Topological Quantum Chemistry and its applications in materials search

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http://edu.iphy.ac.cn/moreintro.php?id=1250

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 and “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. For more versions of “vasp2trace”, please refer to https://github.com/zjwang11/irvsp.

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 contain 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
$ vim PPOSCAR
$ cp PPOSCAR POSCAR

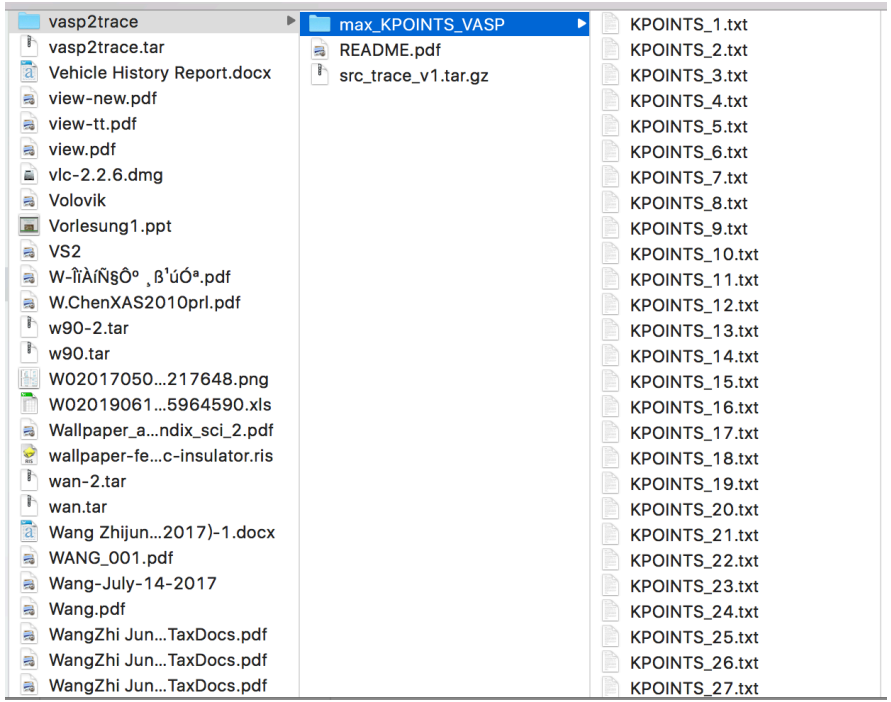
```
/anaconda3/bin/phonopy  --tolerance 0.01 --symmetry -c POSCAR
phonopy_version: '1.13.2'
space_group_type: 'R-3m'
space_group_number: 166
point_group_type: '-3m'
space_group_operations:
- rotation: # 1
  - [ 1,  0 , 0]
  - [ 0,  1 , 0]
  - [ 0,  0 , 1]
  translation: [ 0.00000,  0.00000,  0.00000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

"POSCAR"

```
 1 generated by phonopy
 2    1.0
 3      2.0690000000000000    1.1945377069533354    9.5466666571200012
 4     -2.0690000000000000    1.1945377069533354    9.5466666571200012
 5      0.0000000000000000   -2.3890754139066708    9.5466666571200012
 6 Bi Se
 7    2    3
 8 Direct
 9   0.6009999996010008  0.6009999996010008  0.6009999996010009
10   0.3990000003989990  0.3990000003989991  0.3990000003989989
11   0.7939999997940036  0.7939999997940036  0.7939999997940036
12   0.2060000002059964  0.2060000002059964  0.2060000002059964
13   0.0000000000000000  0.0000000000000000  0.0000000000000000
~
"PPOSCAR" 13L, 560C
```

Step 2:

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



Step 3:

Follow REDME in the folder VASP2trace

a. Run the scf calcualtion 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:
```

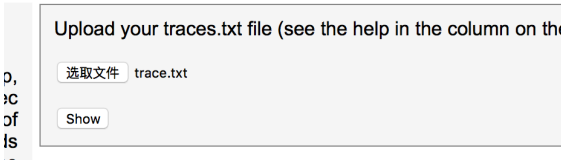
Step 4:

$ 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    0.0
24   3  2   -8.564873    2.000000    0.000000   -2.000000    0.000000    0.000000    0.000000    0.000000    0.0
```

Step 5:

pological Mat



Result of the analysis of the uploaded structure

- The material is a topological insulator.
- List of topological indices:

  z2w,1=0

  z2w,2=0

  z2w,3=0

  z4=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

1. Obtain the eigenstates at maximal high-symmetry k-points in VASP.
   Download the klist for all space groups:
   https://github.com/zjwang11/irvsp/tree/master/max_KPOINTS_VASP.

2. Compute the irreps from the eigenstates. ("vasp2trace" or "irvsp")
   Download and install "vasp2trace":
   https://github.com/zjwang11/irvsp/blob/master/src_trace_v1.tar.gz.
   ref. : https://arxiv.org/abs/2002.04032

3. Solve the compatibility relations: semimetal or Insulator. ("checktopologicalmat"):
   http://www.cryst.ehu.es/cryst/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., Nature, 566, 480-485 (2019)

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Contact us via email : wzj@iphy.ac.cn or zjwang11@hotmail.com

Thanks for your attention!