Hands-on Diagnose Topological Materials

Web:
https://tm.iphy.ac.cn/TopMat_1651msg.html
Source code:
https://github.com/zjwang11/IR2PW
https://github.com/zjwang11/TopMat

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 2025/6/3

Outline

- 1 Installation
- 2 Calculate the SIs of NonMagnetic Topological materials.
- 3 Calculate the SIs of Magnetic Topological materials.
- 4 Calculate the SIs by IR2TB.

1 Installation

1) **lib_irrep_bcs.a**

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

2) **pos2aBR**

```
$ tar -zxvf src_pos2aBR.tar.gz
$ cd src_pos2aBR
$ ./configure.sh
$ source ~/.bashrc
$ make
$ cd ../
```

3) **irvsp**

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

4) **ir2tb**

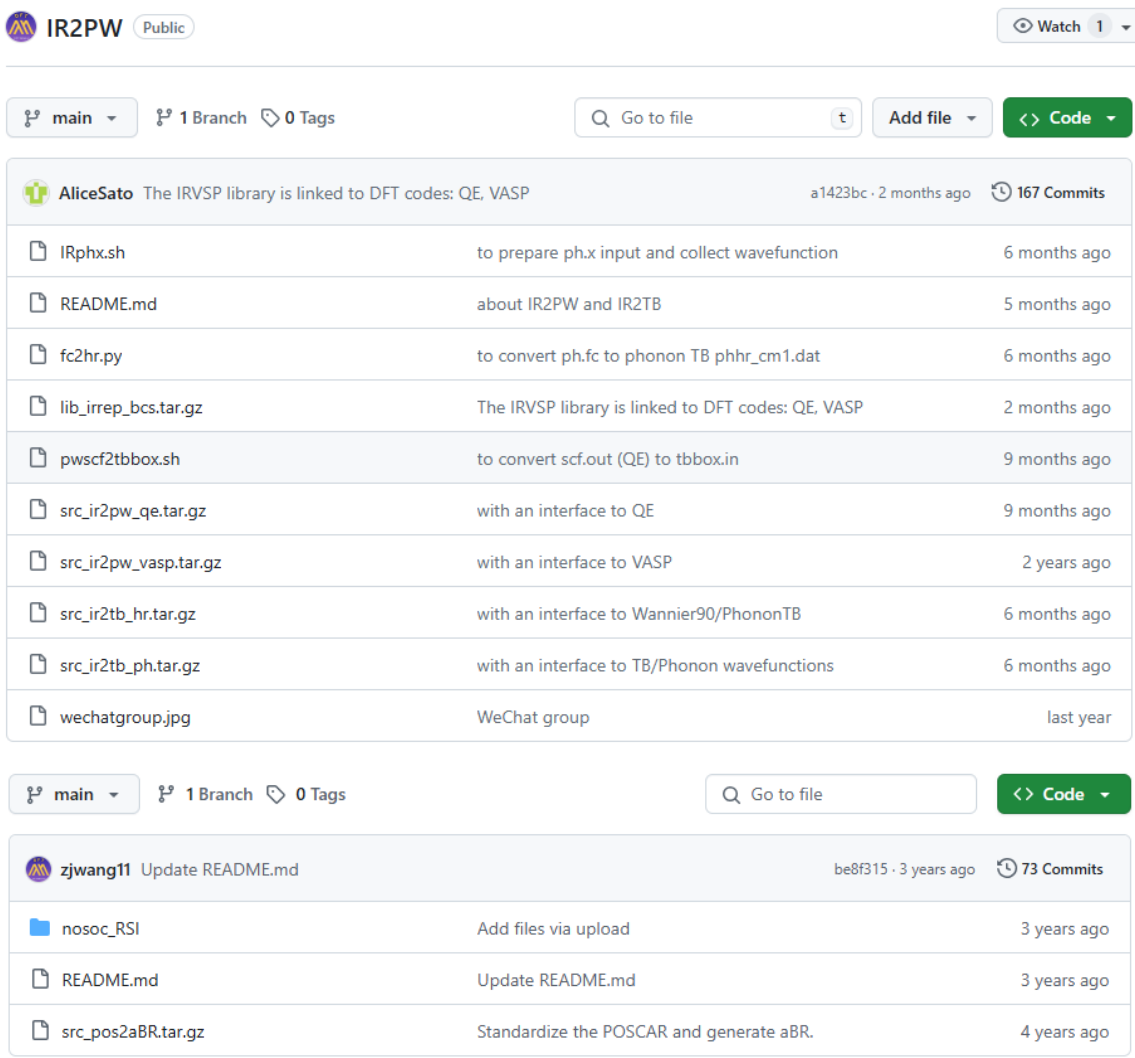
```
$ tar -zxvf src_ir2tb_hr.tar.gz
$ cd src_ir2tb_hr
$ make
$ cd ../
```

5) **ir2pw**

```
$ tar –zxvf src_ir2pw_qe.tar.gz
$ cd src_ir2pw_qe
$ make
$ cd ../
```

6) **ir2ph**

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



https://github.com/zjwang11/IR2PW

https://github.com/zjwang11/UnconvMat

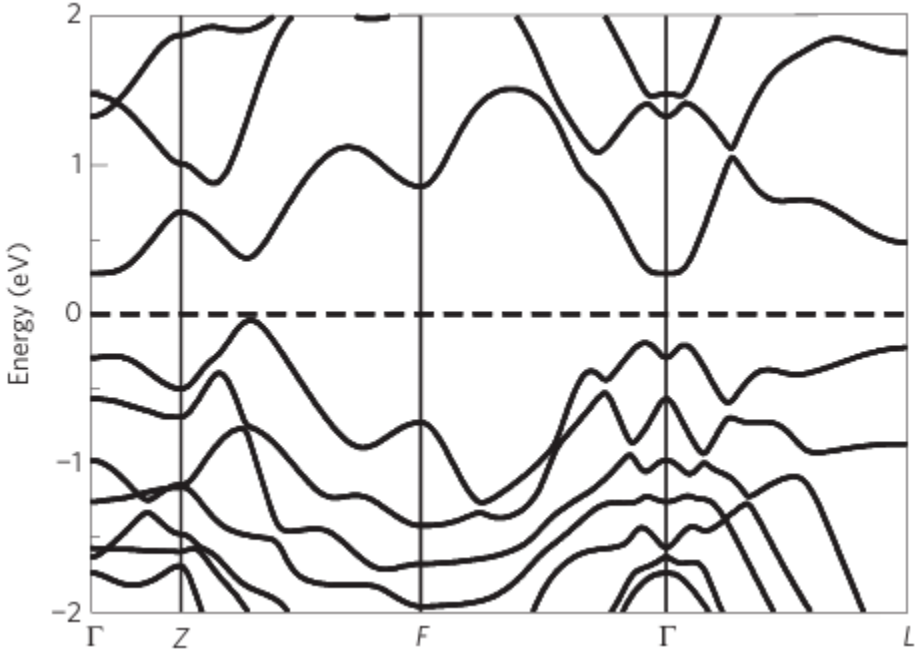
2 Calculate the SIs of NonMagnetic Topological materials

- 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.
- Here we take Bi_2Se_3 and SnSe 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 materials.

2.1 Bi_2Se_3

- Here we take the topological material Bi_2Se_3 as an example to introduce how to calculate Irreps to solve the CR and calculate the 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 (taking Bi_2Se_3 as an example).
2) $ phonopy --symmetry --tolerance 0.01 -c POSCAR
   $ vim PPOSCAR

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

"POSCAR"

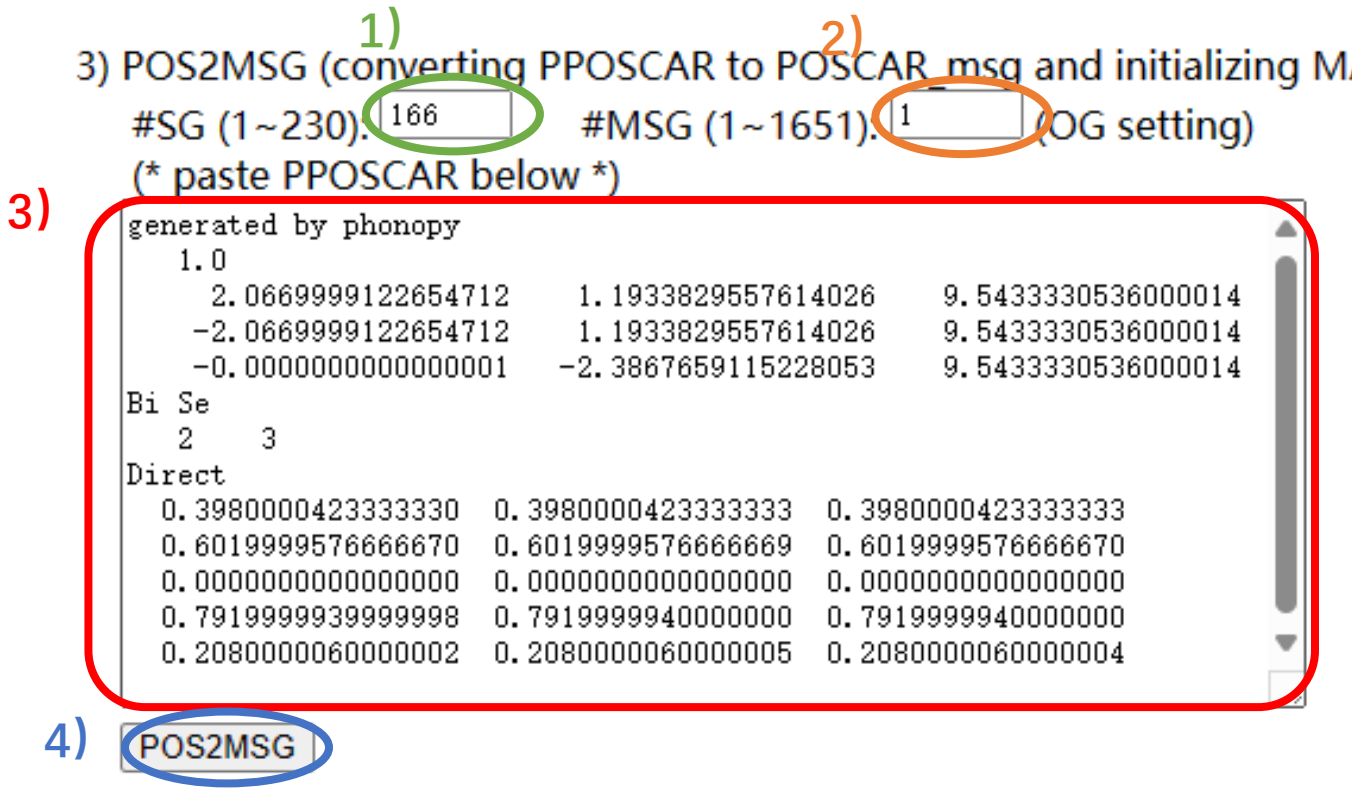
```
Bi2 Se3
1.0
    2.0669999122654712   1.1933829557614029   9.5433330536000032
   -2.0669999122654712   1.1933829557614029   9.5433330536000032
    0.0000000000000000  -2.3867659115228057   9.5433330536000032
Bi Se
2  3
Direct
  0.3980000423333330  0.3980000423333330  0.3980000423333331
  0.6019999576666670  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 space 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.

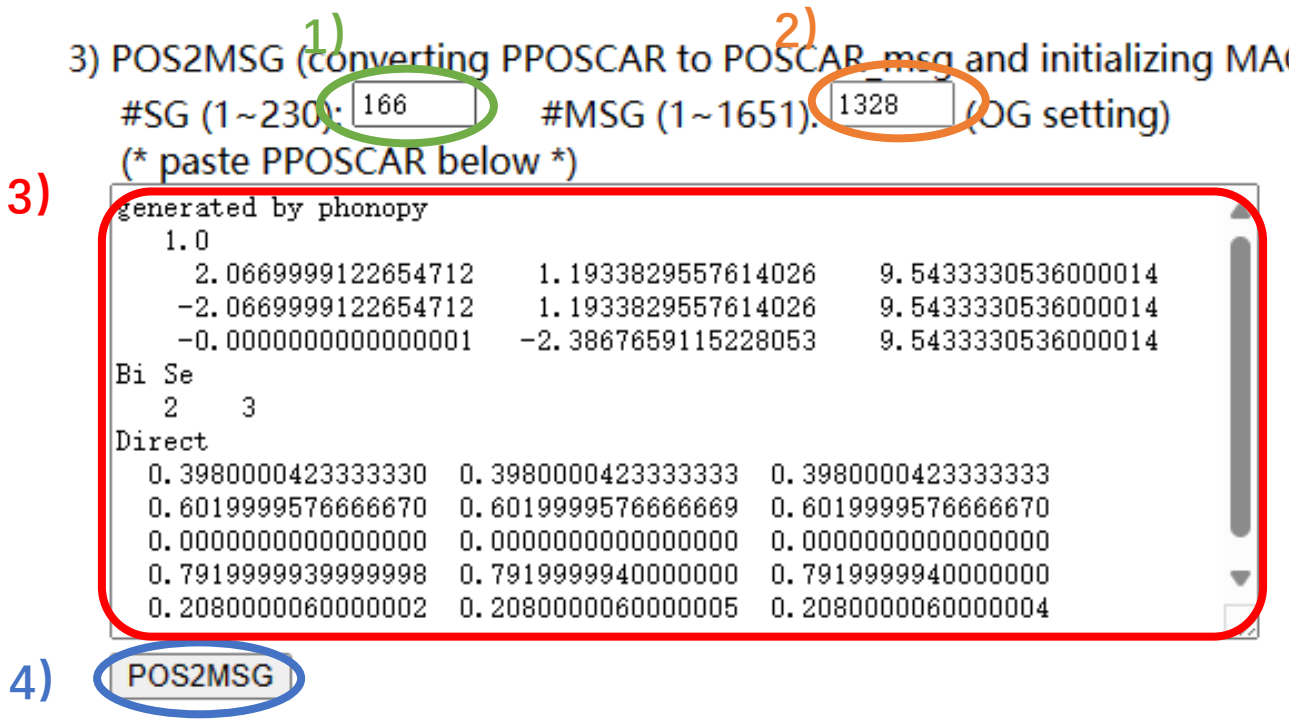
Step 3

```
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 reversal operation.

Step 4

Open 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' high-symmetry k-points (HSKPs) can be found on: https://github.com/zjwang11/IR2PW/lib_irrep_bcs/max_KPOINTS_VASP/

Then we do VASP calculations to get wavefunctions of these HSKPs.

Step 6

The number of valence electrons in Bi_2Se_3 is 48

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

After running IRVSP to get Irreps of HSKPs, the tqc.data file is generated.

"tqc.data"

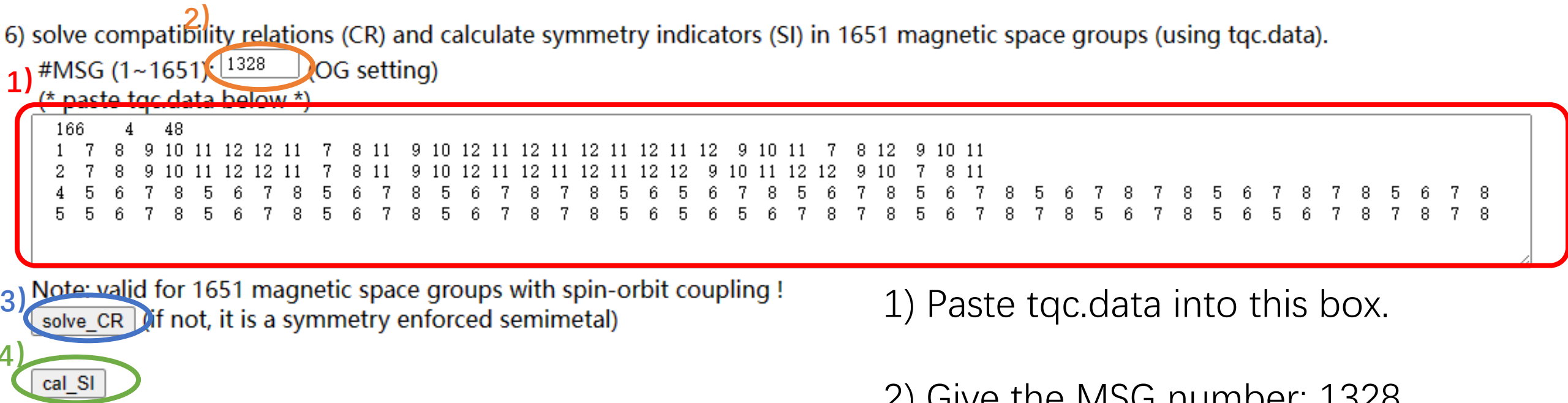
```
166   4   48
 1  7  8  9 10 11 12 12 11  7  8 11  9 10 12 11 12 11 12 11 12 11 12  9 10 11  7  8 12  9 10 11
 2  7  8  9 10 11 12 12 11  7  8 11  9 10 12 11 12 11 12 11 12 12  9 10 11 12 12  9 10  7  8 11
 4  5  6  7  8  5  6  7  8  5  6  7  8  5  6  7  8  7  8  5  6  5  6  7  8  5  6  7  8  5  6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

Open 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 :

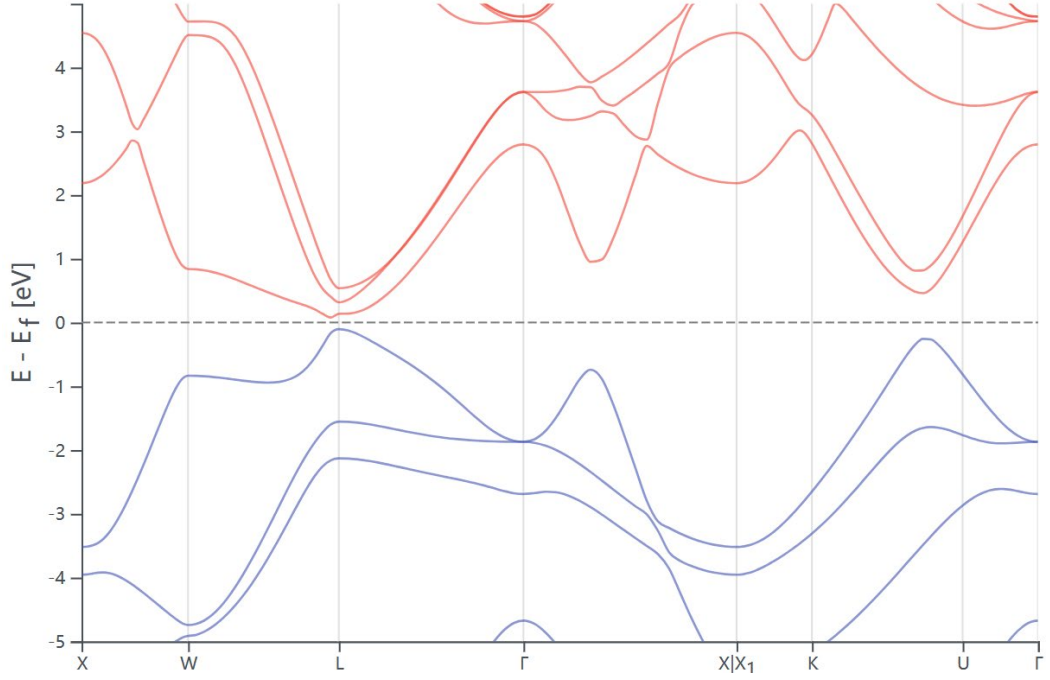
```
The input data is calculated with spin-orbit coupling.
Z2=0,Z4=1,
```

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

2.2 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 example to introduce how to calculate Irreps to solve the CR and calculate the SIs to diagnose topological materials.



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

Step 1

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

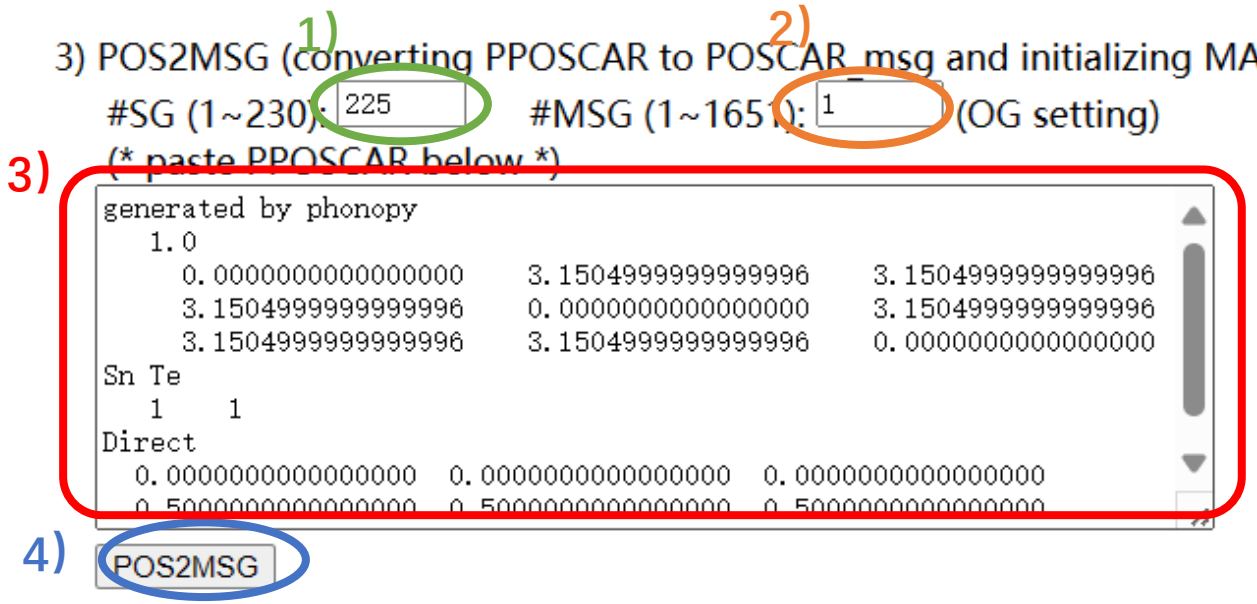
```
phonopy_version: '2.20.0'
space_group_type: 'Fm-3m'
space_group_number: 225
point_group_type: 'm-3m'
```

“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.

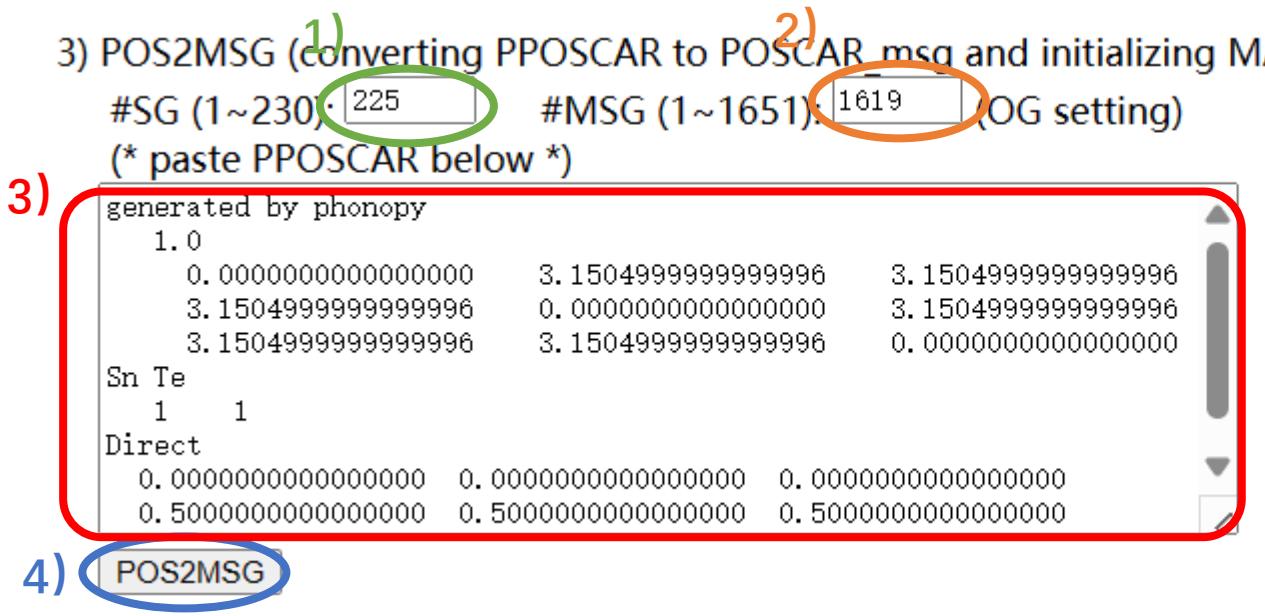
Step 3

```
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

Open 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"

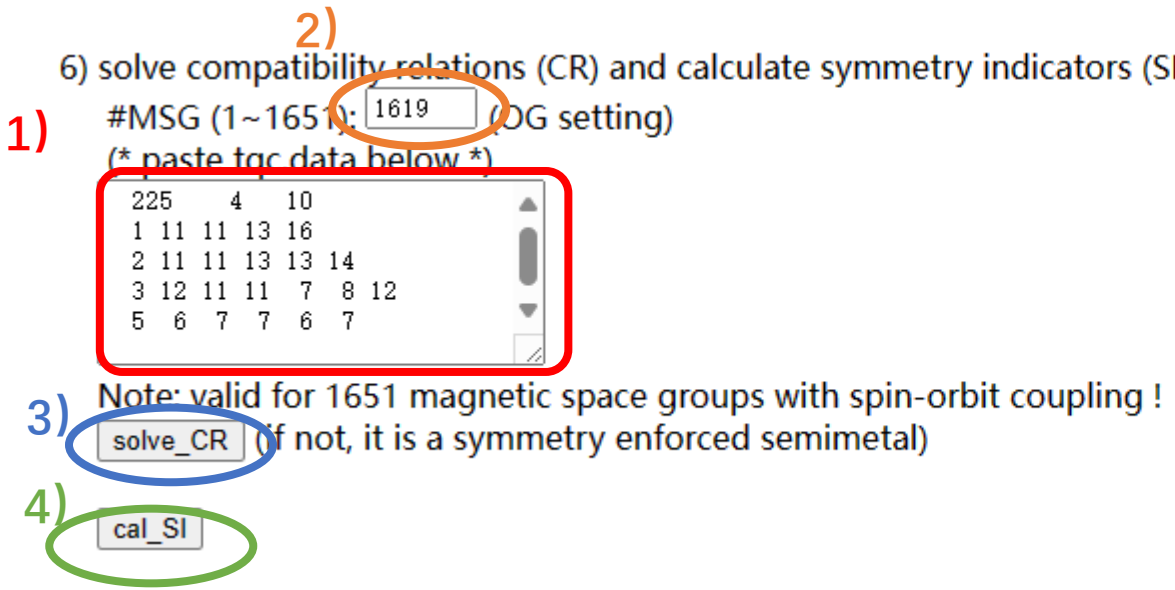
```
225    4   10
 1 11 11 13 16
 2 11 11 13 13 14
 3 12 11 11  7  8 12
 5  6  7  7  6  7
```

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

Open 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 SIs on the website

topological

3 Calculate the SIs of Magnetic Topological materials.

- 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 the 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 $Eu_3In_2As_4$ (AFMc and AFMb)as examples to introduce how to solve the CR and calculate the SIs to magnetic topological materials.

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

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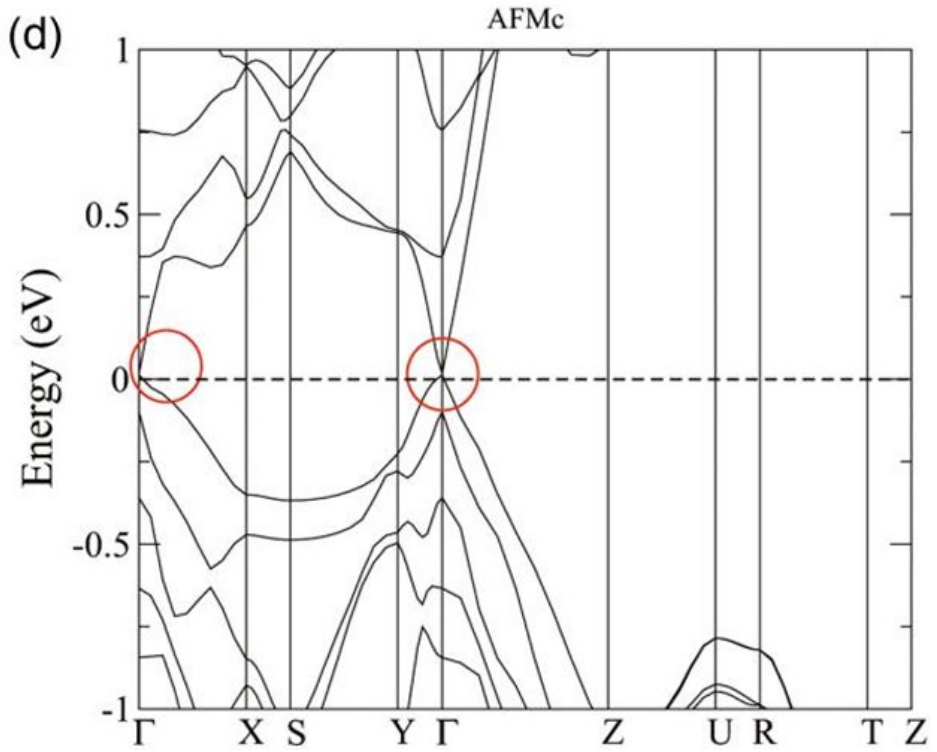
3.1 $Eu_3In_2As_4$-AFMc

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

The band structures of $Eu_3In_2As_4$ for the magnetic configuration AFMc



arXiv:2403.07637(2024)

Step 1

1) Prepare the original POSCAR file (taking $Eu_3In_2As_4$ as an example).
2) $ phonopy --symmetry --tolerance 0.01 -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	$\varnothing$	$\varnothing$
58.4.474	$Pnnm'$	$Pnnm'$	#58.396	III	Table MSG474	$\varnothing$	$\varnothing$
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	$\varnothing$	$\varnothing$
		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		

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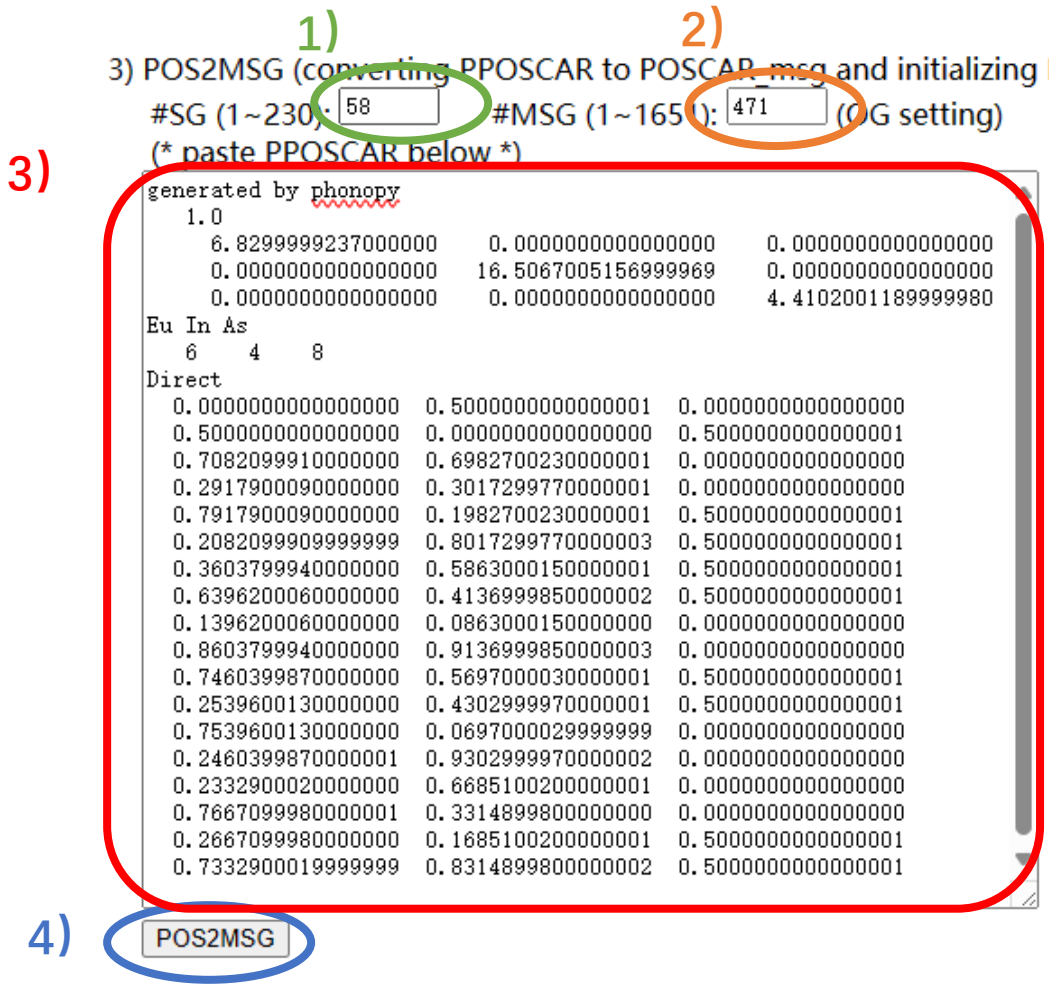
Step 3

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 > outdir

$ vim tqc.data

"tqc.data"

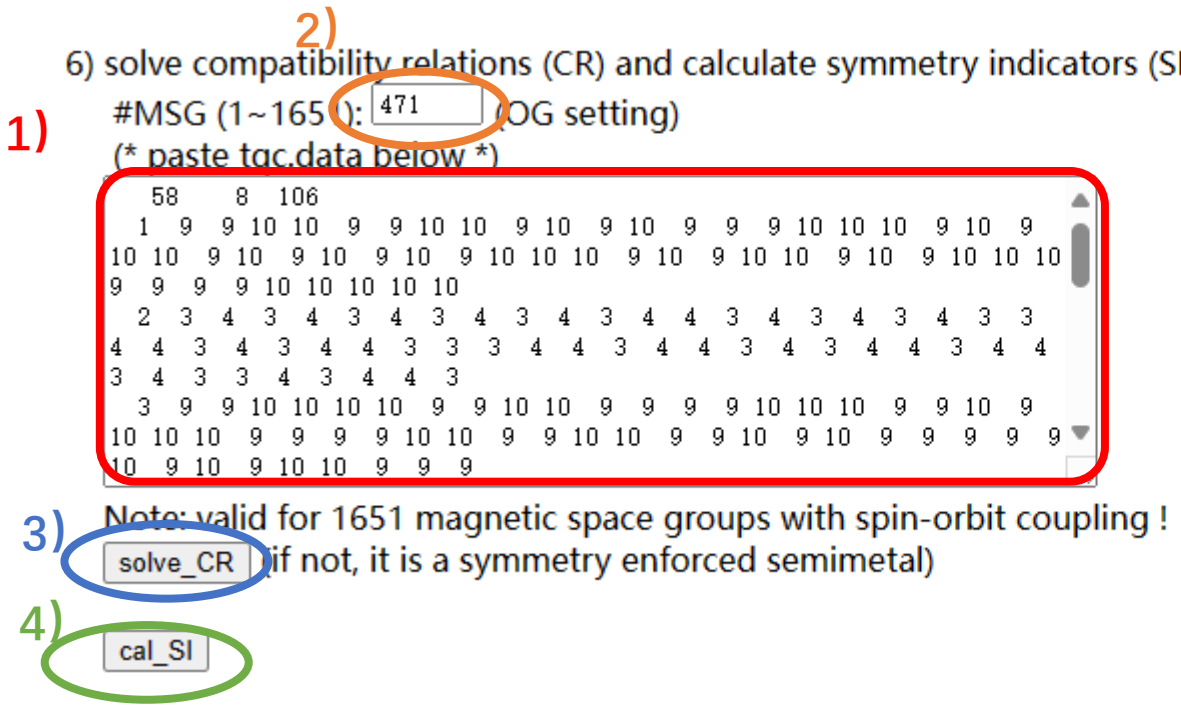
```
 58   8  106
  1  9  9 10 10  9  9 10 10  9 10  9 10  9  9  9 10 10 10  9 10  9 10 10  9 10  9 10  9 10  9 10  9 10 10 10  9 10  9 10 10  9 10 10 10 10 10
  2  3  4  3  4  3  4  3  4  3  4  3  4  4  3  4  3  4  3  4  3  3  4  4  3  4  3  4  4  3  3  3  4  4  3  4  4  3  4  3  4  4  3  4  4  3  4  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  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

Open 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,
```

3.2 $Eu_3In_2As_4$-AFMb

- Here we take the magnetic material $Eu_3In_2As_4$ (AFMb) as an example to introduce how to calculate Irreps to solve the CR and calculate the SIs to diagnose magnetic topological 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 (taking $Eu_3In_2As_4$ 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
2) $ phonopy --symmetry --tolerance 0.01 -c POSCAR_msg

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		

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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 PPOSCAR (with 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 Irreps.

```
$ irvsp -sg 14 -nb 1 154 > outdir
$ vim tqc.data
```

"tqc.data"

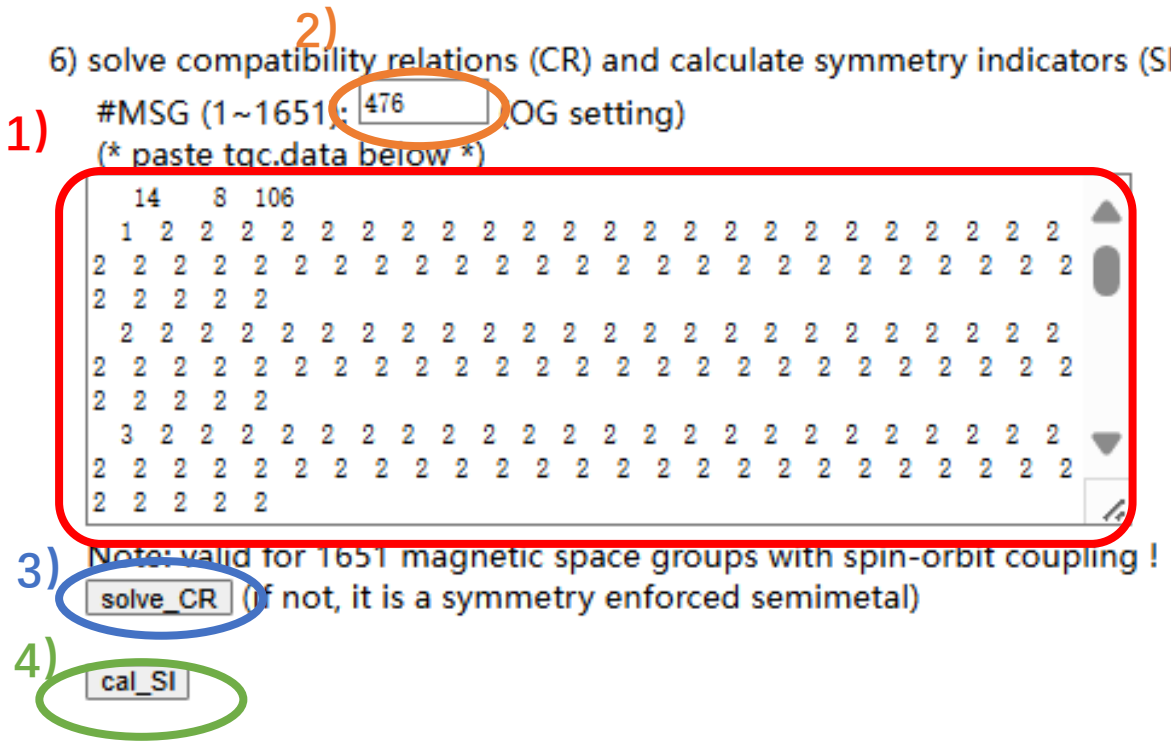
```
 14   8  106
 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 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

Open 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 :

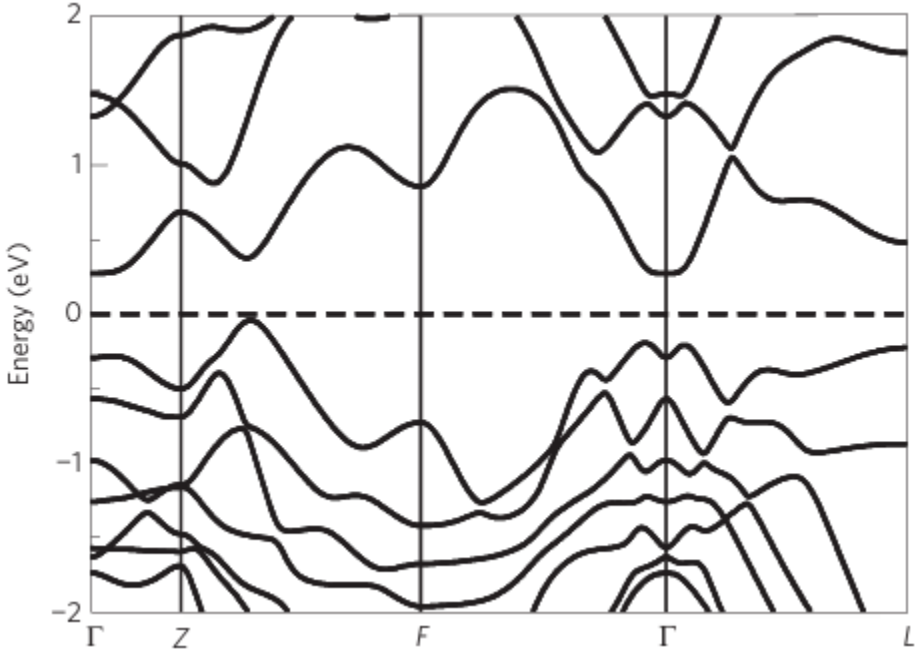
```
The input data is calculated with spin-orbit coupling.
Z2=0,
```

trivial

4 Calculate the SIs by IR2TB.

- Here we take the topological material Bi_2Se_3 as example 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



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Step 1

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

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

"POSCAR"

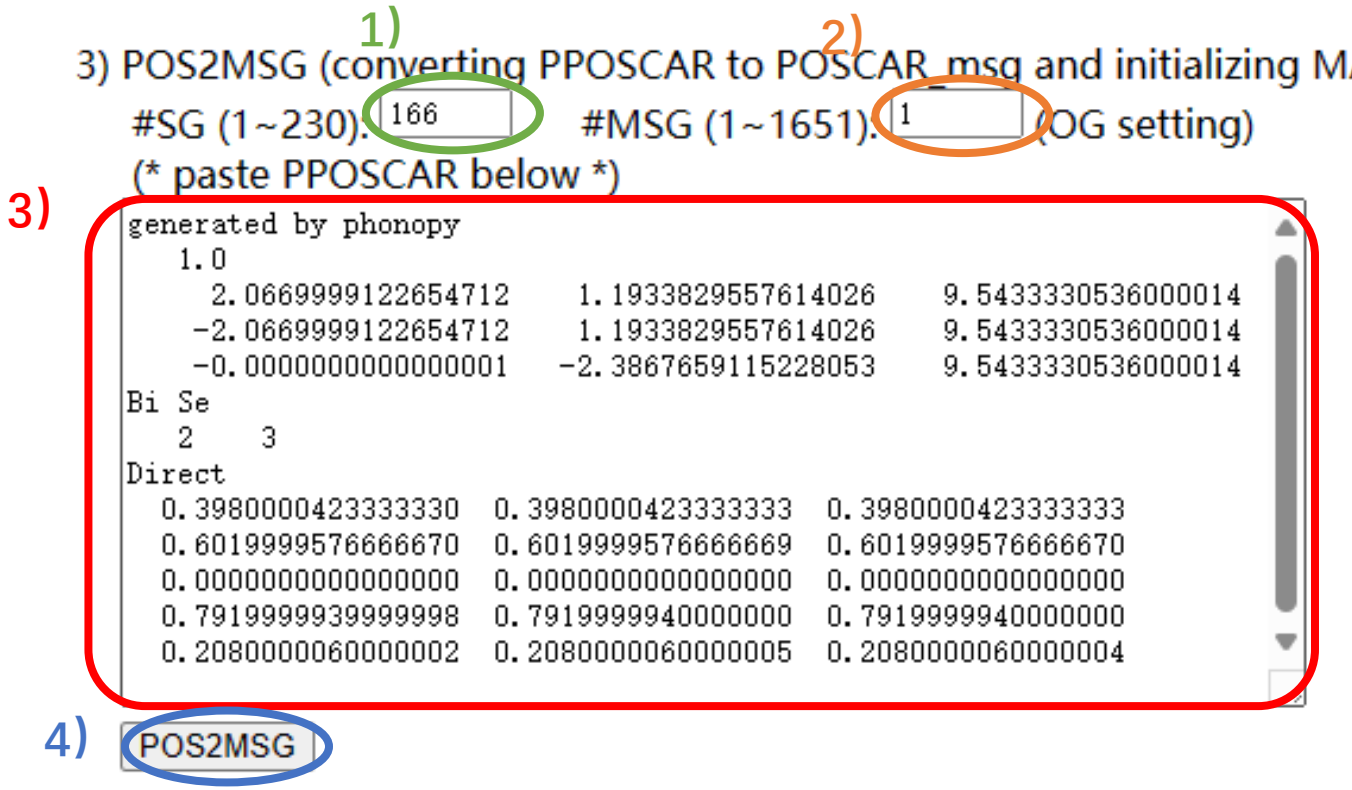
```
Bi2 Se3
1.0
    2.0669999122654712   1.1933829557614029   9.5433330536000032
   -2.0669999122654712   1.1933829557614029   9.5433330536000032
    0.0000000000000000  -2.3867659115228057   9.5433330536000032
Bi Se
2  3
Direct
  0.3980000423333330  0.3980000423333330  0.3980000423333331
  0.6019999576666670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

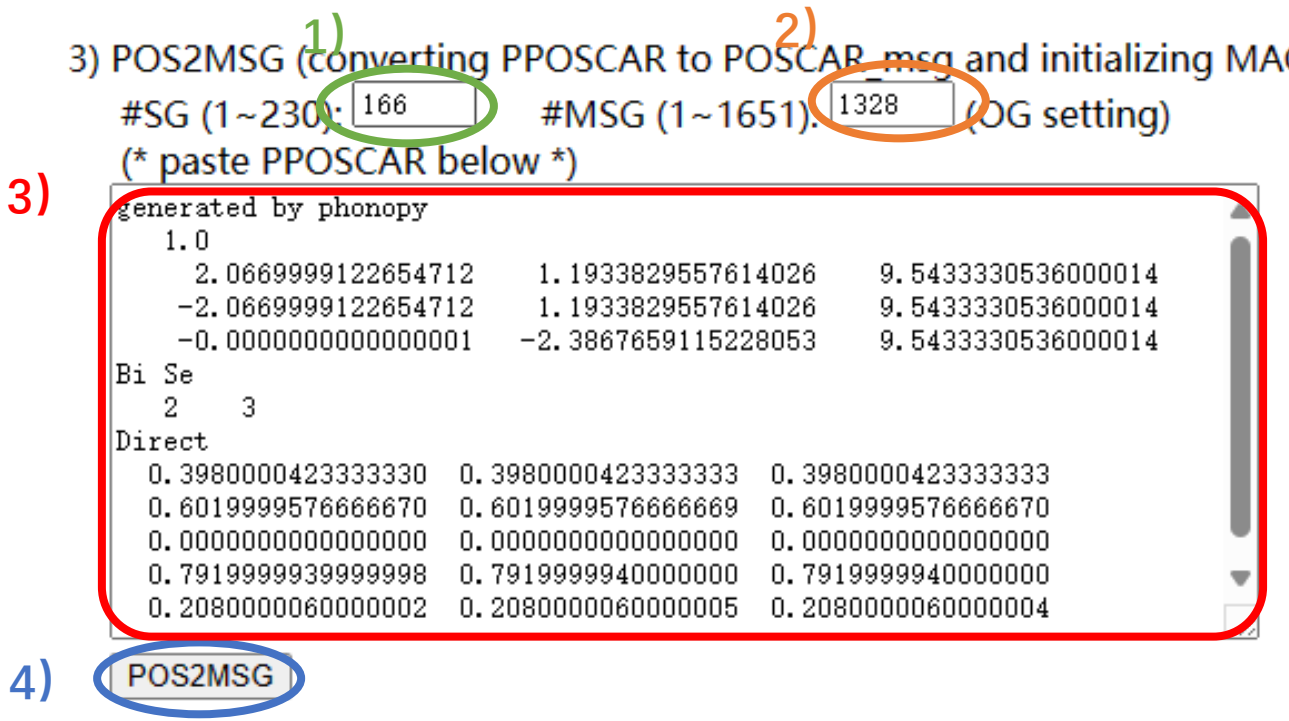
Step 3

```
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

Open 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
```

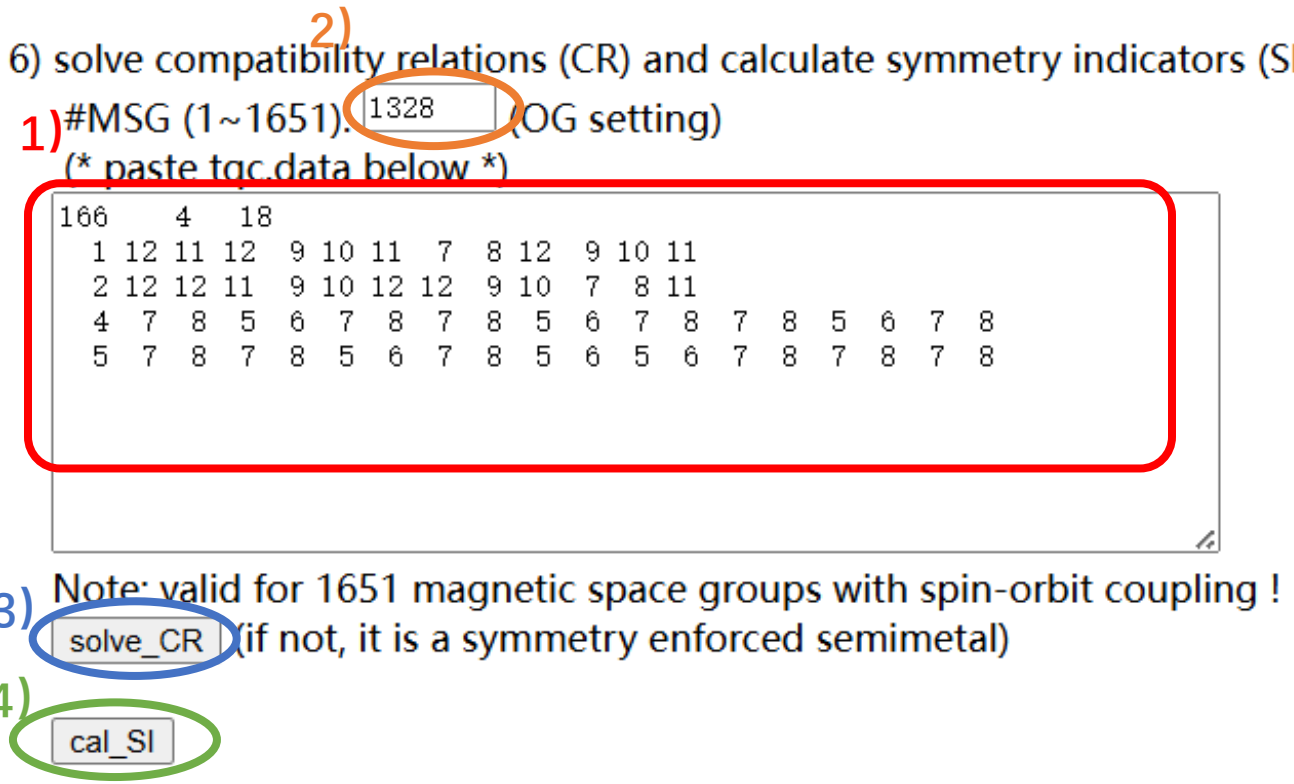
Prepare the Hamiltonian files named lda_hr.dat /soc_hr.dat and tbbox.in

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

Open 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 !!!