Hands-on Diagnose Topological Materials

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

🚳 IR2PW Public

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	1 AliceSato The IRVSP library is linked to DFT codes: 0	QE, VASP		a1423b	oc · 2 months ago	🕙 167 Commits
	🗋 IRphx.sh	to prepare p	to prepare ph.x input and collect wavefunction			
	🗋 README.md	about IR2PV	about IR2PW and IR2TB			
	🗋 fc2hr.py	to convert p	h.fc to phonon TE	9 phhr_cm1.dat		6 months ago
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Z	pwscf2tbbox.sh	to convert s	cf.out (QE) to tbbo	ox.in		9 months ago
	src_ir2pw_qe.tar.gz	with an interface to QE				9 months ago
	src_ir2pw_vasp.tar.gz	with an interface to VASP			2 years ago	
	src_ir2tb_hr.tar.gz	with an interface to Wannier90/PhononTB			6 months ago	
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	nosoc_RSI	Add files via	upload			3 years ago
	🗋 README.md	Update README.md			3 years ago	
	src_pos2aBR.tar.gz	Standardize	the POSCAR and	generate aBR.		4 years ago

https://github.com/zjwang11/IR2PW

https://github.com/zjwang11/UnconvMat

1 Installation

1) lib_irrep_bcs.a

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

3) irvsp

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

5) ir2pw

- \$ tar -zxvf src_ir2pw_qe.tar.gz
- \$ cd src_ir2pw_qe
- \$ make
- \$ cd ../

2) pos2aBR \$ tar -zxvf src_pos2aBR.tar.g: \$ cd src_pos2aBR \$./configure.sh \$ source ~/.bashrc \$ make

- \$ make
- \$ cd ../

4) ir2tb

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

6) **ir2ph**

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

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 Bi₂Se₃ 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.

$$2.1 \text{ Bi}_2\text{Se}_3$$

 Here we take the topological material Bi₂Se₃ as an example to introduce how to calculate Irreps to solve the CR and calculate the SIs to diagnose topological materials. Band structure for Bi₂Se₃ with SOC



Nature Physics volume 5, pages438–442 (2009)

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

"POSCAR"

Bi2 Se3 1.0	
2.0669999122654712 1.1933829557614029 9.543333053600	0032
-2.0669999122654712 1.1933829557614029 9.543333053600	0032
0.00000000000000 -2.3867659115228057 9.543333053600	0032
Bi Se	
2 3	
Direct	
0.3980000423333330 0.3980000423333330 0.3980000423333331	
0.60199995766666670 0.60199995766666670 0.60199995766666668	
0.00000000000000 0.0000000000000 0.000000	1
0.791999993999998 0.791999993999998 0.791999993999998	
0.20800006000003 0.20800006000003 0.20800006000003	

"PPOSCAR"

generated by phonopy		
1.0		
2.0669999122654712	1.193382955761402	26 9.5433330536000014
-2.0669999122654712	2 1.19338295576140	9.5433330536000014
-0.000000000000000	1 -2.38676591152280	053 9.5433330536000014
Bi Se		
2 3		
Direct		
0.39800004233333330	0.3980000423333333	0.3980000423333333
0.6019999576666670	0.6019999576666669	0.60199995766666670
0.0000000000000000000000000000000000000	0.0000000000000000000	0.0000000000000000000000000000000000000
0.791999993999998	0.7919999940000000	0.791999994000000
0.20800006000002	0.2080000060000005	0.20800006000004

phonopy_version: '2.20.0'

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

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



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.

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.

POSCAR msg:					
SG#B 166 OG	(166.	2.1328)	BNS (166.98)	
1.0					
2.06699991	L226547	1.1933	38295576140	9.54333	305360000
-2.06699991	L226547	1.1933	38295576140	9.54333	305360000
-0.0000000	0000000	-2.3867	76591152281	9.54333	305360000
Bi Se					
2 3					
Direct					
0.39800004	1233333	0.3980	000042333333	0.39800	004233333
0.6019999	5766667	0.6019	99995766667	0.60199	995766667
0.0000000	0000000	0.0000	000000000000000000000000000000000000000	0.00000	000000000
0.79199999	9400000	0.7919	99999400000	0.79199	999400000
0.2080000	0600000	0.2080	0000600000	0.20800	000600000
INCAR: LSORBIT = T LNONCOLLINEAR SAXIS = 0 0 1 MAGMOM=300*0.0	= Т)				
KPOINTS:					
MKPOINTS used	for mag	netic spa	ace group		
4					
rec					
0.0000000	0.0	0000000	0.00000	00 1.0	! GM
0.5000000	0.5	0000000	0.500000	00 1.0	! T
0.5000000	0.5	0000000	0.00000	00 1.0	! F
0.0000000	0.5	0000000	0.00000	00 1.0	1 L

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

All space groups' high-symmetry kpoints (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.

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

7 8 11 9 10 12 11 12 11 12 11 12 11 12 9 10 11 7 8 12 9 10 11 910 12 11 12 11 12 11 12 12 9 10 11 12 12 9 10 7 8 11 910 8 1 1 9 8 5 6 8 8 8 8 78 5 5 6 5 8 87856787856785656787878 785678567856 7878565656 556 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 ...

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



4) Press cal_SI button.

solve_CR :

cal_SI :

The input data is calculated with spin-orbit coupling. Satisfy $\ensuremath{\mathsf{CR}}$

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



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

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

"POSCAR"

Sn Te 1.000000000000000000000		
6.3010000000000002	0.00000000000000	00 0.0000000000000000000000000000000000
0.000000000000000000	6.3010000000000	02 0.0000000000000000
0.0000000000000000	0.00000000000000	00 6.301000000000002
Sn Te		
4 4		
Cartesian		
0.0000000000000000000000000000000000000	000000000000000000000000000000000000000	0.0000000000000000
0.00000000000000 3.	1505000000000001	3.1505000000000001
3.150500000000000 0.0	000000000000000000000000000000000000000	3.1505000000000001
3.150500000000001 3.	1505000000000001	0.0000000000000000
3.150500000000001 3.	1505000000000001	3.1505000000000001
3.150500000000000 0.0	000000000000000000000000000000000000000	0.0000000000000000
0.00000000000000 3.	1505000000000001	0.0000000000000000
0.0000000000000000000000000000000000000	000000000000000000000000000000000000000	3.150500000000000

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

"PPOSCAR"

generated by phonopy		
0.0000000000000000000000000000000000000	3,15049999999999999	3,150499999999999996
3.15049999999999996	0.00000000000000000	3.150499999999999996
3.15049999999999996	3.15049999999999996	0.0000000000000000000000000000000000000
Sn Te		
1 1		
Direct		
0.00000000000000 0.	000000000000000000000000000000000000000	000000000000000000000000000000000000000
0.50000000000000 0.	500000000000000 0.5	000000000000000

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.

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.

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.

POSCAR_msg									
SG#B 225	OG (225.2.	1619)	BNS	(225.1	17)		
1.0									
0.0000	000000	00000	3.1505	00000	00000	З.	1505000	00	00000
3.1505	000000	00000	0.0000	00000	00000	З.	1505000	00	00000
3.1505	000000	00000	3.1505	00000	00000	0.	0000000	00	00000
Sn Te									
1 1									
Direct									
0.0000	000000	00000	0.0000	00000	00000	0.	0000000	00	00000
0.5000	000000	00000	0.5000	00000	00000	0.	5000000	00	00000
INCAR: LSORBIT = T LNONCOLLINEAR = T SAXIS = 0 0 1 MAGMOM=300*0.0									
KPOINTS:									
MKPOINTS u 4	sed fo	or magne	tic spa	ce gr	oup				
rec									
0.0000	0000	0.000	00000	0.0	000000	00	1.0	!	GM
0.5000	0000	0.000	00000	0.5	000000	00	1.0	!	х
0.5000	0000	0.500	00000	0.5	000000	00	1.0	!	L
0.5000	0000	0.250	00000	0.7	500000	0	1.0	!	W

DOGGAD -----

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

Then we do VASP calculations.

The number of valence electrons in SnTe is 10



"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 ...

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.

Compound:	Symmetry Group:	Topological Status (Type):	Topological indices:
Sn1 Te1	225 (Fm-3m)	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 $\ensuremath{\mathsf{CR}}$

cal_SI :

The input data is calculated with spin-orbit coupling. $\tt Z8=4\,,$

Consistent with the SIs on the website



3 Calculate the SIs of Magnetic Topological materials.

- Using the CRs and magnetic BRs (MBRs), we reproduce the symmetrybased 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.

 $3.1 \text{ Eu}_3 \ln_2 \text{As}_4 - \text{AFMc}$

The band structures of Eu₃In₂As₄ for the magnetic configuration 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.



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

\$ vim PPOSCAR

EuInAs 1.0 6.82999992370000 0.0000000000000 0.00000000000000 0.000000000000 16.50670051570000 0.00000000000000 0.000000000000 0.000000000000 4.41020011900000 Eu In As 6 4 8 Direct 0.000000000000 0.5000000000000 0.00000000000000 0.500000000000 0.000000000000000 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 0.000000000000000 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"

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	0.0000000000000000000000000000000000000	00 0.0000000000000000000000000000000000
0.0000000000000000000000000000000000000	16.50670051569999	969 0.00000000000000000
0.0000000000000000000000000000000000000	0.0000000000000000000000000000000000000	00 4.4102001189999980
Eu In As		
6 4 8		
Direct		
0.0000000000000000000000	0.5000000000000001	0.00000000000000000
0.500000000000000000000	0.000000000000000000	0.500000000000001
0.7082099910000000	0.6982700230000001	0.00000000000000000
0.2917900090000000	0.3017299770000001	0.00000000000000000
0.7917900090000000	0.1982700230000001	0.500000000000001
0.2082099909999999	0.8017299770000003	0.500000000000000
0.3603799940000000	0.5863000150000001	0.500000000000000
0.6396200060000000	0.4136999850000002	0.500000000000000
0.1396200060000000	0.0863000150000000	0.00000000000000000
0.8603799940000000	0.9136999850000003	0.00000000000000000000
0.7460399870000000	0.5697000030000001	0.500000000000000
0.253960013000000	0.4302999970000001	0.500000000000000
0.753960013000000	0.0697000029999999	0.0000000000000000000000000000000000000
0.2460399870000001	0.9302999970000002	0.0000000000000000000000000000000000000
0.2332900020000000	0.6685100200000001	0.0000000000000000000000000000000000000
0.7667099980000001	0.3314899800000000	0.0000000000000000000000000000000000000
0.2667099980000000	0.1685100200000001	0.5000000000000001
0.7332900019999999	0.8314899800000002	0.5000000000000000000000000000000000000

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 classifications are given below. For each MSG, the detailed information is given in the corresponding MSG table.

OG	setting	BN	S 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	Ø	Ø
58.4.474	Pnnm'	Pnnm'	#58.396	III	Table MSG474	Ø	Ø
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	Ø	Ø
		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		
		$P_C nnm$	#58.403	IV	OG 66 .11.574		
		$P_I nnm$	#58.404	IV	OG 71 .8.628		

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

1 2 POS2MSG (converting PPOSCAR to POSCAP, msg and initializing MAGMOM on magnetic atoms) #SG (1~230 58 #MSG (1~165(): 471 (OG setting) (* paste PPOSCAR below *) generated by phonopy 1.0 6.8299999237000000 16.5067005156999969 4.4102001189999980 Eu In As ĥ Direct 0.50000000000000000 0.000000000000000000 0.500000000000000000 0.7082099910000000 0.6982700230000001 0.2917900090000000 0.3017299770000001 0.7917900090000000 0.1982700230000001 0.50000000000000000 0.2082099909999999 0.8017299770000003 0.500000000000000000 0.3603799940000000 0.5863000150000001 0.50000000000000000 0.639620006000000 0.4136999850000002 0.50000000000000000 0.1396200060000000 0.0863000150000000 0.8603799940000000 0.9136999850000003 0.7460399870000000 0.5697000030000001 0.500000000000000000 0.2539600130000000 0.4302999970000001 0.500000000000000000 0.753960013000000 0.0697000029999999 0.2460399870000001 0.9302999970000002 0.2332900020000000 0.6685100200000001 0.7667099980000001 0.3314899800000000 0.2667099980000000 0.168510020000001 0.50000000000000000 0.7332900019999999 0.831489980000002 0.500000000000000000

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.

3)

POS2MSG

POSCAR msg:				
SG#B 58 OG (58.1.471)	BNS (58.393)	$Ctoo \Lambda$
1.0				
6.8299999237	0000 0.0000	00000000000	0.000000000	
0.000000000	0000 16.5067	0051570000	0.000000000	0000
0.000000000	0000 0.0000	00000000000	4.4102001190	0000
Eu In As				
6 4 8				
Direct				
0.000000000	0000 0.5000	00000000000	0.000000000	0000
0.500000000	0000 0.0000	00000000000	0.500000000	0000
0.7082099910	0000 0.6982	7002300000	0.000000000	0000
0.2917900090	0000 0.3017	2997700000	0.000000000	0000
0.7917900090	0000 0.1982	7002300000	0.500000000	
0.2082099910	0000 0.8017	2997700000	0.500000000	
0.3603799940	0000 0.5863	0001500000	0.500000000	0000
0.6396200060	0000 0.4136	9998500000	0.500000000	$D \cap$
0.1396200060	0000 0.0863	0001500000	0.0000000000	
0.8603799940	0000 0.9136	9998500000	0.0000000000	0000
0.7460399870	0000 0.5697	0000300000	0.500000000	
0.2539600130	0000 0.4302	9999700000	0.500000000	0000 SOI
0.7539600130	0000 0.0697	0000300000	0.0000000000	0000
0.2460399870	0000 0.9302	9999700000	0.0000000000	
0.2332900020	0000 0.6685	1002000000	0.0000000000	
0.7667099980	0000 0.3314	8998000000	0.0000000000	0000
0.2667099980	0000 0.1685	1002000000	0.500000000	0000
0.7332900020	0000 0.8314	8998000000	0.5000000000	0000
INCAR:				The
LSORBIT = T				
LNONCOLLINEAR =	т			
SAXIS = 0 0 1				0 7 20040 0
MAGMOM= 0 0 /	0 0 - 7 0 0		0 0 -7 0	0 -7 300*0.0
KDOTHER.				
MEDOTIME used for	n magnatia ana			
MAPOINIS used to	r magnetic spa	ice group		
0				
0 0000000	0 0000000	0 0000000		м
0.50000000	0.50000000	0 50000000) 10 !G	14
0.5000000	0.5000000	0.0000000) 10 !K	
0.0000000	0.5000000	0 50000000	, 1.0 !s	
0.50000000	0.0000000	0 5000000) 10 11	
0.5000000	0.00000000	0.0000000) 10 IV	
0.0000000	0.5000000	0.00000000) 10 IV	
0.00000000	0.0000000	0.00000000	, T'A IT	

0.50000000

0.00000000

0.00000000

! Z

1.0

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

Then we do VASP calculations.

There is a big gap in the bottom 48 occupied band



"tqc.data"

...

58 8 106
$1 \hspace{0.5mm}9 \hspace{0.5mm}9 \hspace{0.5mm}10 \hspace{0.5mm}10 \hspace{0.5mm}9 \hspace{0.5mm}10 \hspace{0.5mm}9 \hspace{0.5mm}10 $
2 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 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 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 8 910 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 7 910 10 9 8 7
7 9 8 10
6 3 4 3 4 4 3 3 4 4 3 3 4 3 4 3 3 4 3 4
7 3 4 3 4 4 3 4 3 3 4 4 3 3 4 4 3 4 3 4
8 3 4 3 4 4 3 3 4 3 4 3 4 3 4 3 4 3 4 4 4 3 4 3 3 4 4 3 3 4 4 3 3 4 4 3 3 4 4 3 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 3 4 4 4 3 4 4 3 4 4 4 3 4 4 4 3 4 4 4 3 4 4 4 3 4 4 4 3 4 4 4 3 4 4 4 3 4 4 4 3 4 4 3 4 4 4 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 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 ...

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

6) solve compatibility relations (CR) and calculate symmetry indicators (SI) in 1651 magnetic space groups (using tqc.data). #MSG (1~165(): 471 OG setting) 1) (* paste toc.data below *) 106 10 9 10 9 10 9 9 10 10 10 1) Paste tqc.data into this box. Note: valid for 1651 magnetic space groups with spin-orbit coupling ! 3) solve CR () if not, it is a symmetry enforced semimetal) 2) Give the MSG number: 471. cal_SI 3) Press solve_CR button.

4) Press cal_SI button.

solve_CR :

cal_SI: trivial

The input data is calculated with spin-orbit coupling. Satisfy $\ensuremath{\mathsf{CR}}$

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,

 $3.2 \text{ Eu}_3 \ln_2 \text{As}_4 - \text{AFMb}$

- 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 Eu₃In₂As₄ (AFMb) MSG.

The list of results of SG 58 Eu₃ln₂As₄ given by TopMat

	MSG(#OG)	Туре	Configuration	Energy(eV/atom)	SIs
	471	I	AFMc	-6.9430	Z2=0
	472	п	NM	Ø	ø
	473	ш	ZM	Ø	ø
	474	ш	ZM	Ø	ø
Eu ₃ In ₂ As ₄	475	Ш	FMc	-6.9427	Nodal line
SG58			Canted-FM	-6.9428	
	476	ш	FMa	-6.9428	Weyl points
			FMb	-6.9428	
	477	Ш	ZM	ø	Ø

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	0.0000000000000000	0.0000000000000000
0.000000000000000	16.50670051570000	0.000000000000000
0.0000000000000000	0.0000000000000000	4.41020011900000
Eu In As		
6 4 8		
Direct		
0.0000000000000000000000000000000000000	0.50000000000000	0.0000000000000000
0.500000000000000	0.000000000000000	0.50000000000000
0.70820999100000	0.69827002300000	0.0000000000000000
0.29179000900000	0.30172997700000	0.0000000000000000
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	0.000000000000000
0.24603998700000	0.93029999700000	0.00000000000000
0.23329000200000	0.66851002000000	0.00000000000000000
0.76670999800000	0.33148998000000	0.00000000000000000
0.26670999800000	0.16851002000000	0.50000000000000
0.73329000200000	0.83148998000000	0.50000000000000

"POSCAR-add magnetic config"

AFMb				
1.0				
6.82999992370000	0.0000000000000000	0.00000000000000000		
0.0000000000000000	16.50670051570000	0.0000000000000000000000000000000000000		
0.00000000000000000	0.0000000000000000	4.41020011900000		
Eu In As				
6 4 8				
Direct				
0.0000000000000000	0.50000000000000	0.0000000000000000000000000000000000000	0	1 0
0.500000000000000	0.000000000000000	0.500000000000000	0	-10
0.70820999100000	0.69827002300000	0.0000000000000000000000000000000000000	0	1 0
0.29179000900000	0.30172997700000	0.0000000000000000	0	1 0
0.79179000900000	0.19827002300000	0.500000000000000	0	-10
0.20820999100000	0.80172997700000	0.500000000000000	0	-10
0.36037999400000	0.58630001500000	0.500000000000000		
0.63962000600000	0.41369998500000	0.500000000000000		
0.13962000600000	0.08630001500000	0.0000000000000000		
0.86037999400000	0.91369998500000	0.0000000000000000		
0.74603998700000	0.56970000300000	0.500000000000000		
0.25396001300000	0.43029999700000	0.500000000000000		
0.75396001300000	0.06970000300000	0.0000000000000000000000000000000000000		
0.24603998700000	0.93029999700000	0.0000000000000000		
0.23329000200000	0.66851002000000	0.0000000000000000000000000000000000000		
0.76670999800000	0.33148998000000	0.0000000000000000000000000000000000000		
0.26670999800000	0.16851002000000	0.50000000000000		
0.73329000200000	0.83148998000000	0.50000000000000		

- 1) \$ mom2msg > outdir
- 2) \$ phonopy --symmetry --tolerance 0.01 -c POSCAR_msg

ymm 8

> 4 8

We give the MSG classification, number and all operations

Crystalline SG(org.): unitary part (only): unitary +antiunitary:	Int. Pnnm P2_1/c Pnnm	Sch. D2h^12 C2h^5 D2h^12	#SG 58 14 58	#s
Magnetic SG type : Type 1 Magnetic SG number (0G) SG#B 14 0G(58. 6. 470 He: 0.11000000 0.12000000 0.11000000 0.12000000 0.61000000 0.38000000 0.39000000 0.62000000 0.11000000 0.12000000 0.39000000 0.62000000 0.61000000 0.38000000	III (trans : 476 6) 0.150000 0.150000 0.349999 0.650000 0.150000 0.349999 0.650000	01 01 001 001 001 001 001 001 001	eiche)	

"msgout.txt"

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

#9	spg	S	ymm	: 8	
#	1		ur	nit	
	1	0	0	0.00000	
	0	1	0	0.00000	
	0	0	1	0.00000	
#	2		ur	nit	
	-1	0	0	0.00000	
	0	-1	0	0.00000	
	0	0	-1	0.00000	
#	3		ant	ti-unit	
	-1	0	0	0.00000	
	0	-1	0	0.00000	
	0	0	1	0.00000	
#	4		ant	ti-unit	
	1	0	0	0.00000	
	0	1	0	0.00000	
	0	0	-1	0.00000	
#	5		ur	nit	
	1	0	0	0.500000	
	0	-1	0	0.500000	
	0	0	-1	0.500000	
#	6		ur	nit	
	-1	0	0	0.500000	
	0	1	0	0.500000	
	0	0	1	0.500000	
#	7		ant	ti-unit	
	-1	0	0	0.500000	
	0	1	0	0.500000	
	0	0	-1	0.500000	
#	8		ant	ti-unit	
	1	0	0	0.500000	
	0	-1	0	0.500000	
	0	0	1	0.500000	
#9	s ymr	n r	nag,	, #symm:	8

Magnetic SG type : Type III (translationgleiche)

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 classifications are given below. For each MSG, the detailed information is given in the corresponding MSG table.

OG	setting	BNS setting N		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	Ø	Ø
58.4.474	Pnnm'	Pnnm'	#58.396	III	Table $MSG474$	Ø	Ø
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	Ø	Ø
		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		
		$P_I nnm$	#58.404	IV	OG 71 .8.628		

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

2 3) POS2MSG (converting PPOSCAR to POSCAR_meg and initializing MAGMOM on magnetic atoms) #SG (1~2.0): 58 #MSG (1~1661): 476 (OG setting) (* paste PPOSCAR pelow * enerated by phonopy 1.0 6.829999924000000 16.5067005159999987 4.4102001189999998 Eu In As He 6 4 8 8 Direct 0.0000000000000000000 0. 00000000000000000 0.500000000000000000 0.500000000000000000 0.50000000000000000 0.1982700250000000 0.7082099900000000 0.291790010000000 0.8017299750000000 0.791790010000000 0.6982700250000000 0.5000000 0.2082099899999998 0.3017299750000000 0.50000000000000000 0.3603799900000000 0.0863000150000000 0.50000000000000000 0.639620010000000 0.9136999850000000 0.500000000000000000 0.139620010000000 0.5863000150000000 0.8603799900000000 0.4136999850000000 0.7460399900000000 0.0697000050000001 0.253960010000000 0.9302999949999999 0.753960010000000 0.5697000050000001 0.2460399899999999 0.4302999949999999 0.2332900000000000 0.1685100250000000 0.0000000000000000 0.7667100000000000 0.8314899750000000 0.2667100000000000 0.6685100250000000 0.500000000 0.3314899750000000 0.5000000 0.11000000000000000 0.62000005000000 0.150000010000000 0.3799999950000000 0.84999999000000 0.61000000000000000 0.8799999950000000 0.3499999900000000 0.120000050000001 0.650000010000000 0.890000000000000000 0.3799999950000000 0.150000010000000 0.11000000000000000 0.62000005000000 0.8499999900000000 0.39000000000000000 0.1200000050000001 0.3499999900000000 0.61000000000000000 0.8799999950000000 0.650000010000000

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.

POS2MSG

4

3)

SG#B	14	OG	(58	6.47	76)	B	NS	(- 58	3.3	98)					
1.0																		
0.	0000	0000	0000	000	-16.	506	5700	515	700	000		Ο.	000	000	000	0000	00	
6.	8299	9992	2370	000	0.	.000	0000	000	000	000		Ο.	000	000	000	0000	00	
0.	0000	0000	0000	000	16.	506	5700	515	700	000		4.	410	200:	119	9000	00	
Eu	In	1	s	Не														
6	4	-	8	8														
Direct			·															
011000	5000	0000	1000	000	0	000	1000	იიი	nnn	100		n	000	000	nnr	1000	nn	
0.	5000	0000	10000	000	0.	500	10000	000	000	000		n.	5000	0000	000	0000	00	
	2017	2000	7000	000		700	2000	000	000	000		0.	000	0000		0000	00	
	6000	2991	200	000		201	700	221	000	000		÷.	0000	0000		0000	00	
U.	0902	1002	2300	000		291	790	009	000	000		0.	5000			0000	00	
U.	3017	2991		000	U.	. /91	190	009	000	000		υ.	5000			0000	00	
υ.	6982	/002	2300	000	υ.	208	5209	991	000	000		υ.	5000			1000	00	
υ.	9136	9998	500	000	υ.	.360	1379	994	000	000		υ.	500	000	000	1000	00	
0.	0863	0001	1500	000	0.	639	9620	006	000	000		Ο.	500	000	000	0000	00	
0.	9136	9998	3500	000	0.	139	9620	006	000	000		Ο.	000	000	000	0000	00	
0.	0863	0001	1500	000	0.	.860	0379	994	000	000		Ο.	000	000	000	0000	00	
0.	9302	9999	9700	000	0.	.746	5039	987	000	000		Ο.	500	000	000	0000	00	
0.	0697	0000	0300	000	0.	253	3960	013	000	000		Ο.	500	0000	000	0000	00	
0.	9302	9999	9700	000	0.	753	3960	013	000	000		Ο.	000	000	000	0000	00	
0.	0697	0000	0300	000	0.	246	5039	987	000	000		Ο.	000	000	000	0000	00	
0.	3314	8998	8000	000	0.	233	3290	002	000	000		Ο.	000	000	000	0000	00	
0.	6685	1002	2000	000	0.	766	5709	998	000	000		Ο.	000	000	000	0000	00	
0.	3314	8998	8000	000	0.	266	5709	998	000	000		Ο.	500	000	000	0000	00	
0.	6685	1002	2000	000	0.	733	3290	002	000	000		Ο.	500	000	000	0000	00	
0.	0300	0001	000	000	0.	110	0000	000	000	000		Ο.	150	000	010	0000	00	
0.	9699	9999	000	000	0.	890	0000	000	000	000		٥.	849	999	990	0000	00	
0.	9699	9999	000	000	0.	610	0000	000	000	000		٥.	349	999	990	0000	00	
	0300	0001	000	000		390	1000	nnn	nnn	100		n.	650	nnni	110	0000	nn	
0	2700	0001	000	000		807	0000	000	000	000		n.	150	000	110	0000	00	
	7200	0000	2000	000		110	0000	000	000	000		<u> </u>	840	000	0010	0000	00	
	7200	0000	0000	000		200	0000	000	000	000		0.	240	000	000	0000	00	
	0700	2222	0000	000		610	0000	000	000	000		0.	249	999:	990	0000	00	
υ.	2700	0001		000	υ.	. 010	0000	000	000	000		υ.	6001	0000	UTU	1000	UU	
INCAR:																		
LSORB1	T =	Т																
LNONCO	DLLIN	EAR	= T															
SAXIS	= 0	01																
MAGMON	1= 7	7	0	7 -7	0	7	7	0	7	7	0	7	-7	0	7	-7	0	300*0.0
KPOINT	'S:																	
MRPOIN	ITS u	sed	for	magn	netic	s sp	ace	gr	ou	,								
8																		
rec																		
0.	5000	0000)	0.00	00000	000	1	0.5	000	0000	00		1.0		!	А		
0.	0000	0000)	0.00	00000	000		0.5	000	000	00		1.0			в		
0.	5000	0000)	0.50	0000	000		0.0	000	000	00		1.0		1	C		
0	0000	0000	1	0.50	10000	100		0.5	000	1000	10		1.0		i.	D		
0	5000	0000	1	0.50	10000	100		0.5	000	1000	10		1.0		i	Ē		
0.	0000	0000	í	0.00	10000	100		0.0	000	1000	10		1 0			GM		
0.	5000	0000		0.00	10000	100		0.0	000	1000	10		1 0		-	v		
0.	0000	0000		0.00	10000	000		0.0	000	1000	10		1.0		-	7		
υ.	0000	υυυι	,	0.90	10000	000		0.0	υυι	1000	0		1.0		1	4		

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.

I	N	C.	A.	R	:
т	c	O.	D	R	1

POSCAR msg:

INCAR:							
LSORBIT = T							
LNONCOLLINEAR =	Т						
SAXIS = $0 \ 0 \ 1$							
MAGMOM= 0 7 0	0 -7	0 0	7 0	07(0 -7	0 0 -7	0 300*0.0

POSCAL	R_msg:								
SG#B	14	OG	(58.6	.476)	BNS	(58.398)
1.0									
0	.00000	0000	00000	- 00	16.500	570051	57000	00	0.00000000000000
6	.82999	9992	37000	00	0.000	000000	00000	00	0.00000000000000
0	.00000	0000	00000	00	16.500	570051	57000	00	4.41020011900000
Eu	In	A	s						
6	4		8						
Direct	t								
0	. 50000	0000	00000	00	0.000	000000	00000	00	0.00000000000000
0	.50000	0000	00000	00	0.500	000000	00000	00	0.50000000000000
0	.30172	2997	70000	00	0.708	320999	10000	00	0.00000000000000
0	. 69821	7002	30000	00	0.291	179000	90000	00	0.00000000000000
0	.30172	2997	70000	00	0.791	179000	90000	00	0.50000000000000
0	. 69821	7002	30000	00	0.208	320999	10000	00	0.50000000000000
0	.91369	9998	50000	00	0.360	37999	40000	00	0.50000000000000
0	.08630	0001	.50000	00	0.639	62000	60000	00	0.50000000000000
0	.91369	9998	50000	00	0.139	62000	60000	00	0.00000000000000
0	.08630	0001	.50000	00	0.860	37999	40000	00	0.00000000000000
0	.93029	9999	70000	00	0.746	503998	70000	00	0.50000000000000
0	.06970	0000	30000	00	0.253	396001	30000	00	0.50000000000000
0	.93029	9999	70000	00	0.753	396001	30000	00	0.00000000000000
0	.06970	0000	30000	00	0.246	503998	70000	00	0.00000000000000
0	.33148	3998	00000	00	0.233	329000	20000	00	0.00000000000000
0	. 66851	L002	00000	00	0.766	570999	80000	00	0.00000000000000
0	.33148	3998	00000	00	0.266	570999	80000	00	0.50000000000000
0	. 66851	1002	00000	00	0.733	329000	20000	00	0.50000000000000

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 = TLNONCOLLINEAR = T SAXIS = 0 0 1MAGMOM= 0 7 0 -7 0 -7 0 0 -7 0 300*0.0 ... 0 0 0 0 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 ! C 1.0 0.00000000 0.50000000 0.50000000 1.0 ! D 0.50000000 0.50000000 0.50000000 ! E 1.0 0.00000000 0.00000000 0.00000000 1.0 ! GM 0.00000000 0.50000000 0.00000000 1.0 ! Y

0.00000000

1.0

! Z

0.00000000

0.50000000

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 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
556567878787856567878565656565656787878567856
656567878566578875678567856565656877885767878657865
7565678785656787878787856565656785678565878567856
8 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 ...

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.

solve_CR :

The input data is calculated with spin-orbit coupling. Satisfy $\ensuremath{\mathsf{CR}}$

cal_SI :

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



4 Calculate the SIs by IR2TB.

Here we take the topological material Bi₂Se₃ 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 Bi₂Se₃ with SOC



Nature Physics volume 5, pages438–442 (2009)

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

"POSCAR"

Bi2 Se3 1.0	
2.0669999122654712 1.1933829557614029 9.5433330536000	032
-2.0669999122654712 1.1933829557614029 9.5433330536000	032
0.00000000000000 -2.3867659115228057 9.5433330536000	032
Bi Se	
2 3	
Direct	
0.3980000423333330 0.3980000423333330 0.3980000423333331	
0.60199995766666670 0.60199995766666670 0.6019999576666668	
0.00000000000000 0.00000000000000 0.000000	
0.791999993999998 0.791999993999998 0.791999993999998	
0.20800006000003 0.20800006000003 0.20800006000003	

"PPOSCAR"

generated by phonopy	
1.0	
2.0669999122654712	2 1.1933829557614026 9.5433330536000014
-2.066999912265471	2 1.1933829557614026 9.5433330536000014
-0.000000000000000	1 -2.3867659115228053 9.5433330536000014
Bi Se	
2 3	
Direct	
0.3980000423333330	0.3980000423333333 0.3980000423333333
0.6019999576666670	0.60199995766666669 0.60199995766666670
0.00000000000000000	0.0000000000000 0.000000000000000000000
0.7919999939999998	0.7919999940000000 0.7919999940000000
0.20800006000002	0.20800006000005 0.20800006000004

phonopy_version: '2.20.0'

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

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



4)

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.

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.

AR msg	r:								
166	OG	(166	2.1328)	BNS	(166.98)		
0									
2.0669	9991	22	6547	1.193	382955	676140	9.543	33305	360000
2.0669	9991	22	6547	1.193	382955	676140	9.543	33305	360000
0.0000	0000	000	0000	-2.386	765911	52281	9.543	33305	360000
i Se	•								
2 3	;								
ct									
0.3980	0004	1233	3333	0.398	000042	33333	0.398	00004	233333
0.6019	9995	576	6667	0.601	999957	66667	0.601	99995	766667
0.0000	0000	000	0000	0.000	000000	00000	0.000	00000	000000
0.7919	9999	9400	0000	0.791	999994	00000	0.791	99999	400000
0.2080	0000	600	0000	0.208	000006	500000	0.208	00000	600000
R: BIT = COLLIN S = 0 OM=300	T IEAR 0 1 0*0.0	= !	P						
NTS:									
INTS u	sed	foi	r mag	metic spa	ace gr	coup			
0.0000	0000)	0.0	00000000	0.0	0000000	0 1.0	!	GM
0.5000	0000)	0.5	50000000	0.5	0000000	0 1.0	!	т
0.5000	0000)	0.5	50000000	0.0	0000000) 1.0	!	F
0.0000	0000)	0.5	50000000	0.0	0000000) 1.0	!	L
	$\begin{array}{l} \text{R} \\ \text{msg} \\ 166 \\ 0 \\ 2.0669 \\ 2.0669 \\ 0.0000 \\ i \\ \text{Set} \\ 0.3980 \\ 0.6019 \\ 0.6019 \\ 0.6019 \\ 0.6019 \\ 0.0000 \\ 0.7919 \\ 0.2080 \\ \text{R}: \\ \text{BIT} = \\ \text{COLLIN} \\ \text{S} = 0 \\ 0.2080 \\ \text{R}: \\ \text{BIT} = \\ \text{COLLIN} \\ \text{S} = 0 \\ 0.4000 \\ 0.5000 \\ 0.5000 \\ 0.5000 \\ 0.5000 \\ 0.0000 \\ 0.5000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\$	AR msg: 166 OG 0 2.066999991 2.06699991 0.00000000 i Se 2 3 ct 0.39800004 0.601999995 0.000000000 0.791999995 0.208000000 R: BIT = T COLLINEAR S = 0 1 OM=300*0.0 NTS: INTS used 0.00000000 0.50000000 0.50000000	AR msg: 166 OG (0 2.066999991220 2.066999991220 0.000000000000 i Se 2 3 ct 0.39800004233 0.60199995760 0.0000000000 0.79199999400 0.208000000000 0.208000000000 R: BIT = T COLLINEAR = 2 S = 0 0 1 OM=300*0.0 NTS: INTS used for 0.00000000 0.50000000 0.50000000 0.50000000	AR msg: 166 OG (166. 0 2.066999991226547 2.066999991226547 0.000000000000000 i Se 2 3 ct 0.39800004233333 0.60199995766667 0.0000000000 0.79199999400000 0.2080000000000 R: BIT = T COLLINEAR = T S = 0 0 1 OM=300*0.0 NTS: INTS used for mag 0.00000000 0.9 0.5000000 0.9 0.5000000 0.9	AK msg: 166 OG (166.2.1328) 0 2.06699991226547 1.193 2.06699991226547 1.193 0.00000000000000 -2.386 i Se 2 3 ct 0.39800004233333 0.398 0.60199995766667 0.601 0.000000000000 0.000 0.79199999400000 0.791 0.2080000600000 0.208 R: BIT = T COLLINEAR = T S = 0 0 1 OM=300*0.0 NTS: INTS used for magnetic sp 0.0000000 0.5000000 0.5000000 0.5000000	AK msg: 166 OG (166.2.1328) BNS 0 2.06699991226547 1.193382955 2.06699991226547 1.193382955 0.0000000000000 -2.386765911 i Se 2 3 ct 0.39800004233333 0.398000042 0.60199995766667 0.601999957 0.000000000000 0.00000000 0.79199999400000 0.791999994 0.20800000600000 0.208000006 R: BIT = T COLLINEAR = T S = 0 0 1 OM=300*0.0 NTS: INTS used for magnetic space gr 0.00000000 0.0000000 0.00 0.5000000 0.5000000 0.5000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.50000000 0.500000000	AK msg: 166 OG (166.2.1328) BNS (0 2.06699991226547 1.19338295576140 2.06699991226547 1.19338295576140 0.0000000000000 -2.38676591152281 i Se 2 3 ct 0.39800004233333 0.39800004233333 0.60199995766667 0.60199995766667 0.00000000000 0.0000000000 0.7919999940000 0.79199999400000 0.208000060000 0.2080000600000 R: BIT = T COLLINEAR = T S = 0 0 1 OM=300*0.0 NTS: INTS used for magnetic space group 0.0000000 0.5000000 0.5000000 0.5000000 0.5000000 0.0000000	AK msg: 166 OG (166.2.1328) BNS (166.98) 0 2.06699991226547 1.19338295576140 9.543 2.06699991226547 1.19338295576140 9.543 0.0000000000000 -2.38676591152281 9.543 i Se 2 3 ct 0.39800004233333 0.39800004233333 0.398 0.60199995766667 0.60199995766667 0.601 0.00000000000 0.0000000000 0.000 0.79199999400000 0.79199999400000 0.791 0.20800000600000 0.20800000600000 0.208 R: BIT = T COLLINEAR = T S = 0 0 1 OM=300*0.0 NTS: INTS used for magnetic space group 0.0000000 0.0000000 0.0000000 1.0 0.5000000 0.5000000 0.0000000 1.0 0.5000000 0.5000000 0.0000000 1.0 0.5000000 0.5000000 0.0000000 1.0 0.0000000 0.5000000 0.0000000 1.0 0.00000000 0.5000000 0.0000000 1.0 0.00000000 0.5000000 0.0000000 1.0 0.0000000 0.5000000 0.0000000 1.0 0.0000000 0.5000000 0.0000000 1.0 0.0000000 0.5000000 0.0000000 1.0 0.0000000 0.5000000 0.0000000 1.0 0.00000000 0.5000000 0.0000000 1.0 0.00000000 0.5000000 0.0000000 1.0 0.00000000 0.5000000 0.0000000 0.00000000	AK msg: 166 OG (166.2.1328) ENS (166.98) 0 2.06699991226547 1.19338295576140 9.543333053 2.06699991226547 1.19338295576140 9.543333053 0.0000000000000 -2.38676591152281 9.543333053 i Se 2 3 ct 0.3980004233333 0.3980004233333 0.398000042 0.60199995766667 0.60199995766667 0.60199995 0.000000000000 0.0000000000 0.00000000 0.79199999400000 0.79199999400000 0.79199999 0.20800000600000 0.2080000600000 0.20800000 R: BIT = T COLLINEAR = T S = 0 0 1 OM=300*0.0 NTS: INTS used for magnetic space group 0.0000000 0.0000000 0.0000000 1.0 ! 0.5000000 0.5000000 0.0000000 1.0 !

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 Bi₂Se₃ TB model considering soc (or generated by wannier90)

\$ ir2tb -sg 166 -nb 1 18 > outir \$ vim tqc.data The constructed TB model only considers p-orbital, so there are only 18 occupation bands in Bi_2Se_3 .

"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
 5
 6
 7
 8

 5
 7
 8
 7
 8
 5
 6
 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 ...

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

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



4) Press cal_SI button.

solve_CR :

cal_SI :

The input data is calculated with spin-orbit coupling. Satisfy $\ensuremath{\mathsf{CR}}$

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 !!!