Tutorial: 3D-Spin Texture generation

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Please use [ref]: Köksal, O. (2021). *Density functional theory study of Mott and topologically non-trivial phases in oxide heterostructures*. https://doi.org/10.17185/duepublico/74872 for citing in any publication arising from the use of this code

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Report any bugs by sending an e-mail to: koeksal.okan@gmail.com

Contents

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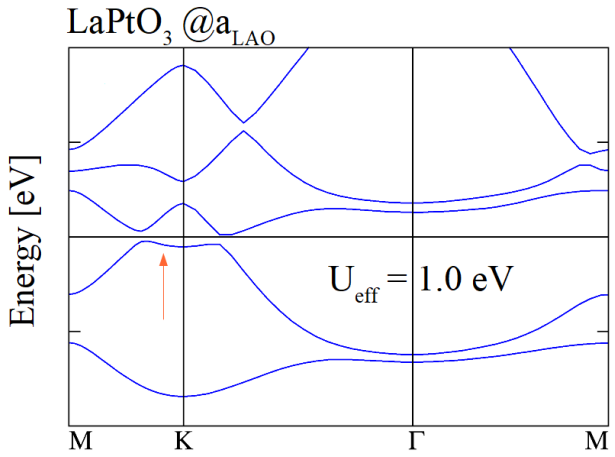
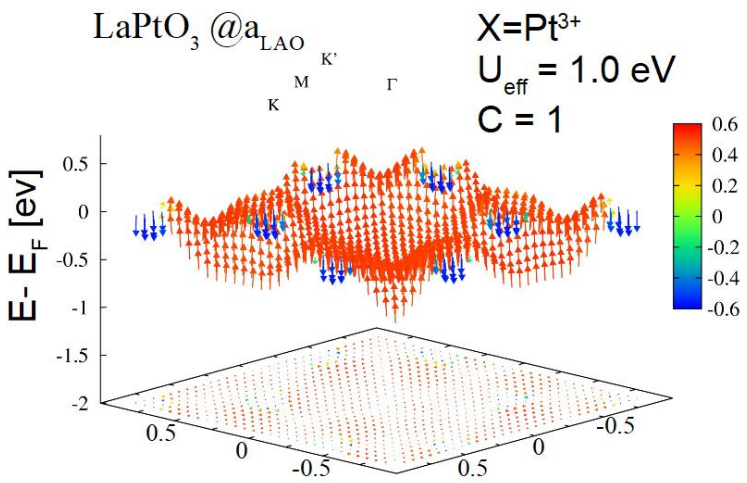
- Definition of the spin texture
- Application of C++: Preparation of the *k*-mesh grid and parsing of the output files obtained from the simulation package VASP
- Drawing of the spin texture via the graphing utility gnuplot

Spin texture of magnetic materials

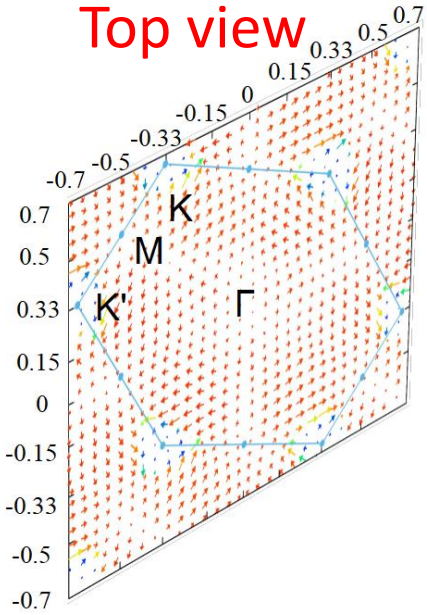
- Spin texture of electronic bands is derived from the coupling of spin and orbital motion of electrons known as spin-orbit coupling (SOC)
- A magnetic field is generated by the orbiting electrons due to their orbital and spin motion
- Useful for investigation of the non-trivial topology nature of systems,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



Side view



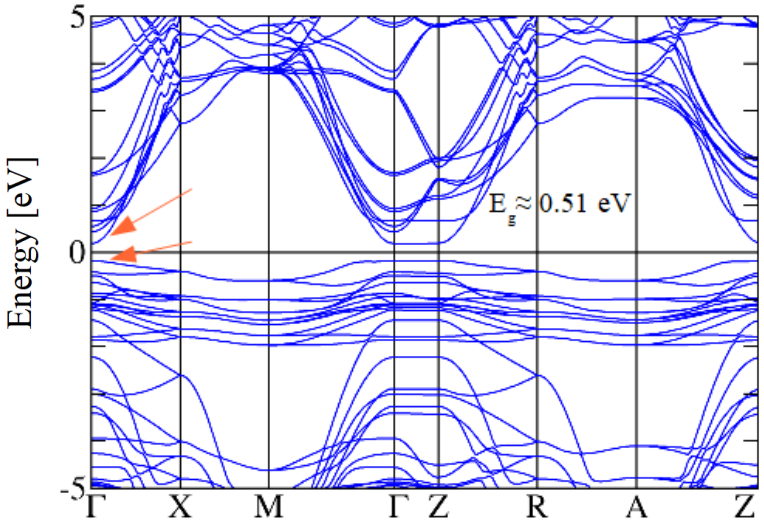
Top view



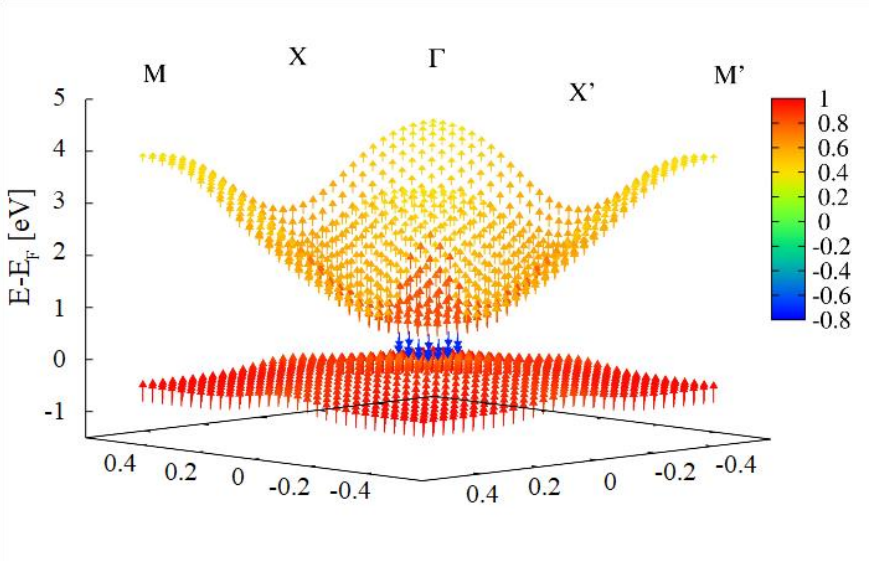
O. Köksal and R. Pentcheva, Scientific Reports **9**, 17306 (2019).

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



O. Köksal and R. Pentcheva, Phys. Rev. B **103**, 045135 (2021).

Step 1: Preparation of the *k*-point grid

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- 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

Step 2: VASP calculation

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- 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

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- 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

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- 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!