SIESTA School 2025

Spin, spin-orbit coupling and magnetism (II)

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siesta

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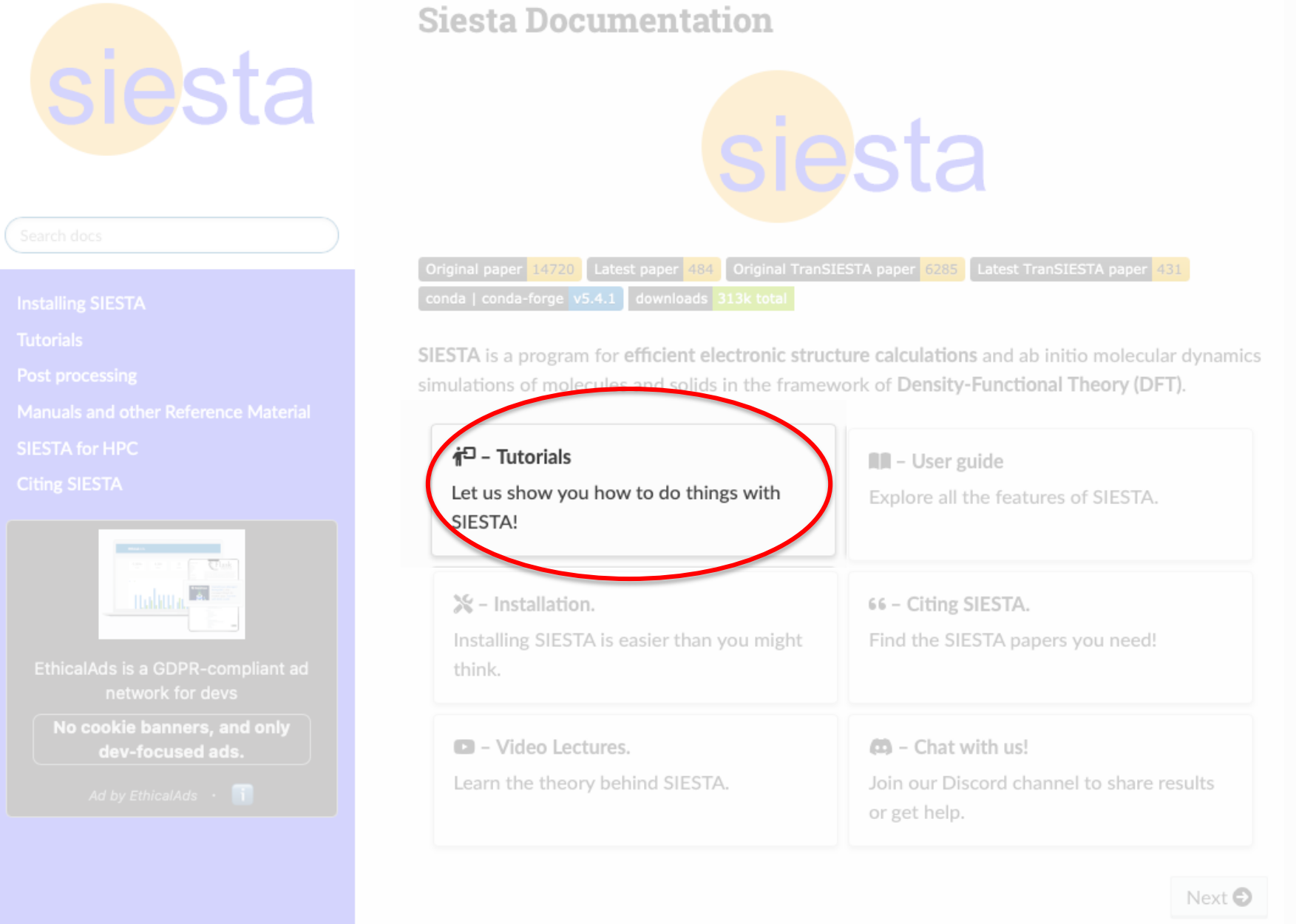
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Tutorials

This set of tutorials will guide you in the exploration of Siesta's features.

Before you do anything else, start here. You need to set up your local working environment to follow the tutorial.

- Setting up the local working environment for the tutorial exercises

If you are interested in the theory behind some of these tutorials, you can have a look at the 2021 videolectures:

- Video Lectures

Basics of Siesta

This section is recommended for all beginners, and also as a refresher for more experienced users.

- A First Encounter with SIESTA
- Basis sets - Optimization
- Basis sets - Special cases
- The real-space grid
- Sampling of the BZ with k-points
- The self-consistent-field cycle
- Analysis tools
- Electronic Structure Analysis
- Structural optimization using forces and stress
- Molecular dynamics
- Vibration modes and phonons
- Spins, Magnetism, and Spin-Orbit Coupling
- First crystals

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Installing SIESTA

Tutorials

- Setting up the local working environment for the tutorial exercises
- Video Lectures
- Basics of Siesta
- Intermediate and Advanced Topics
- Advanced applications
- SISL, Lua and scripting

Post processing

Manuals and other Reference Material

SIESTA for HPC

Citing SIESTA

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- Spins, Magnetism, and Spin-Orbit Coupling
  - First Contact with Spins (10 min)
  - Breaking the Symmetry (5 min)
  - Antiferromagnetic Iron (fcc) (10 min)
  - Spin-Orbit Coupling (10 min)
  - Magnetic anisotropy (15 min)
  - Visualizing the spin density (15 min)
  - Spin resolved density of states (30 min)

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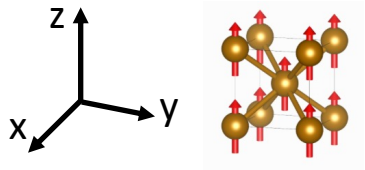
- Spins, Magnetism, and Spin-Orbit Coupling

A
- First Contact with Spins (10 min)
- Breaking the Symmetry (5 min)
- Antiferromagnetic Iron (fcc) (10 min)

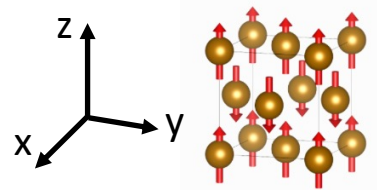
B
- Spin-Orbit Coupling (10 min)
- Magnetic anisotropy (15 min)
- Visualizing the spin density (15 min)
- Spin resolved density of states (30 min)

- Ferromagnetism of Fe bcc: directory '01_Fe_bcc'



-fe_bcc.fdf
-Fe.psf

- Antiferromagnetism of Fe fcc: directory '02_Fe_fcc'



-fe_fcc.fdf
-Fe.psf

- Some tips to remember when SOC in included
- Magnetic anisotropy: directory '04_Pt2'
  - pt2_spin_z.original.fdf
  - pt2_spin_z.fdf
  - Pt.psf
- Bands, proyected density of states and mulliken charges

/siesta-docs/work-files/tutorials/advanced/spin-orbit/Example-1

- example_1.ipynb
- example_1.fdf.original
- example_1.fdf
- dos.gnp
- bands.gnp
- Pt_fept_SOC.psf -> ../Pt_fept_SOC.psf
- Fe_fept_SOC.psf -> ../Fe_fept_SOC.psf

your_directory/siesta-docs/work-files/tutorials/basic/magnetism

- Spins, Magnetism, and Spin-Orbit Coupling

A
- First Contact with Spins (10 min)
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-fe_bcc.fdf
-Fe.psf

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-Fe.psf

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  - pt2_spin_z.original.fdf
  - pt2_spin_z.fdf
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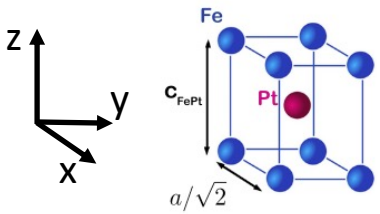
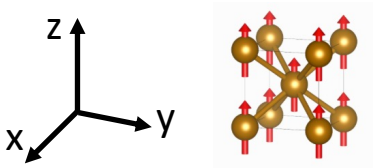
- Bands, proyected density of states and mulliken charges

/siesta-docs/work-files/tutorials/advanced/spin-orbit/Example-1



- example_1.ipynb
- example_1.fdf.original
- example_1.fdf
- dos.gnp
- bands.gnp
- Pt_fept_SOC.psf -> ../Pt_fept_SOC.psf
- Fe_fept_SOC.psf -> ../Fe_fept_SOC.psf

- Ferromagnetism of Fe bcc: directory '01_Fe_bcc'



-fe_bcc.fdf
-Fe.psf

Run it including the following:

```
# Spin options
# >> Edit this part before running siesta
# Spin <OPTION>
# %block DM.InitSpin
#   <AtomIndex> <SpinMoment>
# %endblock DM.InitSpin
```

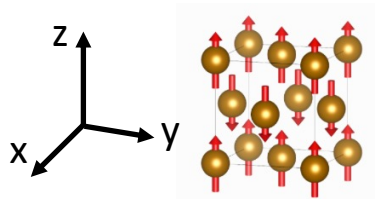
Check:

- Up/down Mulliken population

```
#General system specifications
SystemName          Iron (bcc)
SystemLabel         fe_bcc
NumberOfAtoms       1
NumberOfSpecies     1

%block ChemicalSpeciesLabel
 1  26 Fe      # Species index, atomic numbe
%endblock ChemicalSpeciesLabel

# Basis set definition
PAO.EnergyShift 200 meV
PAO.SplitNorm   0.15
PAO.BasisSize   DZP

# Lattice vectors
LatticeConstant  2.86 Ang
%block LatticeVectors
   -0.5000    0.5000    0.5000
    0.5000   -0.5000    0.5000
    0.5000    0.5000   -0.5000
%endblock LatticeVectors

#Atomic coordinates
AtomicCoordinatesFormat  ScaledCartesian

%block AtomicCoordinatesAndAtomicSpecies
    0.0000    0.0000    0.0000   1
%endblock AtomicCoordinatesAndAtomicSpecies
• • • •
```

HERE (at the end of the file)

- Antiferromagnetism of Fe fcc: directory '02_Fe_fcc'



-fe_fcc.fdf
-Fe.psf

Run it including the following:

```
# Spin options
# >> Edit this part before running siesta
# Spin <OPTION>
# %block DM.InitSpin
#   <AtomIndex> <SpinMoment>
# %endblock DM.InitSpin
```

Check:

- Up/down Mulliken population

```
#General system specifications
SystemName          Iron (fcc) - Antiferromagne
SystemLabel         fe_fcc
NumberOfAtoms       2
NumberOfSpecies     1

%block ChemicalSpeciesLabel
 1  26 Fe      # Species index, atomic number,
%endblock ChemicalSpeciesLabel

# Basis set definition
PAO.EnergyShift 200 meV
PAO.SplitNorm   0.15
PAO.BasisSize   DZP

# Lattice vectors
LatticeConstant  3.66 Ang
%block LatticeVectors
    0.5000   -0.5000    0.0000
    0.5000    0.5000    0.0000
    0.0000    0.0000    1.0000
%endblock LatticeVectors

#Atomic coordinates
AtomicCoordinatesFormat  ScaledCartesian

%block AtomicCoordinatesAndAtomicSpecies
    0.0000    0.0000    0.0000   1
    0.5000    0.0000    0.5000   1
%endblock AtomicCoordinatesAndAtomicSpecies

• • • •
```

HERE (at the end of the file)

- Some tips to remember **when SOC in included**

- carefully converge the k–points sampling.
- carefully converge the mesh cut-off.
- converge the density matrix with a tolerance below 10^-5.
- use relativistic pseudopotentials (PPs) and use the *non–linear core corrections* when the PPs are built.
- For `Spin none` the *.DOS* file contains two columns: energy and DOS.
- For `Spin polarized` the *.DOS* file contains three columns: energy, DOS↑, DOS↓ (DOS for spin-up/spin-down electrons). The integral of DOS↑ (DOS↓) up to E_F will give the number of electrons with spin-up (spin-down). The total density of states is the sum of DOS↑ and DOS↓.
- For `Spin non-colinear` or `Spin spin-orbit` the *.DOS* file contains five columns: energy, DOS↑, DOS↓, Re{DOS↑↓} and Im{DOS↑↓}.
  The integral of Re{DOS↑↓} up to E_F will give the magnetization along *X* axis, Mx, and the integral of Im DOS↑↓ up to E_F , My. The total density of states is the sum of DOS↑ and DOS↓.

All of the information regarding the basis set and all the parameters used in a common SIESTA calculation are also valid for the SOC.

An additional advice: remember to read the SOC section in the main SIESTA manual!

- Magnetic anisotropy: directory '04_Pt2'
  - pt2_spin_z.original.fdf
  - pt2_spin_z.fdf
  - Pt.psf

your_directory/siesta-docs/work-files/tutorials/basic/magnetism

Run it modifying DM.InitSpin:

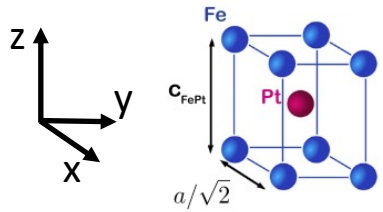
Check both energies E_z and $E_{x/y}$:

```
SystemName              Pt dimer - spin along z
SystemLabel             pt2_spin_z

Spin    spin-orbit

%block DM.InitSpin
 1   +1.   0.   0.
 2   +1.   0.   0.
%endblock DM.InitSpin

AtomicCoordinatesFormat NotScaledCartesianAng
%block AtomicCoordinatesAndAtomicSpecies
     -1.19940    0.00000    0.00000    1
      1.19940    0.00000    0.00000    1
%endblock AtomicCoordinatesAndAtomicSpecies

LatticeConstant  10.0 Ang
%block LatticeVectors
     1.00       .00       .00
      .00      1.00       .00
      .00       .00      1.00
%endblock LatticeVectors

NumberOfAtoms           2
NumberOfSpecies         1
%block Chemical_Species_label
        1       78      Pt
%endblock Chemical_Species_label

 . . . .
```

Now you have to specify the angles

- Bands, proyected density of states and mulliken charges

/siesta-docs/work-files/tutorials/advanced/spin-orbit/Example-1



- example_1.ipynb
- example_1.fdf.original
- example_1.fdf
- dos.gnp
- bands.gnp
- Pt_fept_SOC.psf -> ../Pt_fept_SOC.psf
- Fe_fept_SOC.psf -> ../Fe_fept_SOC.psf

Run it modifying DM.InitSpin:

```
SystemName              FePt-L1_0
SystemLabel             example_1

Spin    spin-orbit
%block DM.InitSpin
 1  +3.  0.  0.
 2  +1.  0.  0.
%endblock DM.InitSpin

NumberOfAtoms           2
NumberOfSpecies         2
%block Chemical_Species_label
        1       26      Fe_fept_SOC
        2       78      Pt_fept_SOC
%endblock Chemical_Species_label

PAO.EnergyShift  100 meV
PAO.SplitNorm      0.15
PAO.OldStylePolOrbs F
Restricted.Radial.Grid  F
%Block PAO.Basis
 Fe_fept_SOC   2
   n=4   0   2
    0.0   0.0
   n=3   2   2
    0.0   0.0
 Pt_fept_SOC   2
   n=6     0       2
    0.00000     0.00000
   n=5     2       2
    0.00000     0.00000
%EndBlock PAO.Basis
```

Modify the angles

• • • •

```
DM.MixingWeight         0.005
DM.NumberPulay          8
DM.UseSaveDM            T
DM.NumberKick           25
DM.MixSCF1  F

WriteMullikenPop        1
WriteForces             T
WriteCoorStep           T


# Band structure options
# ----------------------

BandLinesScale          ReciprocalLatticeVectors

%block BandLines
   1 0.0000 0.0000 0.0000 Gamma
  50 0.5000 0.0000 0.0000 X
  50 0.5000 0.5000 0.0000 M
  50 0.0000 0.0000 0.0000 Gamma
  50 0.0000 0.0000 0.5000 Z
  50 0.0000 0.5000 0.5000 R
  50 0.5000 0.5000 0.5000 A
  50 0.0000 0.0000 0.5000 Z
%endblock BandLines

# Density-of-states options
# -------------------------

%block PDOS.kgrid_Monkhorst_Pack
   30    0    0    0.0
    0   55    0    0.0
    0    0   55    0.0
%endblock PDOS.kgrid_Monkhorst_Pack

%block ProjectedDensityOfStates
  -10.00  5.00  0.02  1000  eV
%endblock ProjectedDensityOfStates
```

Calculation of the magnetic anisotropy of FePt bulk

`/siesta-docs/work-files/tutorials/advanced/spin-orbit/Example-1`

In this example, you will calculate the magnetic anisotropy bulk FePt.

You will find the *example_3z.fdf* file and the PPs of Fe and Pt: *Fe_fept_SOC.psf* and *Pt_fept_SOC.psf*. Each calculation has to be initialized modifying the `DM.InitSpin` block, as above, updating the orientation of each atomic magnetization. As a result one has to have different energy values for each (θ,ϕ) pair.

- A) Obtain the E*tot* for three highly symmetric orientations of the initial magnetization, namely, X, Y and Z, keeping fixed the atoms in their unit cell. Again do not use the same density matrix for same calculations. Allow SIESTA to calculate it from scratch.
- B) Create a magnetization curve changing the angles at intervals of 20 degrees from the Z-axis initial orientation, to finalize along the X axis. Plot the resulting energy as a function of the varied angle. Check the orientation of the final magnetic moment in each output file. Does it coincide with the initial one?

  If this set of calculations takes too much time to be performed completely, you can try to run only a few steps and see how the total energy evolves.

Calculation of the magnetic anisotropy of FePt bulk

```
Spin   spin-orbit

%block DM.InitSpin
 1  +1.  0.  0.
 2  +1.  0.  0.
%endblock DM.InitSpin
```

θ	φ
0º	0º
10º	0º
20º	0º
30º	0º
⋮	⋮