Fat Bands and Spin Texture Analysis

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First steps with SIESTA from zero to hero

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Spin Texture

- **Band structure**: dispersion of eigen energies in k space
- **Spin texture**: dispersion of the spin moments in k space

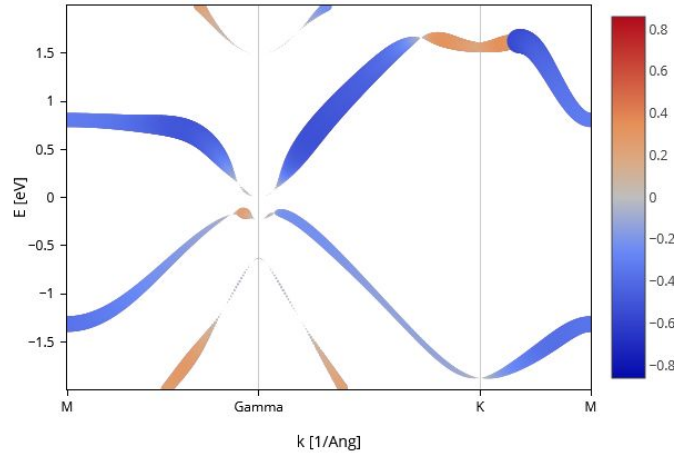
- $\vec{s}_{\nu\mathbf{k}} = \langle \Psi_{\nu\mathbf{k}} | \, \vec{\sigma} \, | \Psi_{\nu\mathbf{k}} \rangle \qquad \vec{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}$

$|\Psi_{\nu\mathbf{k}}\rangle$: wavefunctions

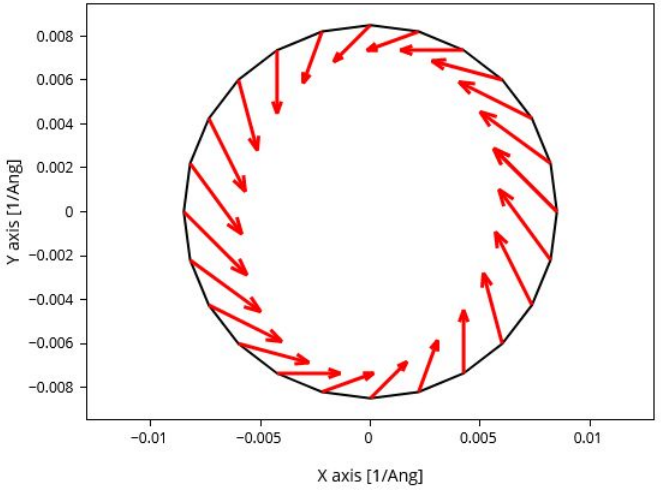
σ_i : Pauli matrices

$\vec{s}_{\nu\mathbf{k}}$: expectation value of the spin operator for each wave function

Visualize Spin as Color



Or as arrows



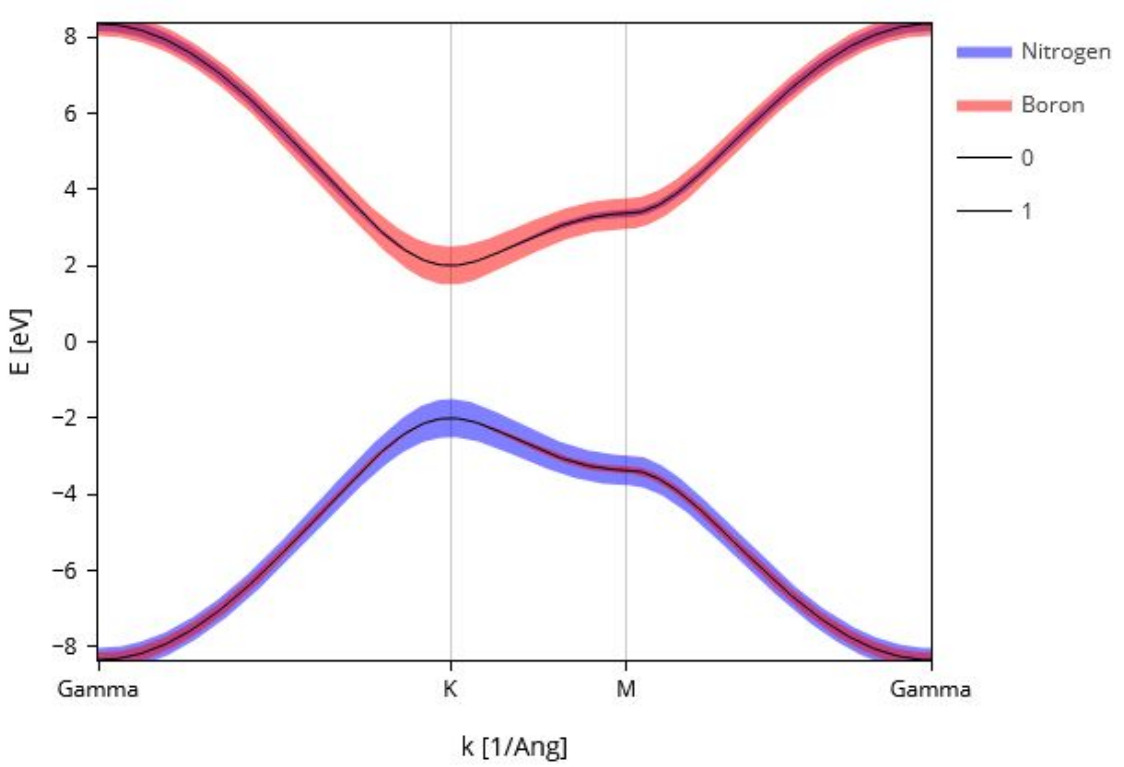
Fat bands analysis

- Very similar to spin texture analysis
- Spin operators = projector on spin subspace
- Fat bands project: projectors on orbital subspaces instead

$$p_\alpha = \langle \Psi_{\nu\mathbf{k}} | \, P_\alpha \, | \Psi_{\nu\mathbf{k}} \rangle$$

- We can project on
  - Specific orbitals
  - All orbitals of one atom or species
  - A specific group of atoms
  - … options are limit-less

Example: hBN



Fat bands input file

SystemLabel

DOS

<ProjectionName1>

<1st subset> <2nd subset>...

<ProjectionName2>

<1st subset> ...

...

Subsets specifications:

```
Si        # All silicon atoms
3         # Atom number 3
O_2           # n=3 orbitals of O
4_2       # n=2 orbitals of atom 4
O_2p          # 2p orbitals of O
O_2py         # only 2py orbitals of O
```

Example

Siesta Documentation

0.1

Search docs

- Tutorials
  - Setting up the local working environment for the tutorial exercises
  - Basics of Siesta
- Intermediate and Advanced Topics
  - Molecular Dynamics
  - Spin-Orbit coupling
  - Polarization calculations with the Berry-phase approach
  - DFT+U calculations
  - Time-Dependent Density-Functional Theory
  - Wannier functions
  - Generation and testing of pseudopotentials
- Advanced analysis of the electronic structure
  - Mulliken charges
  - DOS and projected DOS
  - COOP and COHP curves
  - Fat-bands: orbital-projected band-structure
  - Analysis of the spin texture in reciprocal space

Tutorials / Advanced analysis of

Fat-bands for Si

Here we will use the `fat` program to
band-structure calculation with the o
resulting "fatbands" can later be plott

Hint

Enter the *si_fatbands* directory

Note

It is also possible to perform fatban
check the sisl documentation.

Here we see a si_fatbands.fdf file wit

```
BandLinesScale  pi/a
WFS.Write.For.Bands T            #
Wfs.band.min 1
Wfs.band.max 8
%block BandLines                 #
1  0.000  0.000  0.000  \Gamma   # L
25  2.000  0.000  0.000     X     #
10  2.000  1.000  0.000     W     #
15  1.000  1.000  1.000     L     #
20  0.000  0.000  0.000  \Gamma   #
25  1.500  1.500  1.500     K     #
%endblock BandLines
```

Siesta Documentation

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Tutorials / Advanced analysis of the electronic structure / Spin texture View page so

Spin texture

author Roberto Robles (CFM-CSIC) and Alberto Garcia (ICMAB-CSIC)

Notes on the Siesta implementation

Mathematically, the spin texture is simply a vector field: (non-collinear) spins in reciprocal space
Siesta, the spin vector associated to a given spinor Ψ_{nk}

$$\mathbf{S}_{nk} = < \Psi_{nk} | \sigma | \Psi_{nk} >$$

where σ is a vector of Pauli matrices, can be computed using the coefficients of the spinors and
overlap matrix (appearing because of the space integral implied above).

The wave-function (spinor) coefficients are stored in a WFSX file, which can be created during a
Siesta calculation in several ways:

- Using the 'BandPoints' or 'BandLines' blocks (see manual), *together* with the option:

```
Wfs.Write.For.Bands T
```

- Using the WaveFuncKpoints block to specify k-points and bands
- Using the 'COOP.Write T' option: a wave-function set using the k-point sampling of the BZ
  in the scf cycle will be written (see manual).