Hands-on: symmat

source code：https://github.com/zjwang11/TopMat

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Functions of symmat:

Calculate： Dielectric constants, (spin) Berry curvature, and anomalous/spin Hall conductivity

$: symmat -mu $mu (or -noe $nocc)

function of tags:

By default, the dielectric constant is computed.

-noe $occ	(set the occ and unocc band)
-mu $mu	(or you can set the fermi energy in $mu by -mu)
-nb $band1:$band2	(calulate the berry curvature ... for given bands from $band1 to $band2)
-spin	(set as default, calculate spin berry curvature and SHE (for NONCOLLINEAR) with tag -spin)
-test	(pi mat for given bands from $band1 to $band2)

Notices in VASP calculation before using symmat

1. For VASP6.x, please modify the line "CALL SET_SPINROT_WRAPPER(LATT_CUR%B(1,1),-1)" in mkpoints.F to "CALL SET_SPINROT_WRAPPER(LATT_CUR%B(1,1),IU6)" and recompile VASP before using symmat. We will use the symmerty (irot in the OUTCAR) in the symmat program.

2. set LSORBIT = TRUE; MAGMOM = 900*0

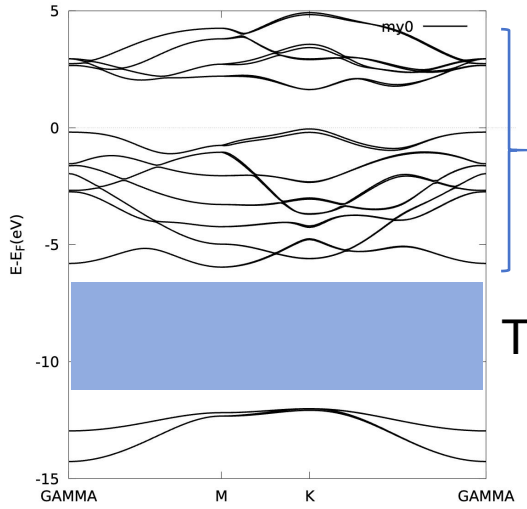
For non-magnetic materials with SOC (+SOC) calculations, please set the MAGMOM tag explicitly in INCAR (for example, MAGMOM=900*0). Default MAGMOM values may unintentionally lower the symmetry of the system. This can result in an increased number of k-points in the irreducible Brillouin zone (IBZKPT), thereby unnecessarily increasing computational cost.

Notices on the choice of bands for hall conductivity calculation

To balance computational accuracy and cost, we typically do not select all energy bands for the calculation of Hall-related parameters. Here are some common selection guidelines:

1. **Note:** When specifying the number of bands (NBANDS) in a DFT calculation (e.g., NBANDS = 128), you should avoid including bands near the highest index (e.g., around the 128th band) in the selection for vasp2mat and subsequent calculations. These bands are often affected by truncation effects and may be less accurate or incomplete.

2. If there is a large gap in the valence bands (similar to the procedure in Wannier calculations), it is often reliable and resource-efficient to select bands starting from this gap for vasp2mat.



select bands

Typically, selecting bands starting from this large gap and upwards is sufficient.

band structure of MoS2 monolayer

EXAMPLE-1： dielectric constants of bulk SiC, without spin-orbit coupling:

Step 1 run "vasp" to obtain the wavefunctions (WAVECAR) of irreducible BZ k points (“ISYM=2” in INCAR).

Step 2 run "vasp2mat" (vmat = 13) to obtain the velocity matrix (vmat: fort.1317, eigmat: fort.1315).
INCAR.mat:

```
&vmat_para
   vmat=13
   vmat_k=72              ! num of k points  in IBZKPT
   bstart=1,  bend=12     ! Velocity is calculated between the 1-12 bands. band 1-4 are occupied, 5-12 are unoccupied.
/
```

Step 3 run "symmat" to obtain the dielectric constants and distribution in k space (dielectric_constants.dat).

$ symmat -noe 4 ! note: 4 is the number of electrons (noe)

Formula of dielectric constants:

$$\varepsilon_{xx} = 1 + \int \frac{d^3k}{(2\pi)^3} 8\pi e^2\hbar^2 \sum_{cv} \mathrm{Re}\{\frac{\langle u_{ck}|v_x|u_{vk}\rangle\langle u_{vk}|v_x|u_{ck}\rangle}{(\varepsilon_{ck}-\varepsilon_{vk})^3}\}$$

Note: The dielectric constant is a tensor.
For three-dimensional materials, six components can be calculated.

```
   # dielectric constant (SUM) :  0.7057E+01 -0.4292E-05 -0.4628E-05  0.7057E+01  0.6109E-05  0.7057E+01
#       ka          kb          kc          xx          xy          xz          yy          yz          zz          epsilon_0 (permittivity of free space)
  0.000000  0.000000  0.000000    0.1173E-01 -0.6887E-06  0.6871E-06  0.1173E-01  0.6813E-06  0.1173E-01
  0.083300  0.000000  0.000000    0.8783E-02 -0.1391E-02  0.1391E-02  0.8783E-02  0.1391E-02  0.8783E-02
  0.166700  0.000000  0.000000    0.6631E-02 -0.2245E-02  0.2245E-02  0.6631E-02  0.2245E-02  0.6631E-02
  0.250000  0.000000  0.000000    0.6253E-02 -0.2655E-02  0.2654E-02  0.6253E-02  0.2654E-02  0.6253E-02
  0.333300  0.000000  0.000000    0.6523E-02 -0.2959E-02  0.2960E-02  0.6523E-02  0.2960E-02  0.6525E-02
  0.416700  0.000000  0.000000    0.6877E-02 -0.3167E-02  0.3167E-02  0.6877E-02  0.3167E-02  0.6879E-02
```

dielectric_constants.dat

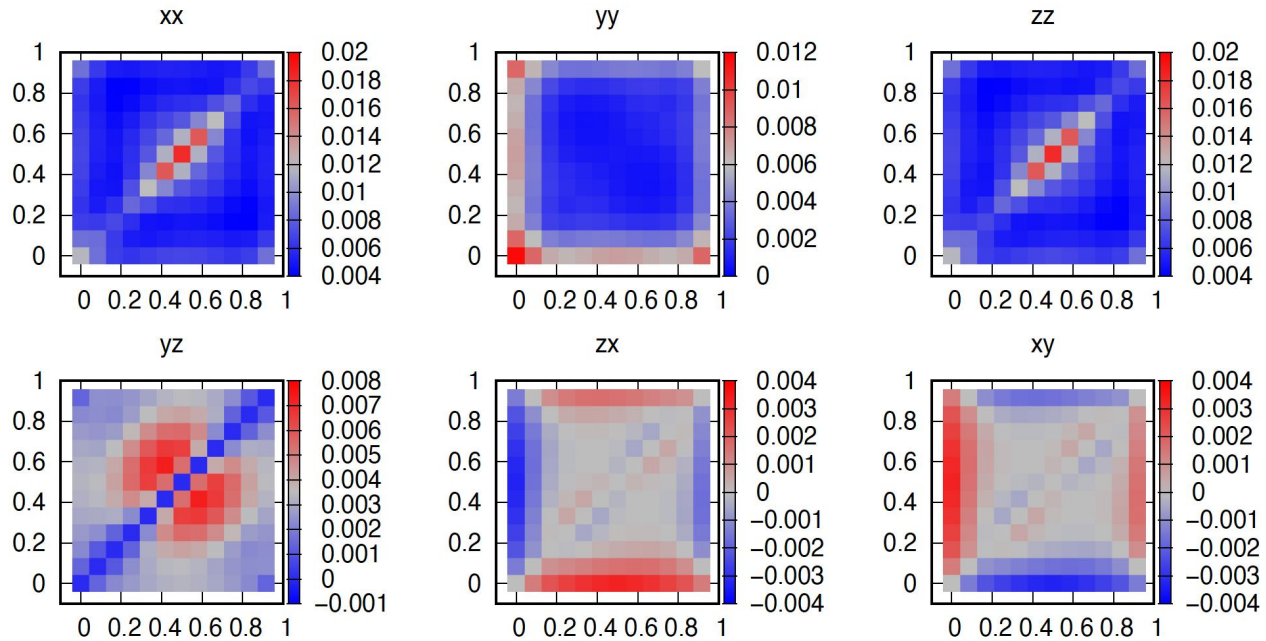
Make sure the following programs are compiled: vasp, vasp2mat, gnuplot and symmat

Enter **EX_SiC** and run the following commands.

Shell commands

```
    ### run vasp scf ###
$ vim INCAR  (set “ISYM = 2; LWAVE = .T. ”)
$ mpirun -np $ncpu $vasp_ncl  > out 2> err
$ cp OUTCAR OUTCAR.scf
$ cp EIGENVAL EIGENVAL.scf
    ### run vasp2mat < INCAR.mat > fort.1315-17 ###
$ vim INCAR  (set “ISTART = 1; ICHARG =  11;  LWAVE = .F.  ”)
$ vasp2mat > mat.out
    ### run symmat   ###
$ symmat -noe 4     # dielectric_constants.dat
$ gnuplot plot_diel.gnu
```

distribution on kc=0 plane



EXAMPLE-2： berry curvature of MoS2:

Step 1 run "vasp" to obtain the wavefunctions (WAVECAR) of irreducible BZ k points (“ISYM=2” in INCAR).

Step 2 run "vasp2mat" (vmat = 13) to obtain the velocity matrix (vmat: fort.1317, eigmat: fort.1315).

INCAR.mat:

```
&vmat_para
   vmat=13
   vmat_k=64                  ! num of k points  in IBZKPT
   bstart=1,  bend=60      ! Velocity is calculated between the 1 -60 bands. band 1-26 are occupied
/
```

Step 3 run "symmat" to obtain the dielectric constants and distribution in k space.

$ symmat -noe 26 ! note: 26 is the number of electrons (noe)

formula of berry curvature and AHE:

$$\Omega_{xy}(k) = -2\hbar^2 \sum_{n=1}^{noe} \sum_{n' \neq n} \mathrm{Im}\{\frac{\langle u_{nk}|v_x|u_{n'k}\rangle\langle u_{n'k}|v_y|u_{nk}\rangle}{(\varepsilon_{nk} - \varepsilon_{n'k})^2}\}$$

$$\sigma_{xy}^{AHE} = -\frac{e^2}{\hbar}\int_{BZ}\frac{d^3k}{(2\pi)^3}\Omega_{xy}$$

```
     # AHE (in e^2/h/angstrom)  : -0.2489E-08  0.1538E-09 -0.3364E-09
     # AHE (in S/cm)            : -0.9641E-05  0.5958E-06 -0.1303E-05
#       ka          kb          kc          xy          yz          zx      ang^2
  0.000000    0.000000    0.000000    0.6554E-05  0.1492E-06  0.2282E-06
  0.055600    0.000000    0.000000   -0.7084E-05  0.1021E-04 -0.1626E-04
  0.111100    0.000000    0.000000    0.2335E-05  0.7261E-05 -0.1031E-04
```

berry_0.dat

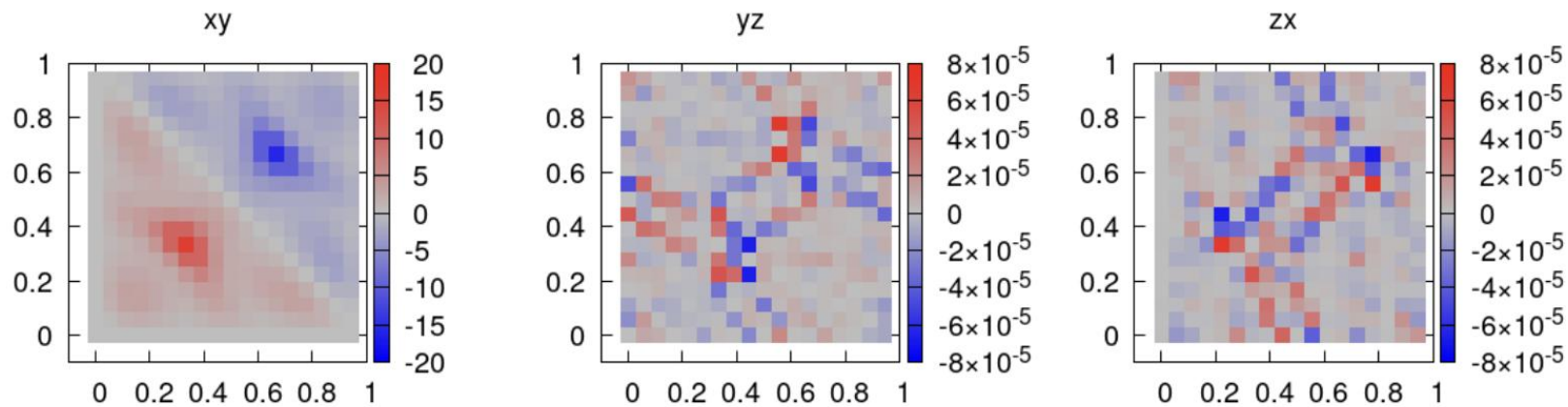
Make sure the following programs are compiled: vasp, vasp2mat, gnuplot, and symmat

Enter **EX_MoS2** and run the following commands.

Shell commands

```
    ### run vasp scf ###
$ vim INCAR  (set “ISYM = 2; LWAVE = .T. ”)
$ mpirun -np $ncpu $vasp_ncl  > out 2> err
$ cp OUTCAR OUTCAR.scf
$ cp EIGENVAL EIGENVAL.scf
    ### run vasp2mat < INCAR.mat > fort.1315-17 ###
$ vim INCAR  (set “ISTART = 1; ICHARG =  11;  LWAVE = .F.  ”)
$ vasp2mat > mat.out
    ### run symmat   ###
$ symmat -noe 26                                          # berry_0.dat is berry curvature
$ cp berry_0.dat berry.dat; gnuplot plot_berry.gnu # plot berry curvature
```

berry curvature



EXAMPLE-3：Spin hall conductivity of 2D QSHI BiH (with SOC):

Step 1 run "vasp" to obtain the wavefunctions (WAVECAR) of irreducible BZ k points (“ISYM=2” in INCAR).

Step 2 run "vasp2mat" (vmat = 13) to obtain the velocity matrix (vmat: fort.1317, eigmat: fort.1315).

INCAR.mat:

```
&vmat_para
   vmat=13
   vmat_k=72                ! num of k points  in IBZKPT
   bstart=1,  bend=100      ! Velocity is calculated between the 1-100 bands. band 1-32 are occupied
/
```

Step 3 run "symmat" to obtain the dielectric constants and distribution in k space.

$ symmat -noe 32 ! note: 32 is the number of electrons (noe)

formula of spin berry curvature and SHE:

$$\Omega_{xy}^{S_z}(k) = -2\hbar \sum_{n=1}^{noe} \sum_{n' \neq n} \mathrm{Im}\{\frac{\langle u_{nk}|J_{z,x}^{S}|u_{n'k}\rangle\langle u_{n'k}|v_y|u_{nk}\rangle}{(\varepsilon_{nk}-\varepsilon_{n'k})^2}\}$$

$$\sigma_{xy}^{O/S} = e\int_{BZ}\frac{d^3k}{(2\pi)^3}\Omega_{xy}^{S_z} \qquad J_{z,x}^{S} = \frac{1}{2}\{v_x, s_z\} \quad s_z = \frac{\hbar}{2}\sigma_z$$

```
        # SHE (in e/(2pi)/ang)  :   0.5010E-01 -0.2169E-10 -0.1361E-11
        # SHE (in (hbar/e)*S/cm) :   0.1941E+03 -0.8403E-07 -0.5274E-08
#       ka          kb          kc          z_xy          z_yz          z_zx       ang^2
  0.000000    0.000000    0.000000     0.8558E+01    0.3157E-07    0.9810E-08
  0.055600    0.000000    0.000000     0.7810E+01    0.2122E-06    0.1744E-06
  0.111100    0.000000    0.000000     0.6167E+01   -0.3658E-06    0.5278E-06
  0.166700    0.000000    0.000000     0.4482E+01    0.2410E-06    0.9289E-07
  0.222200    0.000000    0.000000     0.3121E+01   -0.3611E-06   -0.6672E-06
```

berry_3.dat (spin z)

Make sure the following programs are compiled: vasp, vasp2mat, gnuplot, and symmat

Enter **EX_BiH** and run the following commands.

Shell commands

```
    ### run vasp scf ###
$ vim INCAR  (set “ISYM = 2; LWAVE = .T. ”)
$ mpirun -np $ncpu $vasp_ncl  > out 2> err
$ cp OUTCAR OUTCAR.scf
$ cp EIGENVAL EIGENVAL.scf
    ### run vasp2mat < INCAR.mat > fort.1315-17 ###
$ vim INCAR  (set “ISTART = 1; ICHARG =  11;  LWAVE = .F.  ”)
$ vasp2mat > mat.out
    ### run symmat   ###
$ symmat -noe 32
$ cp berry_3.dat berry.dat; gnuplot plot_berry.gnu # plot spin z berry curvature
```

In the berry_3.dat :

```
      # SHE (in e/(2pi)/ang) :  0.5010E-01 -0.2169E-10 -0.1361E-11
     # SHE (in (hbar/e)*S/cm) :  0.1941E+03 -0.8403E-07 -0.5274E-08
#       ka        kb        kc          z_xy        z_yz        z_zx     ang^2
  0.000000  0.000000  0.000000    0.8558E+01  0.3157E-07  0.9810E-08
  0.055600  0.000000  0.000000    0.7810E+01  0.2122E-06  0.1744E-06
  0.111100  0.000000  0.000000    0.6167E+01 -0.3658E-06  0.5278E-06
  0.166700  0.000000  0.000000    0.4482E+01  0.2410E-06  0.9289E-07
  0.222200  0.000000  0.000000    0.3121E+01 -0.3611E-06 -0.6672E-06
```

Multiply by the c-axis thickness (see POSCAR) to obtain the SHE in quantum units (e/2π).

SHE (in e/(2pi)) : 0.5007E-01*20 = 1.0014

! a 18*18*1 kmesh is needed for 2D-BiH to calculate the quantized spin hall conductivity

Kmesh	e/2pi *1/ang	e/2pi (Multiply by the thickness in the c direction)
12*12	0.5021E-01	1.0042
18*18	0.5007E-01	0.9999
24*24	0.5006E-01	1.0012
30*30	0.5006E-01	1.0012
36*36	0.5006E-01	1.0012

spin z berry curvature