    0.00000000000000    0.00000000000000    0.00000000000000
    0.50000000000000    0.50000000000000    0.50000000000000

INCAR:
LSORBIT = T
LNONCOLLINEAR = T
SAXIS = 0 0 1
MAGMOM=300*0.0

KPOINTS:
MKPOINTS used for magnetic space group
  4
rec
    0.00000000    0.00000000    0.00000000    1.0    ! GM
    0.50000000    0.00000000    0.50000000    1.0    ! X
    0.50000000    0.50000000    0.50000000    1.0    ! L
    0.50000000    0.25000000    0.75000000    1.0    ! W
```

We can get the standard POSCAR (POSCAR_msg) and some setting parameters of INCAR and KPOINTS.

Then we do VASP calculations.

Step 6

The number of valence electrons in SnTe is 10

$ irvsp -sg 225 -nb 1 10 > outir
$ vim tqc.data

"tqc.data"

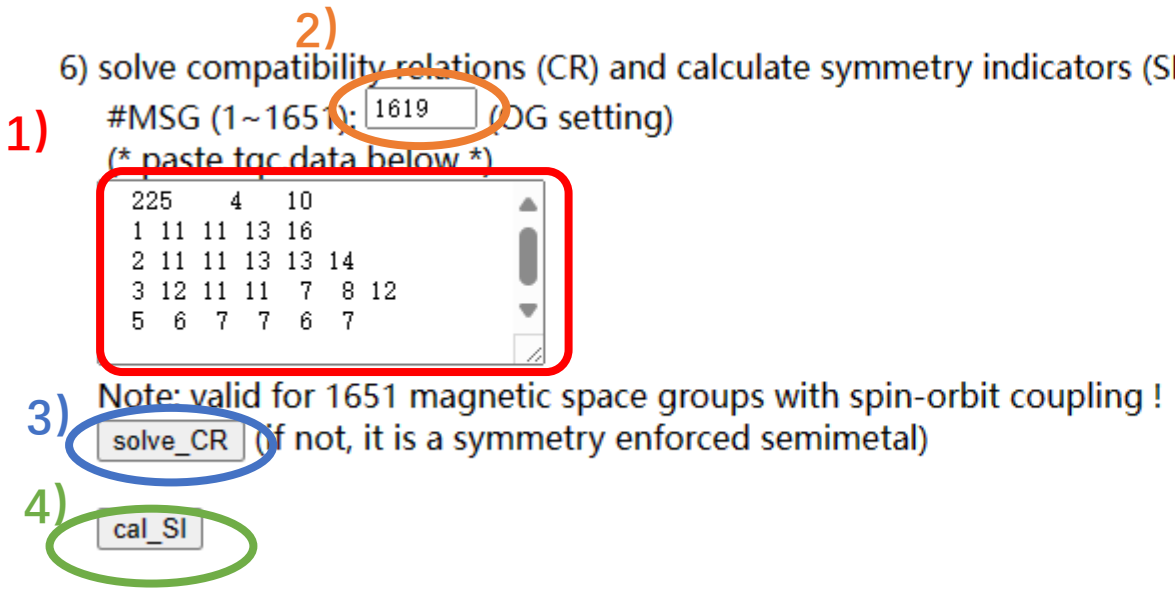
```
225    4   10
 1 11 11 13 16
 2 11 11 13 13 14
 3 12 11 11  7  8 12
 5  6  7  7  6  7
```

Format of tqc.data

```
#SG (space group number)   #nk (number of HSKPs)   #nb (number of bands)
 HSKP#1  irrep(HSKP#1)#1  irrep(HSKP#1)#2  ···
 HSKP#2  irrep(HSKP#2)#1  irrep(HSKP#2)#2  ···
 ...
```

Step 7

Back to the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Paste tqc.data into this box.

2) Give the MSG number: 1619.

3) Press solve_CR button.

4) Press cal_SI button.

Step 8

Compound:	Symmetry Group:	Topological Status (Type):	Topological indices:
Sn1 Te1	225 (*Fm*-3*m*)	TI (SEBR)	$Z_{2w,1} = 0, Z_{2w,2} = 0, Z_{2w,3} = 0, Z_4 = 0, Z_2 = 0, Z_8 = 4$

solve_CR :

```
The input data is calculated with spin-orbit coupling.
Satisfy CR
```

cal_SI :

```
The input data is calculated with spin-orbit coupling.
Z8=4,
```

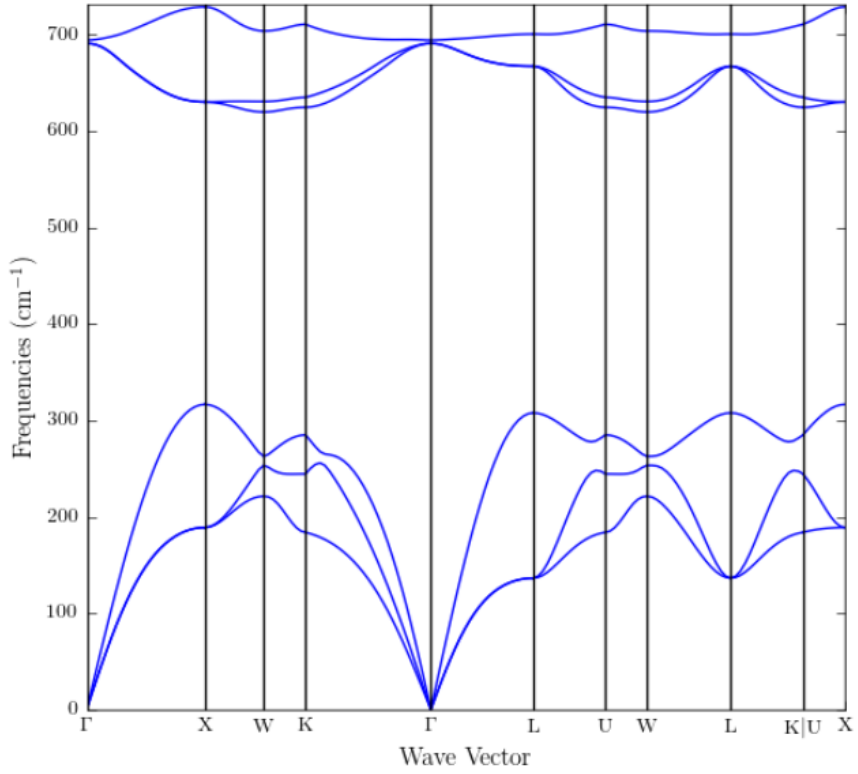
Consistent with the topology indices on the website

topological

4 Calculate the phonon BRs by Quantum Espresso (QE)

MATERIAL	ID:	DOI:
BAs	**mp-10044**	**10.17188/1185076**

- Here we take the BAs as an examples to introduce how to calculate phonon irreps to solve ABR decompositions to diagnose topological /unconventional materials.



https://legacy.materialsproject.org/materials/mp-10044/

Step 1

1) Prepare the original POSCAR file. (BAs as an example)
2) $ phonopy --tolerance 0.01 --symmetry -c POSCAR
   $ vim PPOSCAR

"POSCAR"

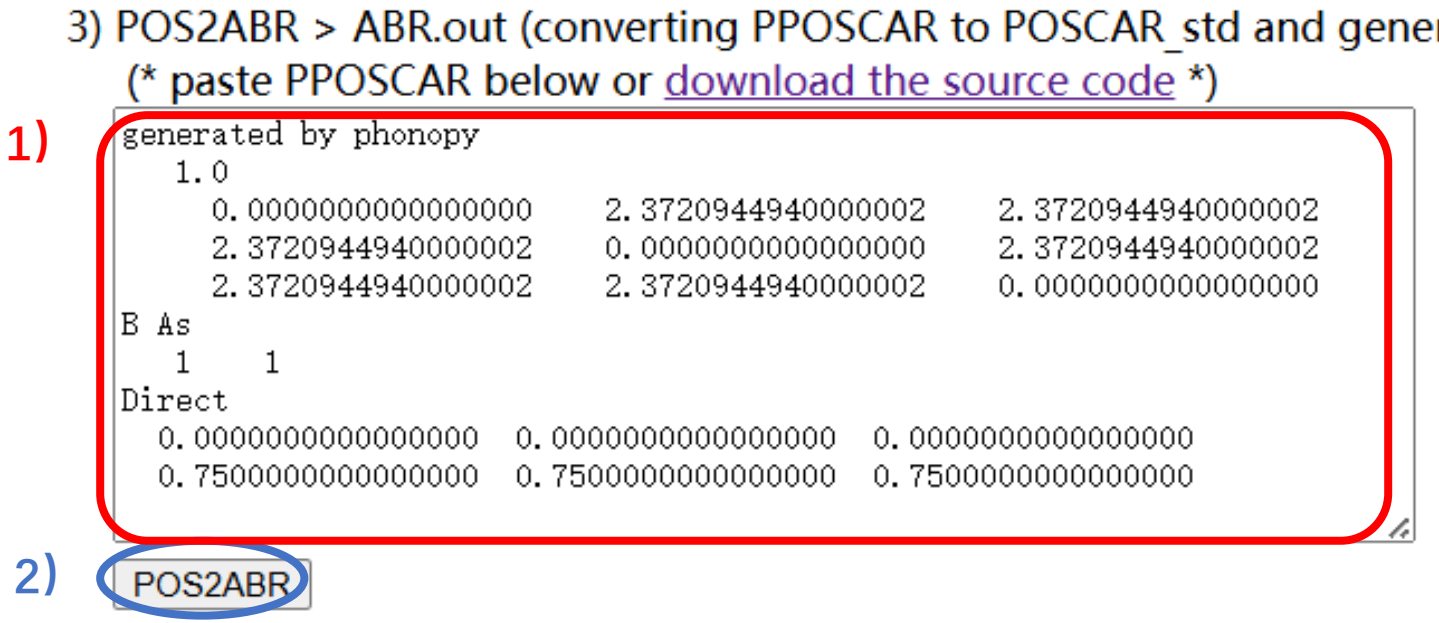
```
qe relaxed
 1.0
   0.000000000   2.372094494   2.372094494
   2.372094494   0.000000000   2.372094494
   2.372094494   2.372094494  -0.000000000
B As
1 1
Direct
        0.0000000000       0.0000000000       0.0000000000
        0.2500000000       0.2500000000       0.2500000000
```

"PPOSCAR"

```
generated by phonopy
   1.0
     0.0000000000000000   2.3720944940000002   2.3720944940000002
     2.3720944940000002   0.0000000000000000   2.3720944940000002
     2.3720944940000002   2.3720944940000002   0.0000000000000000
B As
   1    1
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.7500000000000000  0.7500000000000000  0.7500000000000000
```

Step 2

Open the web: https://tm.iphy.ac.cn/UnconvMat.html



1) Paste PPOSCAR into this box.

2) Press POS2ABR button.

Step 3

We can get the standard POSCAR (POSCAR_std) and the space group number of BAs is 216.

Copy the content in the red box to POSCAR. (Convert to QE input)

```
POSCAR_std :
SG 216   0.000   0.000   0.000 :Generated by pos2aBR for irvsp!
    1.0
     0.0000000000000000     2.3720944940000002     2.3720944940000002
     2.3720944940000002     0.0000000000000000     2.3720944940000002
     2.3720944940000002     2.3720944940000002     0.0000000000000000
 B    As
   1    1
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.7500000000000000  0.7500000000000000  0.7500000000000000
```

Step 4

Note: When we diagnose whether the band structure of a material is unconventional , we only need to calculate irreps at several maximal HSKPs.

All space groups' HSKPs can be found on:
https://github.com/zjwang11/IR2PW/lib_irrep_bcs/max_KPOINTS_VASP/

First, do scf QE calculations.
Second, use **IRphx.sh** to do phonon calculation of the HSKPs.

"KPOINTS_216.txt"

```
k-points
  4
rec
    0.00000000    0.00000000    0.00000000    1.0
    0.50000000    0.00000000    0.50000000    1.0
    0.50000000    0.50000000    0.50000000    1.0
    0.50000000    0.25000000    0.75000000    1.0
```

Step 5

```
tbbox.in for BAs:

  case = ph  ! ph for ir2ph; lda/soc for ir2tb

  proj:
  orbt = 1  ! 1 for px py pz; 2 for pz px py
  ntau = 2  ! number of atoms
    0.000000    0.000000    0.000000    1 3
    0.750000    0.750000    0.750000    2 3
! x1, x2, x3,                itau,             iorbit
! (fraction coordinates)  (kinds of atoms)  (number of orbitals)
  end projections

  kpoint:
  kmesh = 1  ! calculate BRs set 1
  Nk = 4     ! number of k-points
     0.00000000     0.00000000     0.00000000  ! k1, k2, k3
     0.50000000     0.00000000     0.50000000
     0.50000000     0.50000000     0.50000000
     0.50000000     0.25000000     0.75000000
  end kpoint_path


  unit_cell:
  ! Lattice constant and Reciprocal lattice vector
     0.000000    0.707107    0.707107    -0.707107    0.707107    0.707107
     0.707107    0.000000    0.707107     0.707107   -0.707107    0.707107
     0.707107    0.707107    0.000000     0.707107    0.707107   -0.707107
 ! same as OUTCAR:
 ! irot  det(A)     alpha        n_x          n_y          n_z          tau_x         tau_y         tau_z
   1   1.000000    0.000000    1.000000    0.000000    0.000000    0.000000    0.000000    0.000000
   2   1.000000 -180.000000    0.000000    0.000000    1.000000    0.000000    0.000000    0.000000
   3   1.000000 -180.000000    0.000000    1.000000    0.000000    0.000000    0.000000    0.000000
 ...
  end unit_cell_cart
```

Generate tbbox.in using the scf output file of QE

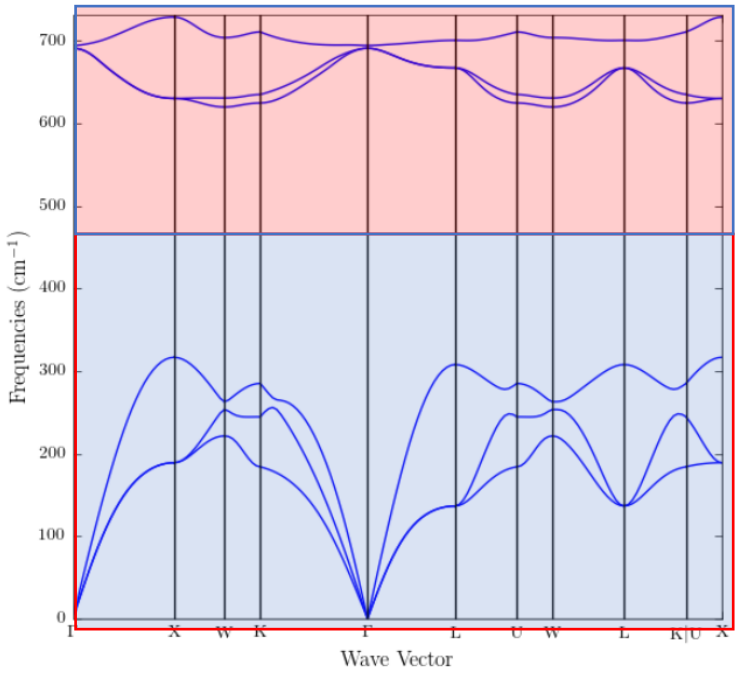
$ pwscf2tbbox.sh 216

Note that the phonon vibration is similar to the p orbital (px py pz). The symmetric operation of QE is converted into the VASP format.

Step 6

$ python dyn2wf.py 4
$ ir2ph -sg 216 –nb 1 3 > outir
$ vim tqc.data

All dynamic matrices are collected and converted to readable ph_wf.dat. (4 HSKPs)



Note that the gap of phonons can be understood as well-separated phonon modes. We can diagnose topological /unconventional at any well-separated phonon modes.

“tqc.data”

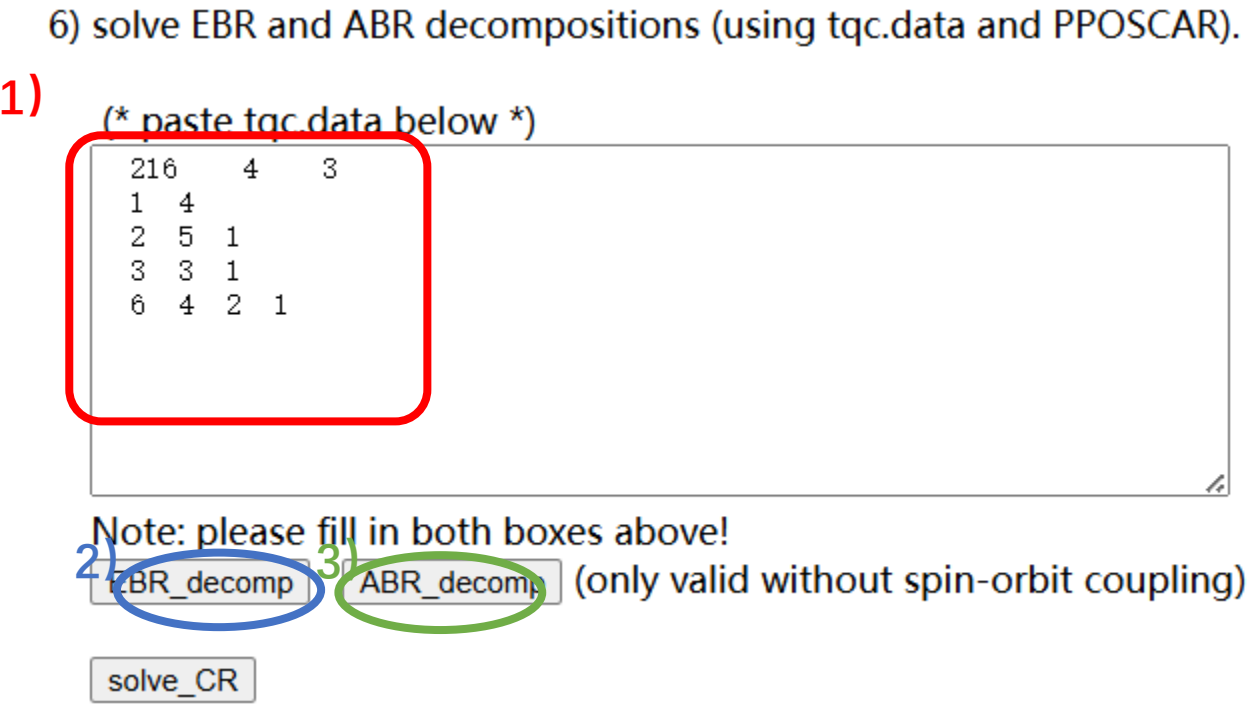
```
216   4   6
1  4  4
2  5  1  5  3
3  3  1  3  1
6  4  2  1  3  2  4
```

Format of tqc.data

```
#SG (space group number)   #nk (number of HSKPs)   #nb (number of bands)
 HSKP#1  irrep(HSKP#1)#1  irrep(HSKP#1)#2  ···
 HSKP#2  irrep(HSKP#2)#1  irrep(HSKP#2)#2  ···
 ...
```

Step 7

Open the web: https://tm.iphy.ac.cn/UnconvMat.html



1) Paste tqc.data into this box.

2) Press EBR_decomp button.

3) Press ABR_decomp button.

Step 8

2) Press EBR_decomp button.

```
There are 1 solutions for eBR decomposition.
      1
   1   1@6      A1@4d    (  1) :  0;
   2   2@6      A2@4d    (  1) :  0;
   3   3@6       E@4d    (  1) :  0;
   4   4@6      T2@4d    (  1) :  1;
   5   5@6      T1@4d    (  1) :  0;
   6   1@7      A1@4c    (  1) :  0;
   7   2@7      A2@4c    (  1) :  0;
   8   3@7       E@4c    (  1) :  0;
   9   4@7      T2@4c    (  1) :  0;
  10   5@7      T1@4c    (  1) :  0;
  11   1@8      A1@4b    (  1) :  0;
  12   2@8      A2@4b    (  1) :  0;
  13   3@8       E@4b    (  1) :  0;
  14   4@8      T2@4b    (  1) :  0;
  15   5@8      T1@4b    (  1) :  0;
  16   1@9      A1@4a    (  1) :  0;
  17   2@9      A2@4a    (  1) :  0;
  18   3@9       E@4a    (  1) :  0;
  19   4@9      T2@4a    (  1) :  0;
  20   5@9      T1@4a    (  1) :  0;
```

topologically trivial

Step 9

3) Press ABR_decomp button.

The irreps induced by atomic-orbital

Note that if there is no ABR for the p-orbital, we can add some atoms in the same Wyckoff Positions. (Including p-orbitals)

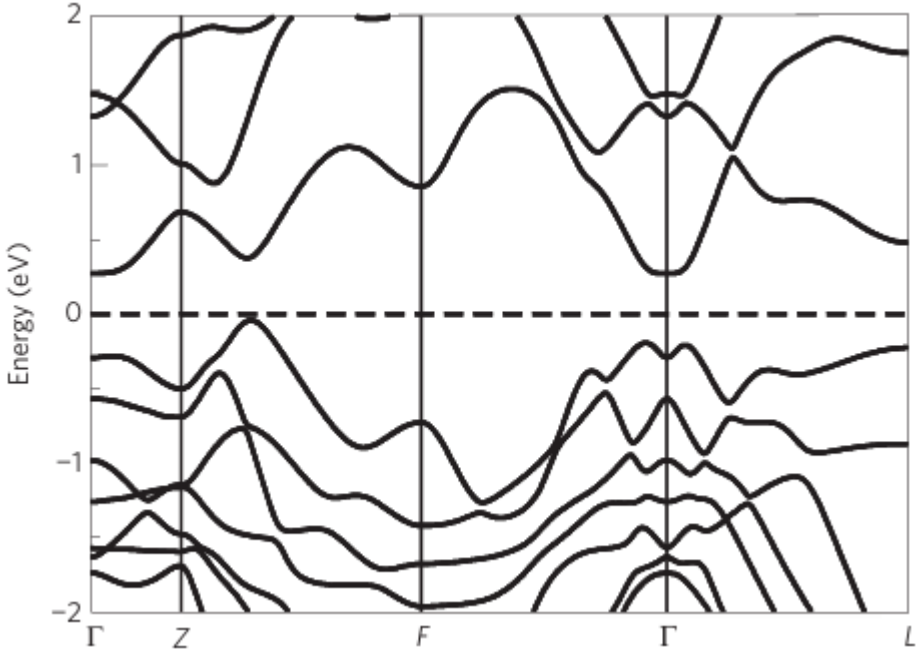
```
        216 F-43m
\\
 SN  Mult. Wyck. Atom   s    p    d  Wyck. Name
   1    1    9    5    2    1    0    4a   B
   2    1    6   33    2    3    0    4d   As
\\
 SN  Orb. @ Site      Symm.          BCS   CJB   MUL
  1   B-s @ 4a( 9)  -43m(31) >>>    (1)   (2)   (3)       Basis
                                 1  GM1 ;GM1 ; A1 ;      x2+y2+z2
  1   B-p @ 4a( 9)  -43m(31) >>>    (1)   (2)   (3)       Basis
                                 4  GM4 ;GM5 ; T2 ;      x,y,z;xy,xz,yz
  2  As-s @ 4d( 6)  -43m(31) >>>    (1)   (2)   (3)       Basis
                                 1  GM1 ;GM1 ; A1 ;      x2+y2+z2
  2  As-p @ 4d( 6)  -43m(31) >>>    (1)   (2)   (3)       Basis
                                 4  GM4 ;GM5 ; T2 ;      x,y,z;xy,xz,yz

There are 1 solutions for eBR decomposition.

There are 1 solutions for aBR decomposition.
It is an atomic insulator.        1
   1   1@9      A1@4a     (  1) :  0;
   2   4@9      T2@4a     (  1) :  0;
   3   1@6      A1@4d     (  1) :  0;
   4   4@6      T2@4d     (  1) :  1;
```

Atomic insulator

5 Solve CR and calculate SI by IR2TB

- Here we take the topological material Bi_2Se_3 as examples to introduce how to calculate TB Hamiltonian irreps to solve EBR decompositions and the compatibility relationship (CR) and symmetry indicators (SIs) to diagnose topological materials.

Band structure for Bi_2Se_3 with SOC



Nature Physics volume 5, pages438–442 (2009)

Step 1

1) Prepare the original POSCAR file. (Bi_2Se_3 as an example)
2) $ phonopy --tolerance 0.01 --symmetry -c POSCAR
   $ vim PPOSCAR

phonopy_version: '2.20.0'
space_group_type: 'R-3m'
space_group_number: 166
point_group_type: '-3m'

"POSCAR"

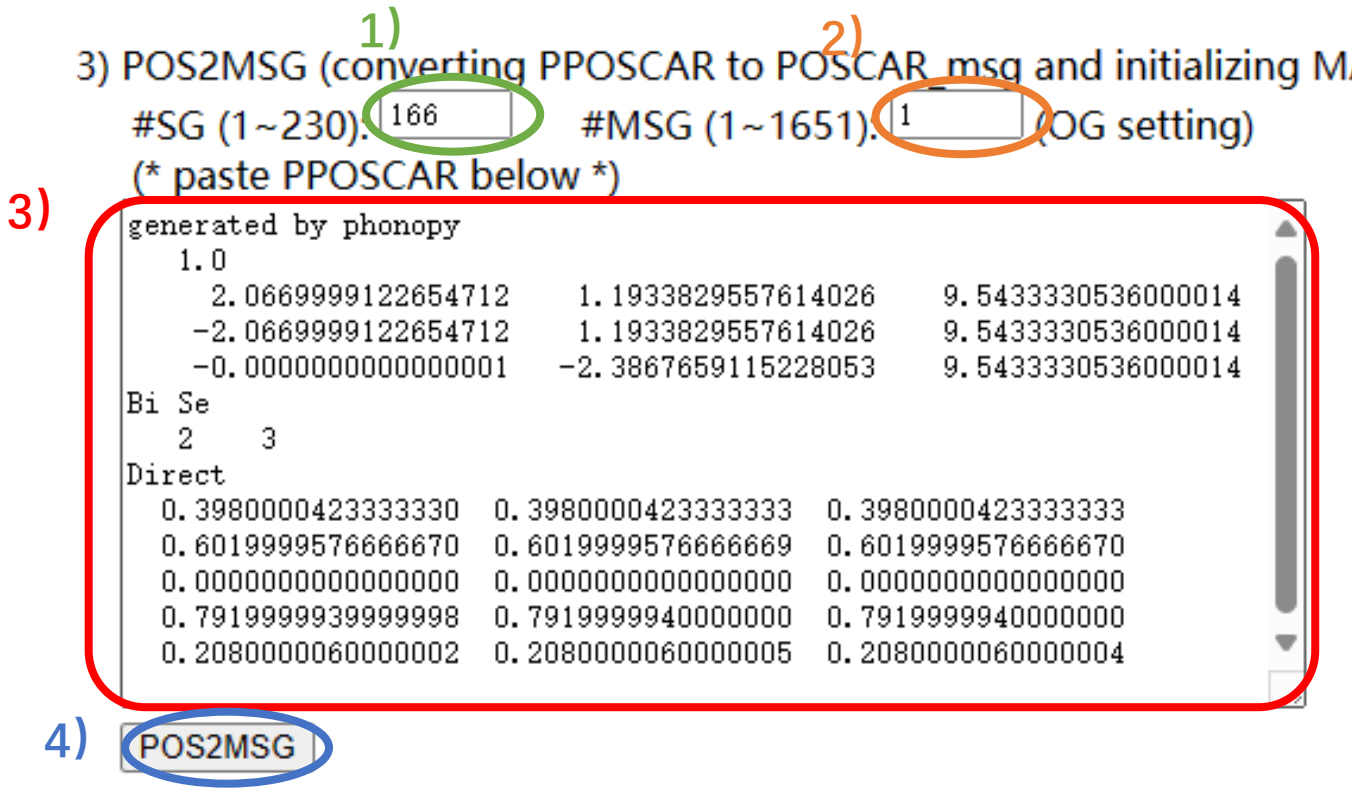
```
Bi2 Se3
1.0
    2.0669999122654712   1.1933829557614029   9.5433330536000032
   -2.0669999122654712   1.1933829557614029   9.5433330536000032
    0.0000000000000000  -2.3867659115228057   9.5433330536000032
Bi Se
2  3
Direct
  0.3980000423333330  0.3980000423333330  0.3980000423333331
  0.6019999576666670  0.6019999576666670  0.6019999576666668
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.7919999939999998  0.7919999939999998  0.7919999939999998
  0.2080000060000003  0.2080000060000003  0.2080000060000003
```

"PPOSCAR"

```
generated by phonopy
   1.0
    2.0669999122654712   1.1933829557614026   9.5433330536000014
   -2.0669999122654712   1.1933829557614026   9.5433330536000014
   -0.0000000000000001  -2.3867659115228053   9.5433330536000014
Bi Se
   2    3
Direct
  0.3980000423333330  0.3980000423333333  0.3980000423333333
  0.6019999576666670  0.6019999576666669  0.6019999576666670
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.7919999939999998  0.7919999940000000  0.7919999940000000
  0.2080000060000002  0.2080000060000005  0.2080000060000004
```

Step 2

Open the web:https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Give the group number(SG) from phonopy: 166.

2) Give any reasonable magnetic space group (MSG) number, such as 1.

3) Paste PPOSCAR into this box.

4) Press POS2MSG button.

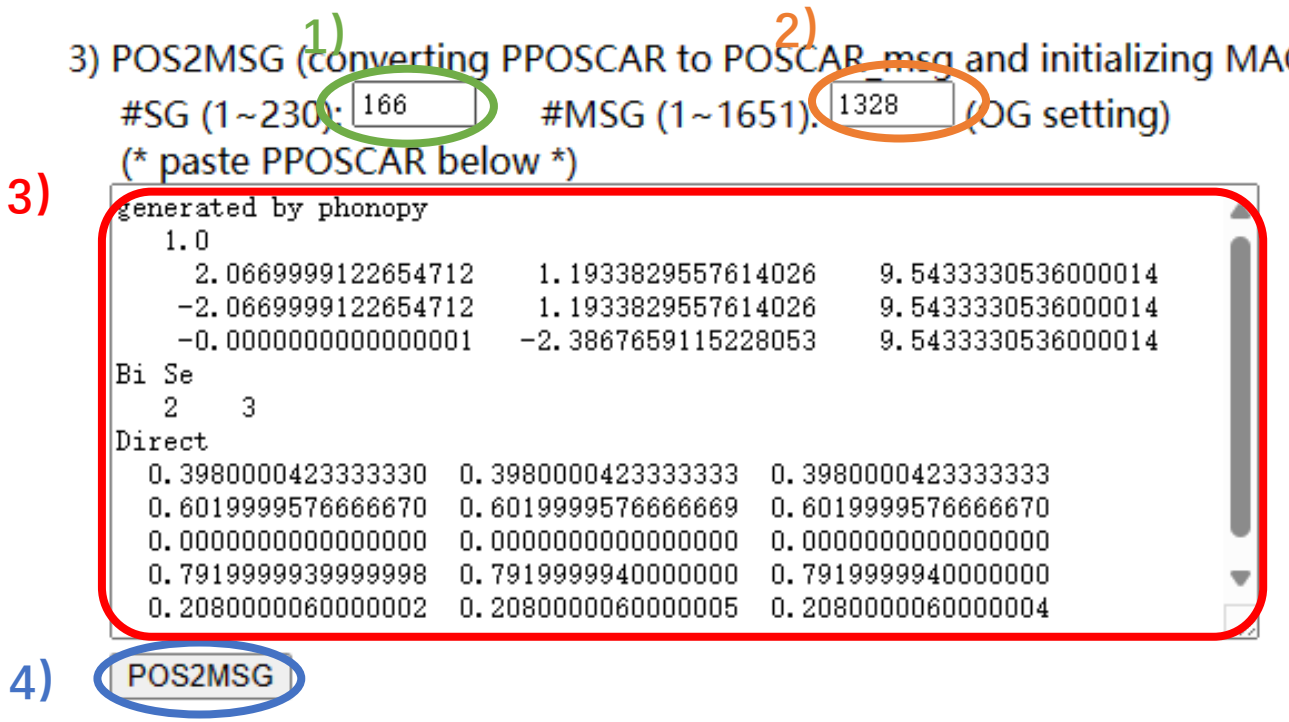
Step 3

```
The OG magnetic space group number do not match with the given space group number.
Possible OG magnetic space group numbers are given below:
1327, type 1
1328, type 2
1329, type 3
1330, type 3
1331, type 3
1332, type 4
1333, type 4
```

Nonmagnetic materials are the type-2 MSGs, which include time inversion operation.

Step 4

Back to the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Give the correct space group (SG) number: 166.

2) Give the correct magnetic space group(MSG) number: 1328.

3) Paste PPOSCAR into this box.

4) Press POS2MSG button.

Step 5

```
POSCAR_msg:
SG#B 166    OG (  166.2.1328)    BNS (      166.98)
  1.0
    2.06699991226547     1.19338295576140     9.54333305360000
   -2.06699991226547     1.19338295576140     9.54333305360000
   -0.00000000000000    -2.38676591152281     9.54333305360000
    Bi    Se
     2     3
Direct
    0.39800004233333     0.39800004233333     0.39800004233333
    0.60199995766667     0.60199995766667     0.60199995766667
    0.00000000000000     0.00000000000000     0.00000000000000
    0.79199999400000     0.79199999400000     0.79199999400000
    0.20800000600000     0.20800000600000     0.20800000600000

INCAR:
LSORBIT = T
LNONCOLLINEAR = T
SAXIS = 0 0 1
MAGMOM=300*0.0

KPOINTS:
MKPOINTS used for magnetic space group
  4
rec
    0.00000000    0.00000000    0.00000000    1.0    ! GM
    0.50000000    0.50000000    0.50000000    1.0    ! T
    0.50000000    0.50000000    0.00000000    1.0    ! F
    0.00000000    0.50000000    0.00000000    1.0    ! L
```

We can get the standard POSCAR (POSCAR_msg) and some setting parameters of INCAR and KPOINTS.

All space groups' HSKPs can be found on: https://github.com/zjwang11/IR2PW/lib_irrep_bcs/max_KPOINTS_VASP/

Then we construct a Bi_2Se_3 TB model considering soc (or generated by wannier90)

Step 6

The constructed TB model only considers p-orbital, so there are only 18 occupation bands in Bi_2Se_3.

```
$ ir2tb -sg 166 -nb 1 18 > outir
$ vim tqc.data
```

"tqc.data"

```
166    4   18
1 12 11 12  9 10 11  7  8 12  9 10 11
2 12 12 11  9 10 12 12  9 10  7  8 11
4  7  8  5  6  7  8  7  8  5  6  7  8  7  8  5  6  7  8
5  7  8  7  8  5  6  7  8  5  6  5  6  7  8  7  8  7  8
```

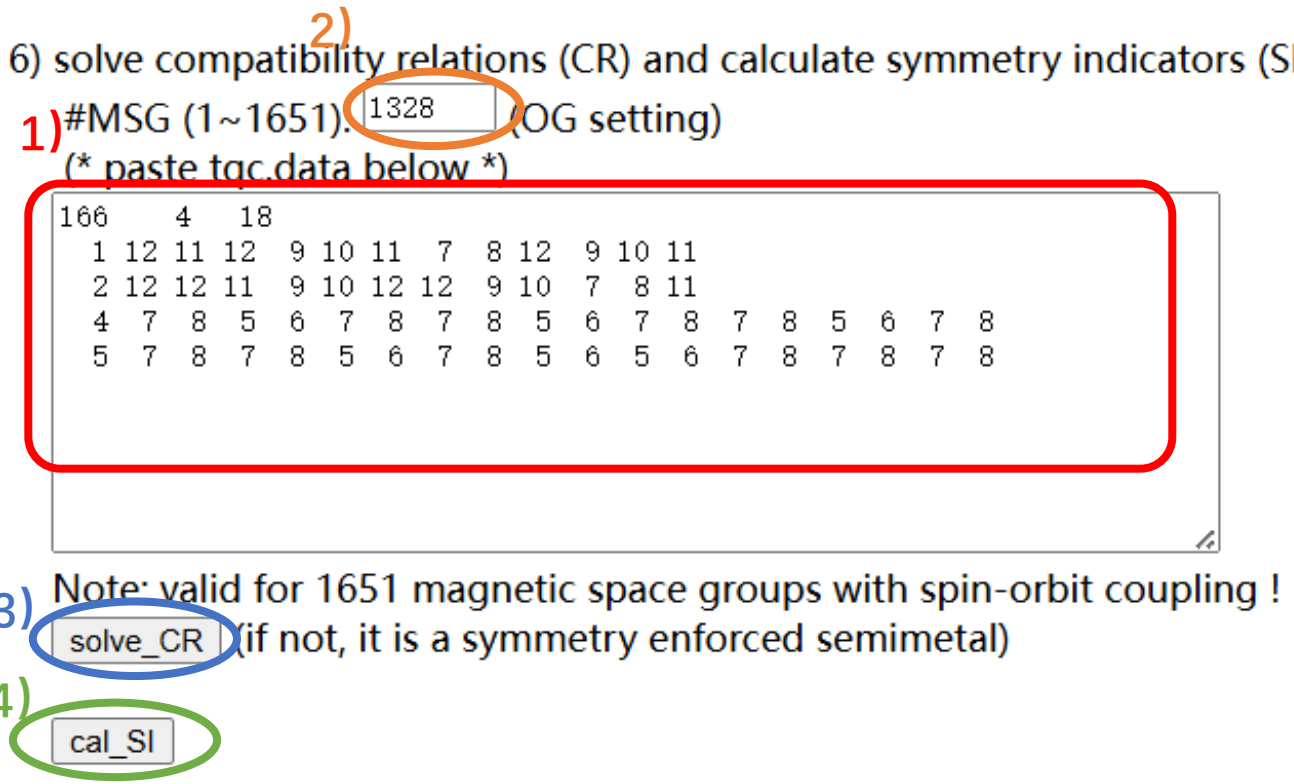
Prepare the Hamiltonian files named lda_hr.dat /soc_hr.dat and tbbox.in

Format of tqc.data

```
#SG (space group number)   #nk (number of HSKPs)   #nb (number of bands)
 HSKP#1  irrep(HSKP#1)#1  irrep(HSKP#1)#2  ···
 HSKP#2  irrep(HSKP#2)#1  irrep(HSKP#2)#2  ···
 ...
```

Step 7

Back to the web: https://tm.iphy.ac.cn/TopMat_1651msg.html



1) Paste tqc.data into this box.

2) Give the MSG number: 1328.

3) Press solve_CR button.

4) Press cal_SI button.

Step 8

solve_CR :

```
The input data is calculated with spin-orbit coupling.
Satisfy CR
```

cal_SI :

```
The input data is calculated with spin-orbit coupling.
Z2=0,Z4=1,
```

We can see that Bi_2Se_3 satisfies the CR, and its SI is Z4=1,
so we can diagnose that this is a topological material.

Thank you !!!