Hands-on Diagnose Unconventional Materials

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

Ref:

Gao, J. et al. "IRVSP: to obtain irreducible representations in the VASP", Comput. Phys. Comm. 261, 107760 (2021).
Gao, J. et al. "Unconventional materials: the mismatch between electronic charge centers and atomic positions", Sci. Bull. 67, 598 (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 Solve the EBR/ABR decomposition.
- 3 Example 1: Diagnose unconventional material 1H-$NbSe_2$.
- 4 Example 2: Calculate BAs phonon Irreps.

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**

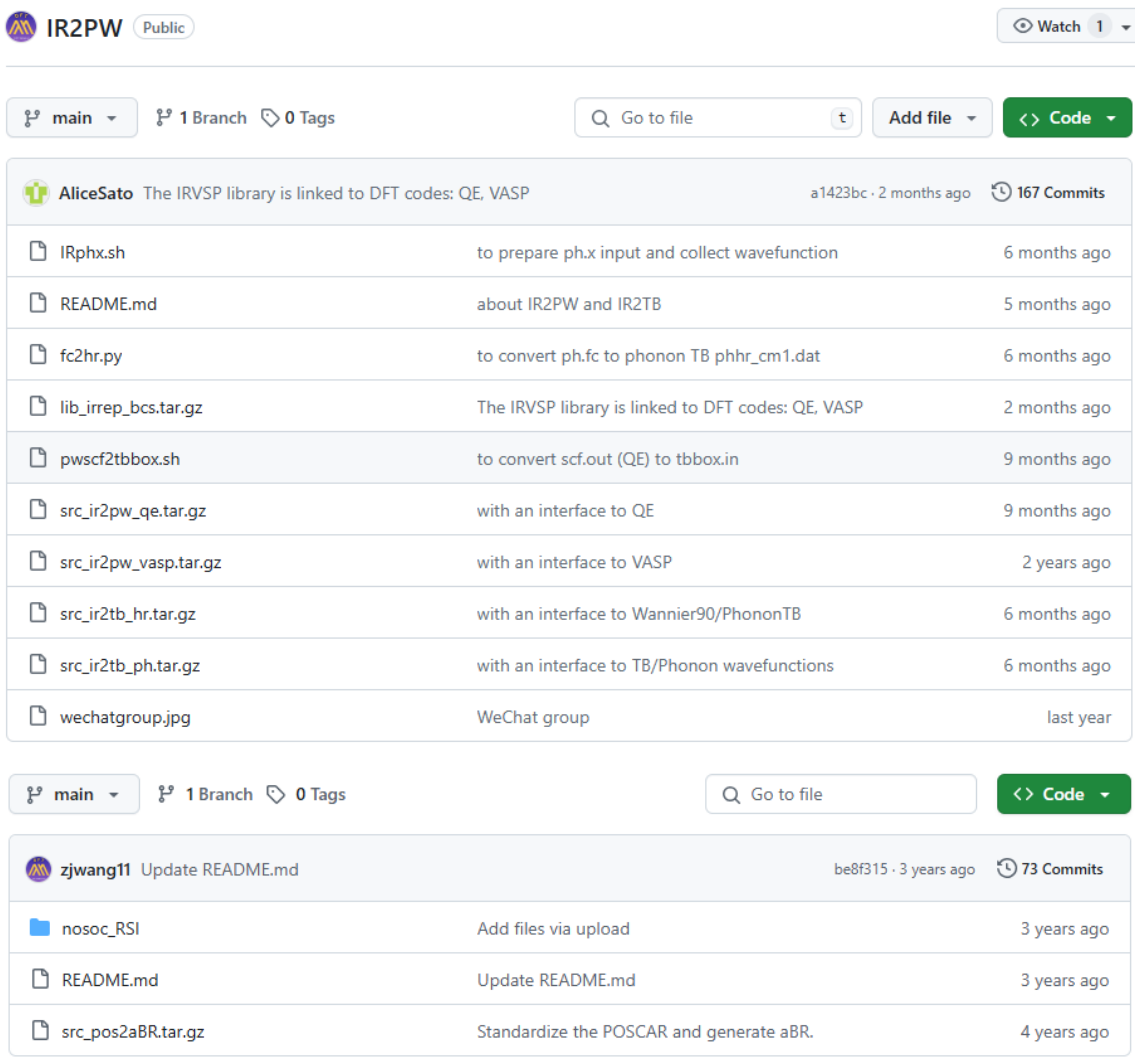
```
$ tar -zxvf src_ir2tb_hr.tar.gz
$ cd src_ir2tb_hr
$ make
$ cd ../
```

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

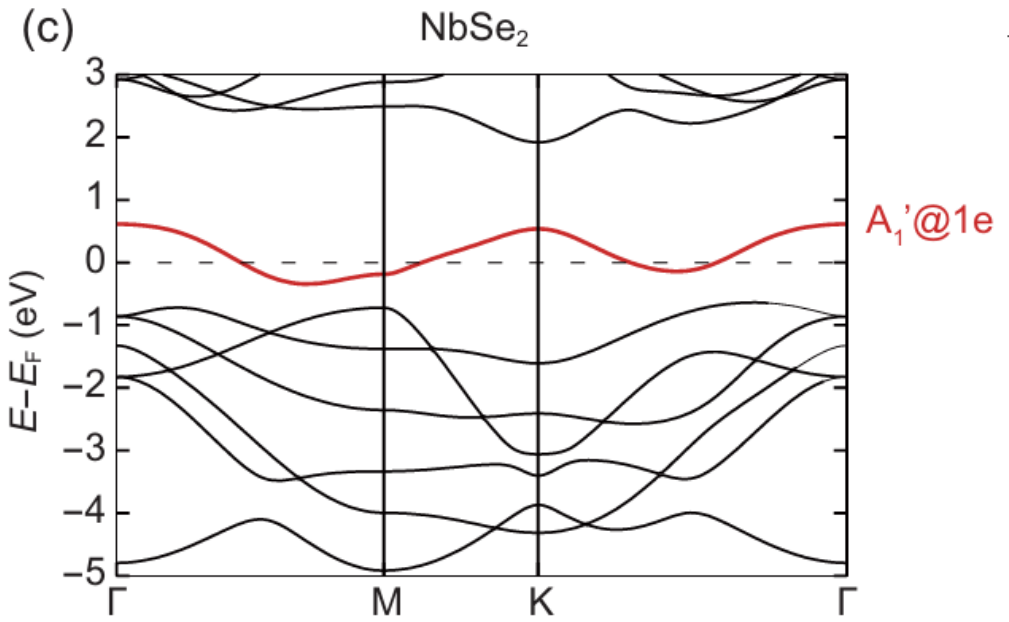
2 Solve the EBR/ABR decomposition

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

3 Example 1: Diagnose unconventional material 1H-$NbSe_2$.

- Here we take the unconventional material 1H-$NbSe_2$ as an example to introduce how to calculate Irreps to solve ABR decompositions to diagnose unconventional materials / obstructed atomic limit materials.

Band structure for $NbSe_2$ without SOC



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

Step 1

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

"POSCAR"

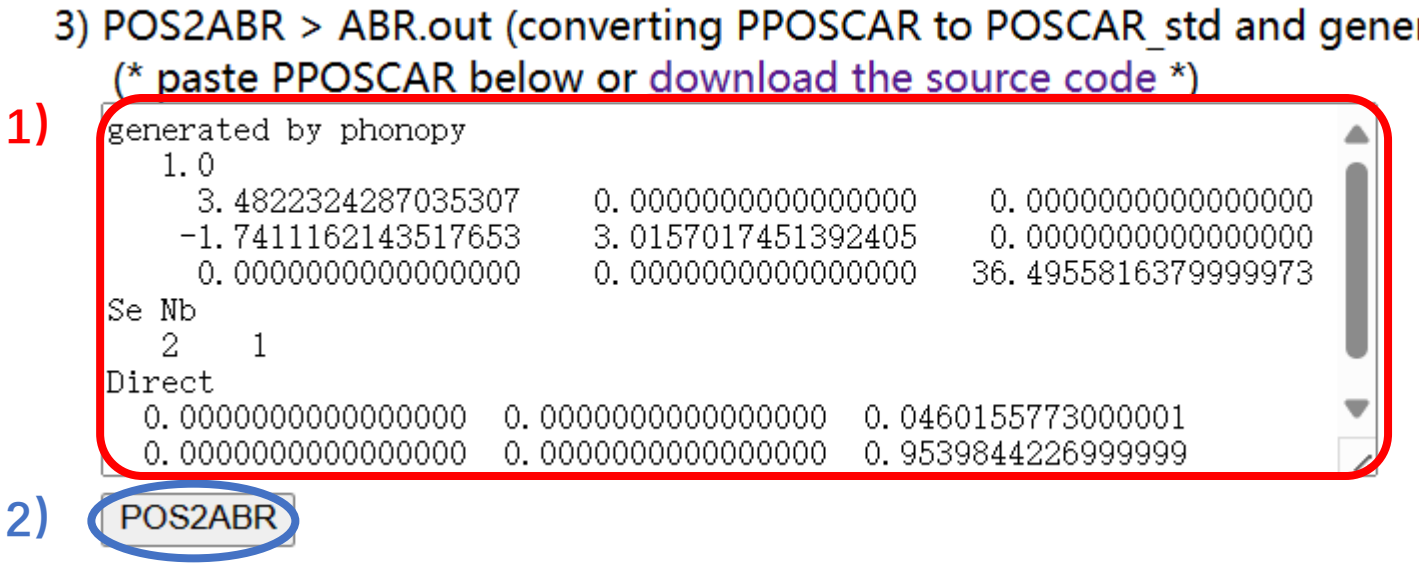
```
qe relaxed
1.0
   3.482232429  -0.000000000   0.000000000
  -1.741116214   3.015701745   0.000000000
  -0.000000000  -0.000000000  36.495581638
Se Nb
2 1
Direct
 0.333332986   0.666666985  0.0460155773000000
 0.333332986   0.666666985  0.9539844227000000
 0.666666985   0.333332986  0.0000000000000000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

"PPOSCAR"

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

Step 2

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



1) Paste PPOSCAR into this box.

2) Press POS2ABR button.

Step 3

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

Copy the content in the red box to POSCAR.

```
POSCAR std :
SG 187  0.000  0.000  0.000 :Generated by pos2aBR for irvsp!
    1.0
     3.4822324287035307     0.0000000000000000     0.0000000000000000
    -1.7411162143517653     3.0157017451392405     0.0000000000000000
     0.0000000000000000     0.0000000000000000    36.4955816379999973
 Se  Nb
   2   1
Direct
  0.0000000000000000  0.0000000000000000  0.0460155773000001
  0.0000000000000000  0.0000000000000000  0.9539844226999999
  0.3333333333333334  0.6666666666666667  0.0000000000000000
```

Step 4

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

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

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

"KPOINTS_187.txt"

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

Step 5

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

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

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

"tqc.data"

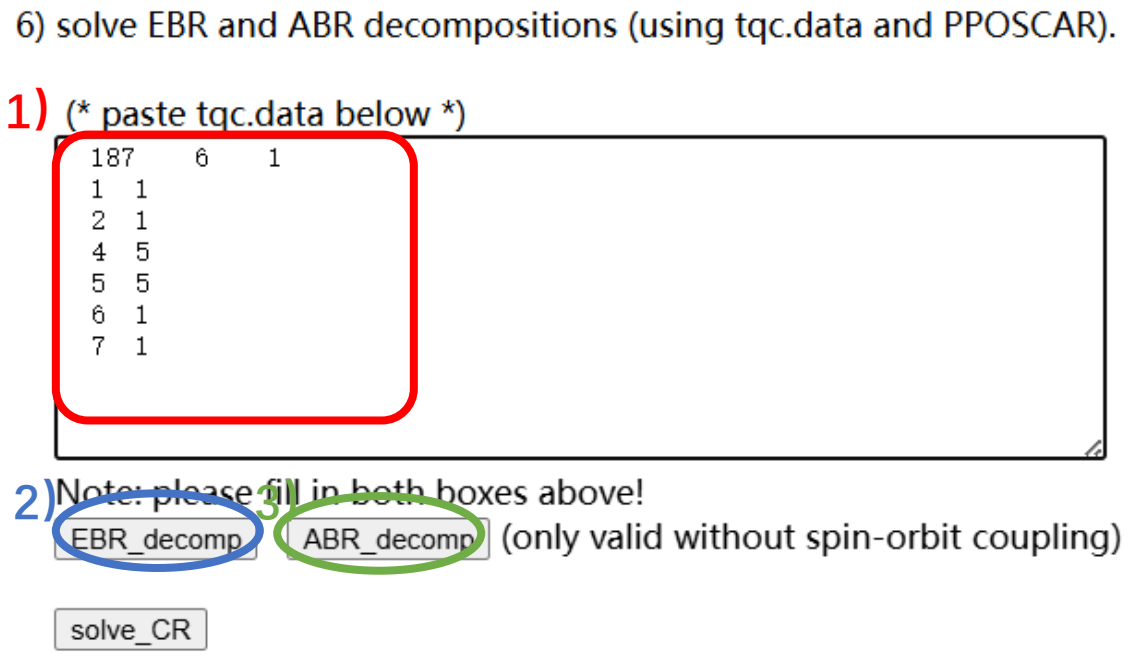
```
187   6   1
1  1
2  1
4  5
5  5
6  1
7  1
```

Format of tqc.data

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

Step 6

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



1) Paste tqc.data into this box.

2) Press EBR_decomp button.

3) Press ABR_decomp button.

Step 7

2) Press EBR_decomp button.

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

topologically trivial

Step 8

3) Press ABR_decomp button

The Irreps induced by atomic-orbital

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

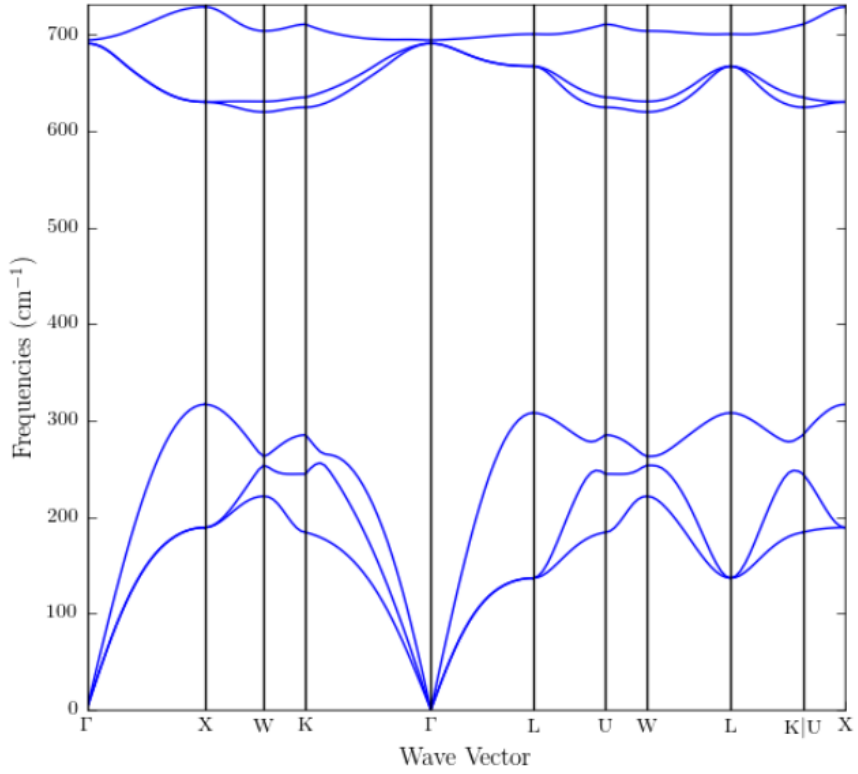
```
There are 1 solutions for eBR decomposition.

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

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

unconventional material

4 Example 2: Calculate BAs phonon Irreps.

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

- Here we take the BAs as an example to introduce how to calculate phonon Irreps to solve ABR decompositions to diagnose unconventional materials.



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

Step 1

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

"POSCAR"

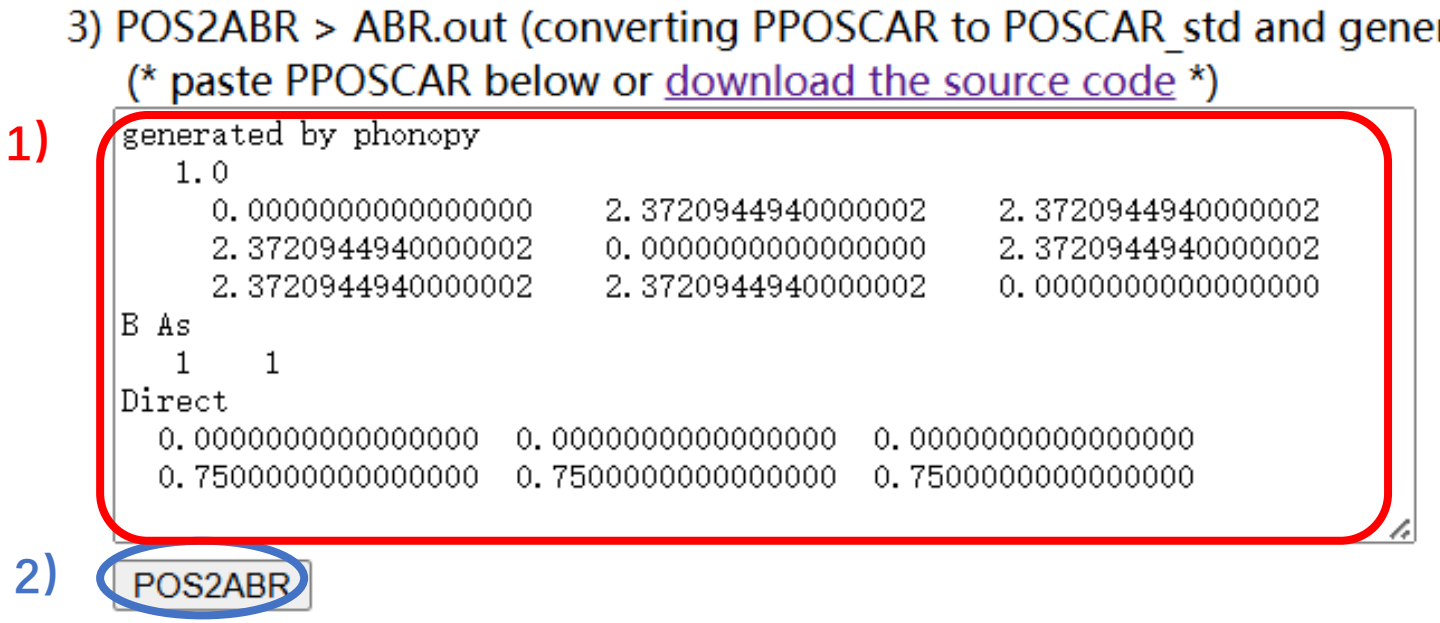
```
qe relaxed
 1.0
   0.000000000   2.372094494   2.372094494
   2.372094494   0.000000000   2.372094494
   2.372094494   2.372094494  -0.000000000
B As
1 1
Direct
        0.0000000000       0.0000000000       0.0000000000
        0.2500000000       0.2500000000       0.2500000000
```

"PPOSCAR"

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

Step 2

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



1) Paste PPOSCAR into this box.

2) Press POS2ABR button.

Step 3

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

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

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

Step 4

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

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

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

"KPOINTS_216.txt"

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

Step 5

```
tbbox.in for BAs:

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

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

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


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

Generate tbbox.in using the scf output file of QE

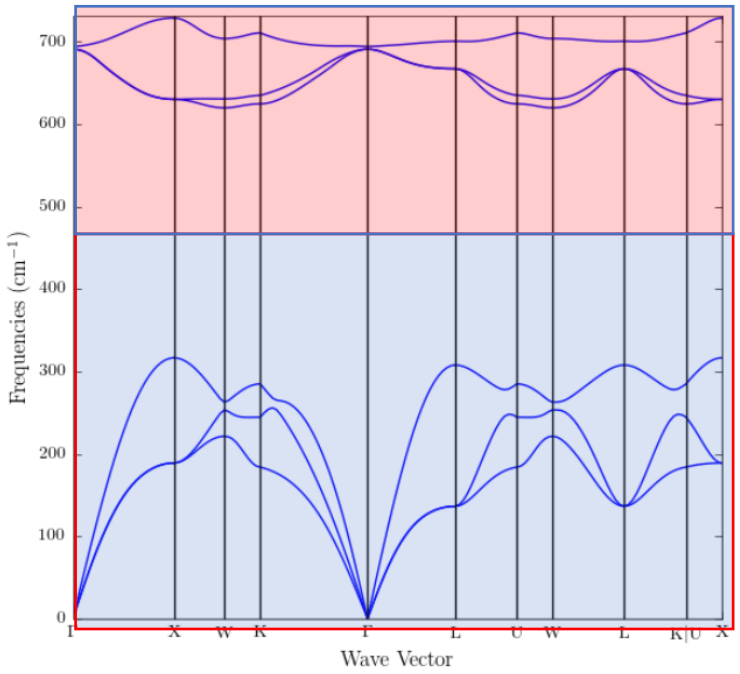
$ pwscf2tbbox.sh 216

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

Step 6

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

```
$ python dyn2wf.py 4
$ ir2ph -sg 216 –nb 1 6 > outir
$ vim tqc.data
```



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

"tqc.data"

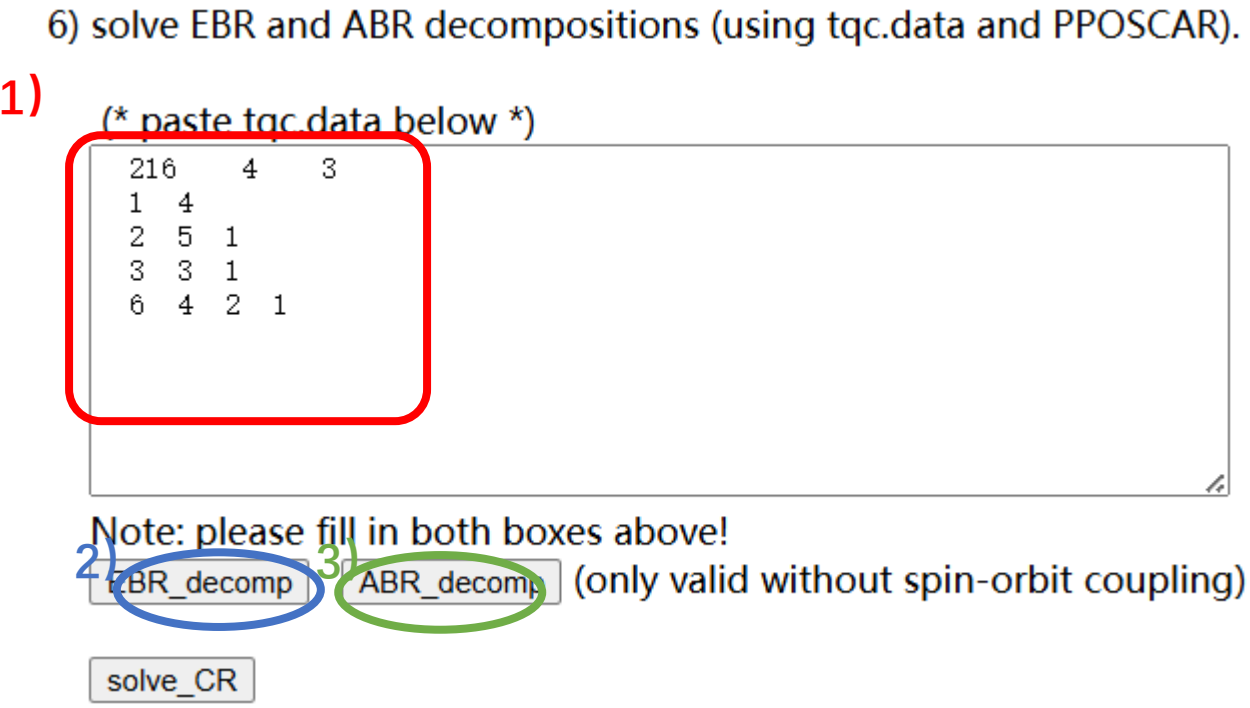
```
216   4   6
1  4  4
2  5  1  5  3
3  3  1  3  1
6  4  2  1  3  2  4
```

Format of tqc.data

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

Step 7

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



1) Paste tqc.data into this box.

2) Press EBR_decomp button.

3) Press ABR_decomp button.

Step 8

2) Press EBR_decomp button.

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

topologically trivial

Step 9

3) Press ABR_decomp button.

The Irreps induced by atomic-orbital

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

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

There are 1 solutions for eBR decomposition.

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

Atomic insulator

Thank you !!!