Tutorial: 3D-Spin Texture generation

Computational Materials Physics

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Work funded by the German Science Foundation within CRC TRR 80, project G03.

Contents



- Definition of the spin texture
- Application of C++: Preparation of the k-mesh grid and parsing of the output files obtained from the simulation package VASP
- Drawing of the spin texture via the graphing utility gnuplot

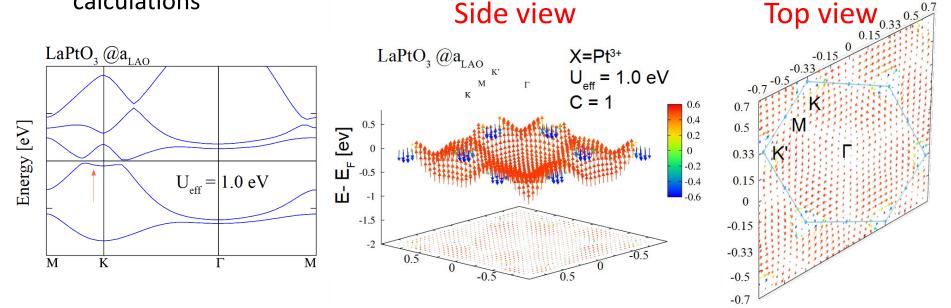
Spin texture of magnetic



materials

- Spin texture of electronic bands is derived from the coupling of spin and orbital motion of electrons known as spin-orbit coupling (SOC)
- A magnetic field is generated by the orbiting electrons due to their orbital and spin motion
- Useful for investigation of the non-trivial topology nature of systems, i.e.
 Chern insulators by analyzing the band structures obtained from non-collinear calculations

 Side view



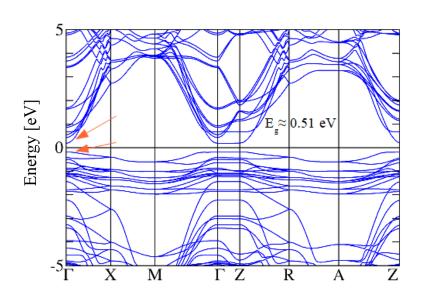
Spin texture of magnetic

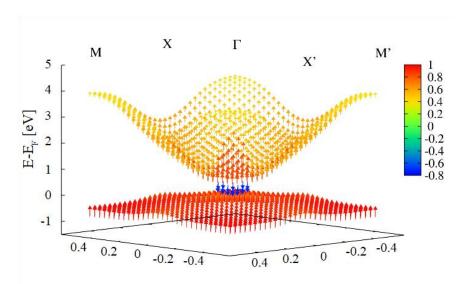


materials

 Spin texture plots are not only restricted to systems with a hexagonal structure but also possible for systems with a tetragonal structure

Side view





Step 1: Preparation of the



k-point grid

- The written code generates 900 number of points along the reciprocal axis k_x , k_y and k_z
- Execute the already compiled code using the executable file "main.exe"
- Choose the desired k-point path (see exemplary message):

```
Choose the path you want to take!
Enter 'y' (yes) for Gamma-M-K-Gamma or type in 'n' (no) for the default path of Gamma-X-M-Gamma:
```

• The KPOINTS file for vasp should look like the output example below:

foo			
900 rec			
-0.700	-0.700	0.000	1.0
-0.700	-0.652	0.000	1.0
-0.700	-0.603	0.000	1.0
-0.700	-0.555	0.000	1.0
-0.700	-0.507	0.000	1.0
-0.700	-0.459	0.000	1.0
-0.700	-0.410	0.000	1.0
-0.700	-0.362	0.000	1.0
-0.700	-0.314	0.000	1.0
-0.700	-0.266	0.000	1.0
-0.700	-0.217	0.000	1.0
-0.700	-0.169	0.000	1.0
-0.700	-0.121	0.000	1.0
-0.700	-0.072	0.000	1.0
-0.700	-0.024	0.000	1.0

- 1st line: Arbitrary comment line
- 2nd line: Total number of *k*-points
- 3rd line: Reciprocal coordinates option
- 4th line: Reciprocal coordinates of each k-point and its weight of 1.0 $_{5}$

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Step 2: VASP calculation

- Use CHGCAR for the non SCF calculation from the pre-converged non-collinear SCF calculation
- Flags for INCAR: ICHARG = 11, ISMEAR = 0, ISYM = -1, LSORBIT = .TRUE.,
 LNONCOLLINEAR = .TRUE., SAXIS = 0 0 1 (by default)
- Required files for plotting the spin texture:

PROCAR: Magnetization components S_x , S_y and S_z for atoms arranged in the order of the POSCAR file

EIGENVAL: Eigen energy values for the chosen band

OUTCAR: Fermi energy E_F of the system

Step 3: Running the main



program

- Before running "main.exe" copy all necessary files "PROCAR, EIGENVAL and generated KPATH.txt into the current folder where you execute "main.exe"
- Run "main.exe", note that the size of the PROCAR file can be huge (several GBs)!
- After having performed the calculation with the finer grid, the main code can be executed (follow instructions on screen):

```
Did you already run this program in order to generate the kpath?
Please type in 'y' for yes and 'n' for no: n
Just type in 'y' for yes: y
Choose the path you want to take!
Enter 'f' for first path G-M-K-G or 's' (or any other character) for the second path G-X-M-G: f
Do you wish to run the entire code (use same kpath as used for the DFT calculations)?
Please type in 'y' for yes and 'n' for no: y
```

 If there was no error encountered, then it can be continued with the next step of plotting the spin texture

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Step 4: Post-Processing/Gnuplot

 Use delivered gnuplot scripts for plotting side and top view of spin textures (example here: 2D-material hosting the honeycomb lattice)

Run sequentially the scripts (adjust the energy scale before running):

- 1. gnuplot -p top_view.gnu
- 2. gnuplot –p side_view.gnu(optional: labelling positions of the high-symmetry points by using 'KPATH.dat')

Output filenames (recommendation: *.ps files for high quality figures, see produced figures on page 3):

- 1. top_view.ps
- 2. side_view.ps

Congratulations, the spin texture was plotted!