

Topological Quantum Chemistry and its applications

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Check any material by yourself

The open-source code VASP2Trace and end-user button CheckTopologicalMat are available online at <http://www.cryst.ehu.es/cryst/checktopologicalmat>.

1. Obtain the eigenstates at several k-points. (VASP)
2. Compute the irreps from the eigenstates. (“irvsp”, “vasp2trace”)
 - a. Download “vasp2trace” : www.cryst.ehu.es/cryst/checktopologicalmat, which includes a folder of “max_KPOINTS_VASP/” and a source code of “src_trace_v1.tar.gz”
 - b. Install “vasp2trace” with the source: vasp2trace/src_trace_v1.tar.gz
3. Solve the compatibility relations: semimetal or **Insulator**. (“checktopologicalmat”).
Insulator: check If it's can be decomposed into a sum of EBRs.
(Yes: Trivial **No: Topological**)
Topological: Compute the symmetry indicators

Ref: Vergniory, M.G., et al., “A complete catalogue of high-quality topological materials”, Nature, 566, 480-485 (2019)

www.cryst.ehu.es/cryst/checktopologicalmat

Check Topological Mat

Check Topological Mat.

Given a file that contains the eigenvalues at each maximal k-vec of a space group, the program gives the set of irreducible representations at each maximal k-vec (time-reversal is assumed). Then, using the compatibility relations and the set of Elementary Band Representations (EBRs), it checks whether the set of bands can be put as linear combinations of EBRs. This (self-explanatory) file shows the format of the file to be uploaded in the menu on the right:

File_Description

You can download examples of input files here:

[Example_Ag1Ge1Li2](#)

[Example_Ag1O2Sc1](#)

[Example_B2Ca3Ni7](#)

[Example_of_Bad_File](#)

[Example_Ba3Ca1O9Ru2](#)

You can generate the "trace.txt" file in your own computer using VASP and this program (fortran).

[vasp2trace](#)

Read the "README.pdf" file for help on the use of vasp2trace.

If you are using "Check Topological Mat." and/or "vasp2trace" programs in the preparation of an article, please cite this reference:

M.G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B.A. Bernevig, Z. Wang
Nature(2019) **566**, 480-485. doi:10.1038/s41586-019-0954-4

Upload your traces.txt file (see the help in the column on the left).

选取文件 未选择文件

Show

Ex: Bi₂Se₃

- 1. The SG number(166) and crystal structure.
(run “Phonopy” to make sure the POSCAR is given in a standard setting.)
- 2. Get the high-symmetry k points for that SG (166).
(Vasp2trace/max_KPOINTS_VASPKPOINTS_166.txt).
- 3. Run “VASP”, to obtain the eigen-states(WAVECAR) at those kpoints.
(check the symmetry operators in OUTCAR, simply by counting the total number of the operators)
- 4. Run “vasp2trace” that you have just installed locally in the folder.
(trace.txt would be generated automatically)
- 5. Upload “trace.txt” and press the button.

Step 1:

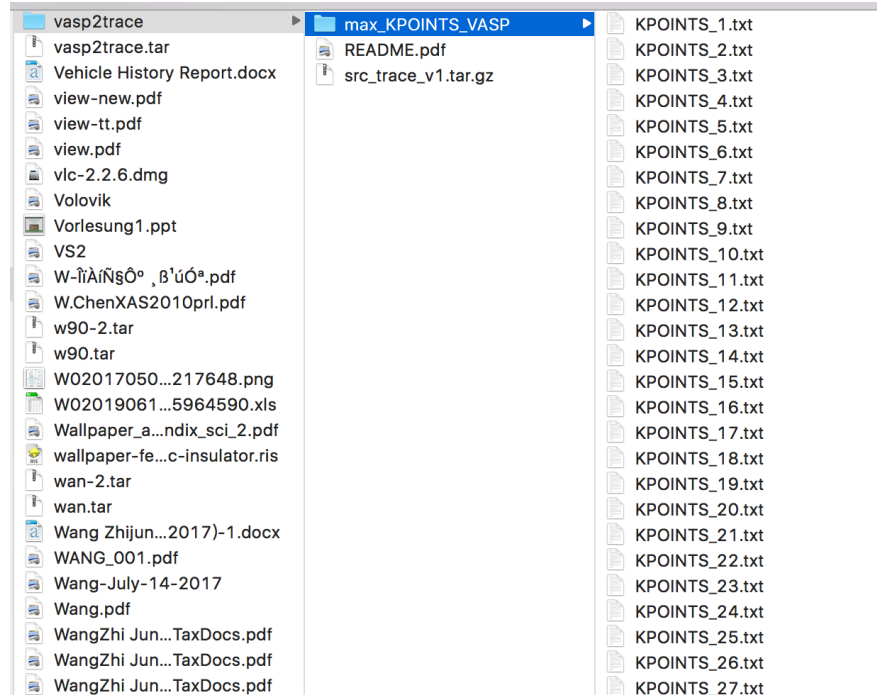
```
$ phonopy --tolerance 0.01 --symmetry -c POSCAR
```

```
$ cp PPOSCAR POSCAR
```

```
/anaconda3/bin/phonopy --tolerance 0.01 --symmetry -c POSCAR
phonopy_version: '1.13.2'
space_group_type: 'R-3m'
space_group_number: 166
point_group_type: '-3m'
space_group_operations:
- rotation: # 1
  - [ 1, 0, 0]
  - [ 0, 1, 0]
  - [ 0, 0, 1]
  translation: [ 0.00000, 0.00000, 0.00000 ]
- rotation: # 2
  - [-1, 0, 0]
  - [ 0, -1, 0]
  - [ 0, 0, -1]
  translation: [ 0.00000, 0.00000, 0.00000 ]
```

Step 2:

\$ cp xx/vasp2trace/max_KPOINTS_VASP/KPOINTS_166.txt KPOINTS.high



Step 3:

Follow README in the folder VASP2trace

a. Run the scf calculation in vasp

b. Run the band calculation in vasp with KPOINTS.high

\$ vim OUTCAR; :/ irot

399 Automatic generation of k-mesh.

400 Space group operators:

401	irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
402	1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000
403	2	-1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000
404	3	1.000000	180.000000	0.866025	0.500000	0.000000	0.000000	0.000000	0.000000
405	4	-1.000000	180.000000	0.866025	0.500000	0.000000	0.000000	0.000000	0.000000
406	5	1.000000	120.000000	0.000000	0.000000	-1.000000	0.000000	0.000000	0.000000
407	6	-1.000000	120.000000	0.000000	0.000000	-1.000000	0.000000	0.000000	0.000000
408	7	1.000000	179.999999	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000
409	8	-1.000000	179.999999	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000
410	9	1.000000	120.000000	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000
411	10	-1.000000	120.000000	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000
412	11	1.000000	180.000000	0.866025	-0.500000	0.000000	0.000000	0.000000	0.000000
413	12	-1.000000	180.000000	0.866025	-0.500000	0.000000	0.000000	0.000000	0.000000

414

415 Subroutine IBZKPT returns following result:

Step 4:

\$ vasp2trace / vasp2trace \$nele

```
1 28
2 1
3 12
4 1 0 0 0 1 0 0 0 1 0.000000 0.000000 0.000000 1.000000 0.000000 0.000000 0.0000
5 -1 0 0 0 -1 0 0 0 -1 0.000000 0.000000 0.000000 1.000000 0.000000 0.000000 0.0000
6 -1 0 0 0 0 -1 0 -1 0 0.000000 0.000000 0.000000 0.000000 0.000000 0.500000 0.8660
7 1 0 0 0 0 1 0 1 0 0.000000 0.000000 0.000000 0.000000 0.000000 0.500000 0.8660
8 0 0 1 1 0 0 0 1 0 0.000000 0.000000 0.000000 0.500000 -0.866025 0.000000 0.0000
9 0 0 -1 -1 0 0 0 -1 0 0.000000 0.000000 0.000000 0.500000 -0.866025 0.000000 0.0000
10 0 -1 0 -1 0 0 0 0 -1 0.000000 0.000000 0.000000 0.000000 0.000000 1.000000 0.0000
11 0 1 0 1 0 0 0 0 1 0.000000 0.000000 0.000000 0.000000 0.000000 1.000000 0.0000
12 0 1 0 0 0 1 1 0 0 0.000000 0.000000 0.000000 0.500000 0.866025 0.000000 0.0000
13 0 -1 0 0 0 -1 -1 0 0 0.000000 0.000000 0.000000 0.500000 0.866025 0.000000 0.0000
14 0 0 -1 0 -1 0 -1 0 0 0.000000 0.000000 0.000000 0.000000 0.000000 -0.500000 0.8660
15 0 0 1 0 1 0 1 0 0 0.000000 0.000000 0.000000 0.000000 0.000000 -0.500000 0.8660
16 4
17 0.000000 0.000000 0.000000
18 0.500000 0.500000 0.500000
19 0.500000 0.500000 0.000000
20 0.000000 0.500000 0.000000
21 12
22 1 2 3 4 5 6 7 8 9 10 11 12
23 1 2 -9.773922 2.000000 0.000000 2.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.0
24 3 2 -8.564873 2.000000 0.000000 -2.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.0
```


Step 5:

Topological Mat

Upload your traces.txt file (see the help in the column on the left)

trace.txt

Result of the analysis of the uploaded structure

- The material is a topological insulator.
- List of topological indices:
 $z_{2w,1}=0$
 $z_{2w,2}=0$
 $z_{2w,3}=0$
 $z_4=3$
- The material belongs to the strong topological class: 6
- Clicking on [See the irreps](#) you can see the details about the number of bands and the identified irreps at each maximal k-vector.
- The set of bands can be put as linear combination of Elementary Band Representations (EBR) and parts of decomposable EBRs with integer positive coefficients. Click on [Linear Combinations](#) to get some possible linear combinations of EBRs and partial EBRs.
- Click on [Subgroups](#) to check the topological character of the structure in each of its (translationengleiche) subgroups.

Take-home message

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欢迎各位学生学者联系我们 (wzj@iphy.ac.cn) , 来本组学习访问! !

Thanks for your attention!