

Tutorial: 3D-Spin Texture generation

Computational Materials Physics

University Duisburg-Essen

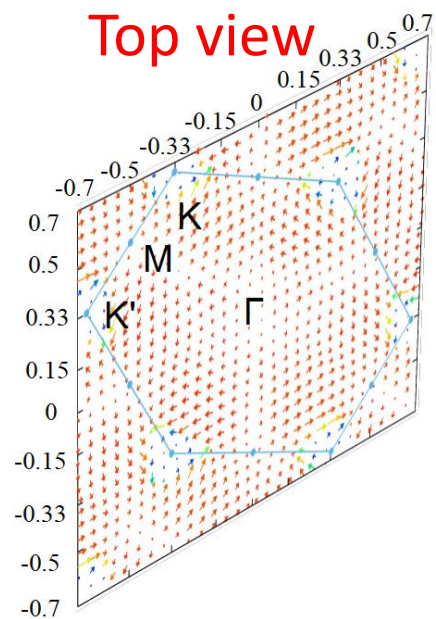
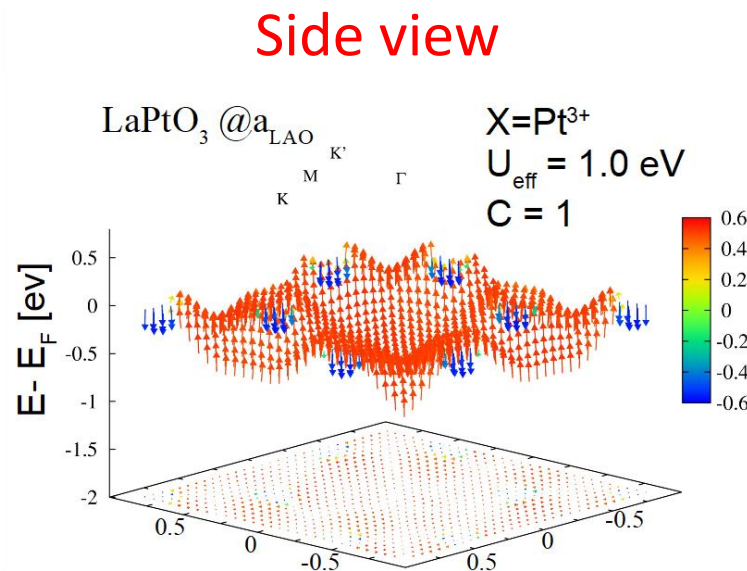
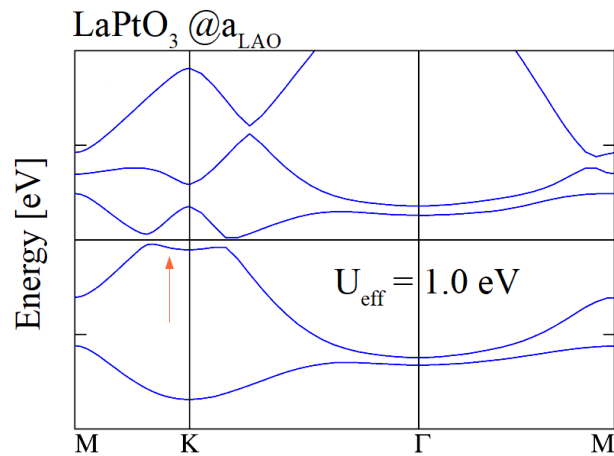
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- Definition of the spin texture
- Application of C++: Preparation of the k -mesh grid and parsing of the output files obtained from the simulation package VASP
- Drawing of the spin texture via the graphing utility gnuplot

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



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 eample 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
```

- 1th line: Arbitrary comment line
- 2nd line: Total number of k -points
- 3rd line: Reciprocal coordinates option
- 4th line: Reciprocal coordinate of each k -point and its weight of 1.0

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

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!