# TBKOSTER

Tight-Binding Magnetic Molecular Dynamics for everyone

C. Barreteau, P. Thibaudeau*

Release 0.0.3
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**Abstract**

# Contents



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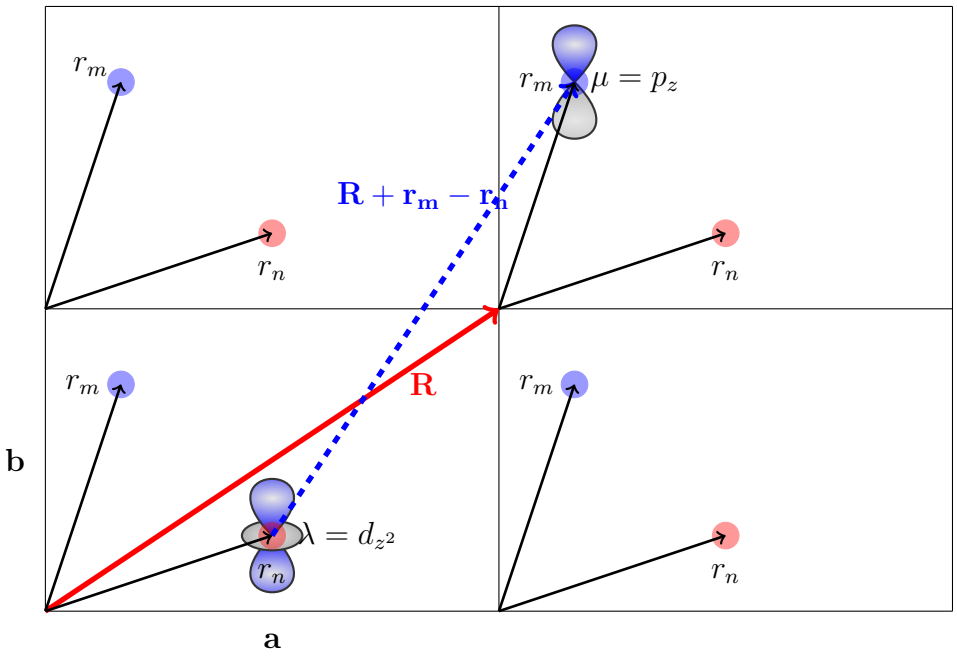
# Preface

In this manual we describe the TBKOSTER code.




**The manual contains:**

• Background theory for magnetic Tight-Binding with several atoms per unit-cell, periodic boundary conditions and overlaps.
• Installation guide
• Instructions to run the code
• TBKOSTER process and post-process options.
• Description of input and output files.

CHAPTER 1

# Background theory

• **General TB formalism** with several atoms per unit-cell, non-collinear magnetism, overlap integrals and periodic boundary conditions is described thoroughly in file TB.pdf.

• **NRL TB** Hamiltonian is described in the review paper: *An efficient magnetic tight-binding method for transition metals and alloys* C. Barreteau, D. Spanjaard, MC Desjonqueres Comptes Rendus Physique **17** 406-429 (2016).

• **Magnetic Force Theorem (MFT)** and its application to the calculation of magneto-crystalline anisotropy can be found in: *Magnetocrystalline anisotropy energy of Fe(001) and Fe(110) slabs and nanoclusters: A detailed local analysis within a tight-binding model* D. Li, A. Smogunov, C. Barreteau, F. Ducastelle, and D. Spanjaard Phys. Rev. B **88** 214413 (2013).

• **TB spin dynamics** is described in *Spin dynamics from a constrained magnetic tight-binding model* Ramon Cardias, Cyrille Barreteau, Pascal Thibaudeau, and Chu Chun Fu Phys. Rev. B **103**, 235436 (2021).

CHAPTER 2

# Installation

The first step is to download the latest release of TBKOSTER from its github repository. To proceed, you have to check that git is installed :

```
$ locate git
```

Then, clone the distant repository to your local one :

```
$ git clone https://github.com/araven/TBKOSTER.git
```

In order to build this documentation, a LaTeX distribution is mandatory, including some external packages such as pdflatex, bibtex and htlatex.

## 2.1 Linux

Preferred method : on Ubuntu 16.04 and later, install gfortran and cmake to compile TBKOSTER. Be sure to get the mandatory related dependencies of these packages.

```
$ sudo apt install cmake gfortran clang doxygen graphviz \
libblas-dev liblapack-dev libomp-dev texlive-latex-base \
texlive-latex-extra tex4ht
```

Be sure to update to cmake release 3.9 or higher. In order to build the code, to the root of TBKOSTER directory :

```
$ if ! test -d linux; then mkdir linux; fi
$ cd linux
$ cmake ..
$ make
```

To get access to the OpenMP implementation, then update your packages with openmp support.

If you want to use Intel compiler, MKL and Intel Lapack libraries, you have to tell this to cmake as, in sequential :

```
$ BLA_VENDOR=Intel10_64lp_seq FC=ifort cmake ..
```

Be sure that the variable MKLROOT is set accordingly.

In order to get good numerical performance, you have to produce a Release version as :

```
$ cmake -DCMAKE_BUILD_TYPE=Release ..
```

You can combine all these options. If you prefer to prepare an installation with a given installed Lapack library and gfortran try :

```
$ BLA_VENDOR=OpenBLAS FC=gfortran cmake ..
```

## 2.2 MacOS

Preferred method : on MacOS 10.11 and later, install the cmake, lapack and gfortran with llvm support, with the ports subsystem (http://www.macports.org)

```
$ sudo port install cmake gcc6 libgcc6 gcc_select \
llvm-3.9 llvm_select lapack libomp
```

In order to build the code, to the root of TBKOSTER directory :

```
$ if ! test -d macos; then mkdir macos; fi
$ cd macos
$ cmake ..
$ make
```

For both Linux and MacOS platform, you can invoke cmake with Release or Debug option in order to deploy these releases. Simply try

```
$ cmake -DCMAKE_BUILD_TYPE=Release/Debug ..; make
```

To get access to the OpenMP implementation, then update your ports with openmp package. You can easily change your settings with

```
$ port select --summary
$ port select --set llvm mp-llvm-3.9
$ port select --set gcc mp-gcc6
```

In order to get good numerical performance, you may use the OpenBLAS library and produce a Release version as :

```
$ port install openblas
$ BLA_VENDOR=OpenBLAS cmake -DCMAKE_BUILD_TYPE=Release ..
```

## 2.3 MS Windows

For Windows earlier than 10 release 1709, you have to consider the following method: download and follow the instructions to install MSYS2 software distro and building platform (http://www.msys2.org/). Open an MSYS console and first upgrade the whole system :

```
$ pacman -Syu
```

get the compilation toolchain :

```
$ pacman -S mingw-w64-x86_64-toolchain
```

get the gfortran compiler and lapack library :

```
$ pacman -S mingw-w64-x86_64-gcc-libgfortran
$ pacman -S mingw-w64-x86_64-openblas
```

get the cmake program to control the software compilation process using simple platform and compiler independent configuration files, and to generate native makefiles and workspaces that can be used in the compiler environment of your choice :

```
$ pacman -S cmake
```

In order to build the code, open a MSYS MINGW 64-bit console. To the root of TBKOSTER directory :

```
$ if ! test -d win; then mkdir win; fi
$ cd win
$ cmake -G"MinGW Makefiles" -DCMAKE_SH="CMAKE_SH-NOTFOUND" ..
$ mingw32-make
```

In order to run TBKOSTER.exe, be sure you have the TERM and TERMINFO environment variables up to date into your .bashrc file :

```
$ export TERM=xterm
$ export TERMINFO=/c/Program Files/msys/mingw64/share/terminfo
```

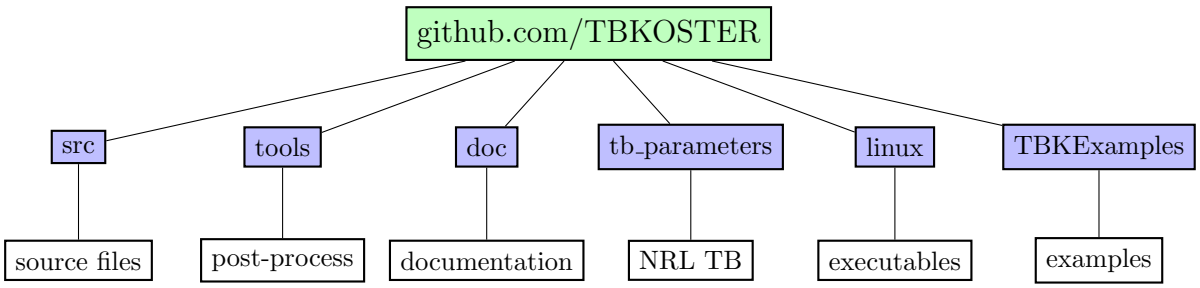
No OpenMP implementation for MS Windows has been tested.

For Windows higher than 10 release 1709, you simply have to activate the optional Windows SubSystem for Linux, download the Ubuntu Package from the Microsoft Marketplace and follow the instructions of the Linux section of this manual.

CHAPTER 3

# Running the code

## 3.1 Directories




## 3.2 linux directory

The "linux" directory should contain...

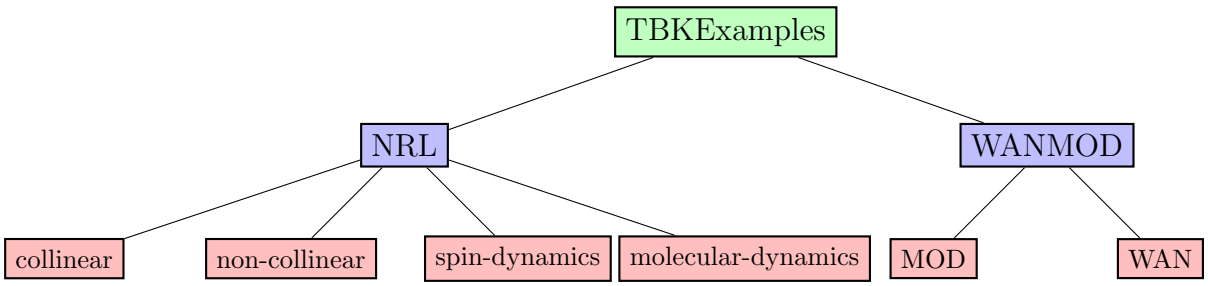
## 3.3 running TBKOSTER

TBKOSTER needs an `in_master.txt` file to run. `in_master.txt` contains all the parameters of the calculation. This file will be described in details in Input File Command Reference section.

CHAPTER 4

# Getting Started

To get started we recommend to first run the various examples that are provided within the TBKOSTER git repository.
In the TBKOSTER directory one can find a TBKExamples directory organized as follow;




In each sub-directory one can find a `README.md` file and a list of examplesxx directories each containing a `jobs.sh` file. This `jobs.sh` can be executed by the command `./jobs.sh`

CHAPTER 5

# Input File Command Reference

## 5.1 input files

### in_master.txt

The file `in_master.txt` is the main input file of TBKOSTER.

| namelist | Variable | Description |
|---|---|---|
| &calculation | | |
| | `pre_processing` (char) | type of pre-processing calculation:<br>'txt2xyz'→ write geometry in xyz format, |
| | `pre_processing_dir` (char) | directory for saving pre-processing calculation:<br>'txt2xyz'→ default value, |

| | | |
|---|---|---|
| | `processing` (char) | type of processing calculation:<br>'scf'→ **self-consistent**,<br>'md'→ molecular-dynamics.<br>'sd'→ spin-dynamics. |
| | `post_processing` (char) | type of post-processing calculation (always preceded by a scf calculation):<br>'band'→ band structure calculation,<br>'dos'→ density of states calculation.<br>'forces'→ forces calculation.<br>'mft'→ magnetic force theorem. |
| &units | | |
| | `energy` (char) | Energy unit:<br>'hau'→ **Hartree atomic units** ,<br>'rau'→ Rydberg atomic units,<br>'ev'→ electronvolts. |
| | `length` (char) | Length unit:<br>'hau'→ **Hartree atomic units**,<br>'rau'→ Rydberg atomic units,<br>'nm'→ nanometer.<br>'ang'→ angstrom. |

| | | |
|---|---|---|
| | `time` (char) | time unit:<br>'hau'→ **Hartree atomic units**,<br>'rau'→ Rydberg atomic units,<br>'fs'→ femtoseconds. |
| | `mass` (char) | Mass unit:<br>'hau'→ **Hartree atomic units**,<br>'rau'→ Rydberg atomic units,<br>'g/mol'→ g/mol. |

| &element | | |
|---|---|---|
| | `ne` (int) | Number of different elements in the system. |
| | `symbol(i)` (char) | Symbol of the elements in the system $i = 1, \cdots, ne$ |
| | `no(i)` (int) | number of orbitals of element $i = 1, \cdots, ne$ (optional) |
| | `o(i,1:no(i))` (int) | list of orbitals $i = 1, \cdots, ne$ |
| | `q(i)` (real) | input charge of element $i = 1, \cdots, ne$ |
| | `q_s(i)` (real) | $s$ input charge of element $i = 1, \cdots, ne$ |
| | `q_p(i)` (real) | $p$ input charge of element $i = 1, \cdots, ne$ |
| | `q_d(i)` (real) | $d$ input charge of element $i = 1, \cdots, ne$ |
| | `u_lcn(i)` (real) | U (in eV) value of element $i = 1, \cdots, ne$ for local charge neutrality |
| | `u_lcn_d(i)` (real) | Ud (in eV) value of element $i = 1, \cdots, ne$ for local $d$ charge neutrality |
| | `i_stoner_d(i)` (real) | Stoner parameter of element $i = 1, \cdots, ne$ for of $d$ orbitals for magnetic systems. |
| | `xi_so_p(i)` (real) | spin-orbit coupling constant of element $i = 1, \cdots, ne$ for $p$ orbitals |

| | | |
|---|---|---|
| | `xi_so_d(i)` (real) | spin-orbit coupling constant of element $i = 1, \cdots, ne$ for $d$ orbitals |
| &element_tb | | |
| | `tb_type` (char) | type of TB calculation<br>'nrl'→ **NRL TB**,<br>'mod'→ model TB (input=mod.dat),<br>'wan'→ Wannier TB (input=hr.dat). |
| | `filename(i)` (char) | file with the NRL TB parameters of element $i = 1, \cdots, ne$. |
| &lattice | | |
| | `v_factor` (real) | Multiplication factor applied to the lattice vectors. |
| | `v(1:3,3)` (real) | 3 translation vectors $\mathbf{a} = v(1,:)$,$\mathbf{b} = v(2,:)$,$\mathbf{c} = v(3,:)$, |
| &atom | | |
| | `ns` (int) | Type of magnetic system.<br>'1'→ **non magnetic system**,<br>'2'→ collinear spin,<br>'4'→ non-collinear spin. |
| | `na` (int) | Number of atoms in the system. |
| | `k_spiral(3)` (real) | spiral vector for spin-spiral calculations (defaut k_spiral=(0,0,0)). |
| | `ntag` (int) | Number of tags to give names to differents atoms. |
| | `stag(i)` (int) | Number of atoms of tag $i = 1, \cdots, ntag$. |
| | `tag(i)` (char) | tag of atom $i = 1, \cdots, ntag$. |
| | `pbc(3)` (int) | number of unit-cell in the three periodic directions to search for neighbours. if pbc($i$)=0 then there is no periodicity in direction $i$. |

| | |
|---|---|
| `r_coord` (char) | type of coordinate for atom positions,<br>'**direct**'→ in fractions of $a$, $b$ and $c$ coordinate,<br>'cartesian'→ $xyz$ coordinates, |
| `x(i,3)` (real) | coordinates of atom $i = 1, \cdots, na$, |
| `m_coord` (char) | type of coordinate for magnetism,<br>'**spherical**'→ $m$, $\theta$ and $\phi$ coordinate,<br>'cartesian'→ $xyz$ oordinates, |
| `m_listing` (char) | type of magnetic assignation,<br>'**by_atom**'→ by atom,<br>'by_tag'→ by tag, |
| `m(i,3)` (real) | magnetic coordinates of atom $i = 1, \cdots, na$ or $i = 1, \cdots, ntag$ |
| `lambda_pen_listing` (char) | type of magnetic assignation,<br>'**by_atom**'→ by atom,<br>'by_tag'→ by tag, |
| `lambda_pen(i)` (real) | magnetic penalization factor of atom $i = 1, \cdots, na$ or $i = 1, \cdots, ntag$ |
| &mesh | |
| `type` (char) | type of $k$ mesh<br>'**mp**'→ monkhorst pack mesh,<br>'path'→ path in k-space,<br>'list'→ list of $k$-vectors. |

| | |
|---|---|
| `x_coord` (char) | type of $k$ mesh<br>'**direct**'→ in fractions of $a$, $b$ and $c$ coordinate,<br>'cartesian'→ $xyz$ coordinates, |
| `gx(3)` (int) | $gx = (n_a, n_b, n_c)$, $n_i$ integer, when type=mp. |
| `dx(3)` (int) | $dx = (d_a, d_b, d_c)$ $d_i = 0, 1$ shift when type=mp. |
| `nxs` (int) | number of symmetry point when type=path. |
| `gxs` (int) | number of points between two consecutive symmetry-point when type=path. |
| `xs(1:nxs,3)` (int) | coordinate of the symmetry points when type=path |
| `xs_label(1:nxs)` (int) | label (G,X,M,K etc..) of the symmetry points when type=path |
| `nx` (int) | number of $k$ points when type=list. |
| `x(1:nx,3)` (int) | coordinate of the $k$ points when type=list |

&hamiltonian_tb

| | |
|---|---|
| `e_e_interaction` (char) | type of electronic interaction<br>'**stoner**'→ monkhorst pack mesh,<br>'ujb'→ TB+U(J,B), |
| `m_penalization` (char) | type of magnetic penalization<br>'**none**'→ no penalization<br>'r'→ penalization of the amplitude of the spin moment $m(i)$ for each atom.<br>'r,$\theta$'→ penalization of the amplitude of the spin moment $m(i)$ and on the $\theta(i)$ angle for each atom.<br>'r,$\theta$,$\phi$'→ penalization of the amplitude of the spin moment $m(i)$ and on the $\theta(i)$ and $\phi(i)$ angles for each atom.<br>'$\theta$'→ penalization of the the $\theta(i)$ angle for each atom.<br>'$\theta$,$\phi$'→ penalization of the $\theta(i)$ and $\phi(i)$ angles for each atom.<br>'$\phi$'→ penalization of the $\phi(i)$ angles for each atom. |

| &energy | | |
|---|---|---|
| | `smearing` (char) | type of smearing<br>'**mp**'→ Methfessel Paxton,<br>'fd'→ Fermi Dirac,<br>'mv'→ Marzari-Venderbilt,<br>'g'→ Gaussian, |
| | `degauss` (real) | electronic broadeding |
| | `fixed_fermi_level` (logical) | '**false**'→ Fermi level determined by number of electrons in the system,<br>'true'→ Fermi level fixed to a given value `en_f_ffl`, |
| | `en_f_ffl` (entier) | value of the fixed "Fermi level" if fixed_fermi_level=true |
| | `fixed_spin_moment` (logical) | '**false**'→ ,<br>'true'→ Fermi spin moment calculation, the total magnetization being equal to `m_fsm`, |
| | `m_fsm` (entier) | value of the fixed spin moment when fixed_spin_moment=true |
| &mixing | | |
| | `type` (char) | type of smearing<br>'**broyden**'→ Broyden mixing<br>'linear'→ linear mixing, |

| | | |
|---|---|---|
| | `alpha` (real) | mixing coefficient $0 < \alpha < 1$ |
| | `n_init` (int) | first step of Broyden mixing (default 1) |
| | `n_hist` (int) | number of history steps of Broyden mixing (default 50) |
| &scf | | |
| | `verbose` (logical) | type of smearing<br>'**false**'→ minimum writing in out_log.txt file<br>'true'→ verbose writing in out_log.txt file, |
| | `delta_en` (real) | energy crtiterium for scf calculation |
| | `delta_q` (real) | charge crtiterium for scf calculation |
| | `ni_min` (int) | miniumum number of iteration (default 2) |
| | `ni_max` (int) | maximum number of iteration (default 50) |

## post-processing

### a) band

`band/in_band.txt`

| namelist | Variable | Description |
|---|---|---|
| &band | | |
| | `proj` (char) | type of projection<br>'**none**'→ no projection,<br>'site'→ atomic site projection,<br>'spin'→ spin projection (only if $ns = 4$) to plot spin-textures.<br>'orbit'→ orbit projection (only if $ns = 4$) to plot orbit-textures.<br>'spin,orbit'→ spin and orbit projection (only if $ns = 4$) to plot spin and orbit-textures. |

| | | |
|---|---|---|
| | `i_min` (int) | lowest band index to include in the calculation (default $i_min = 1$) |
| | `i_max` (int) | largest band index to include in the calculation (default $i_max = nmax$) |
| | `na_band` (int) | number of atomic sites on which projection should be done (default na_band=0). |
| | `ia_band(1:na_band)` | index of the atomic sites. |

`band/in_mesh.txt`

| namelist | Variable | Description |
|---|---|---|
| | `type` (char) | type of $k$ mesh<br>'**mp**'→ monkhorst pack mesh,<br>'path'→ path in k-space,<br>'list'→ list of $k$-vectors. |
| | `x_coord` (char) | type of $k$ mesh<br>'**direct**'→ in fractions of $a$, $b$ and $c$ coordinate,<br>'cartesian'→ $xyz$ coordinates, |
| | `gx(3)` (int) | $gx = (n_a, n_b, n_c)$, $n_i$ integer, when type=mp. |
| | `dx(3)` (int) | $dx = (d_a, d_b, d_c)$ $d_i = 0, 1$ shift when type=mp. |
| | `nxs` (int) | number of symmetry point when type=path. |
| | `gxs` (int) | number of points between two consecutive symmetry-point when type=path. |
| | `xs(1:nxs,3)` (int) | coordinate of the symmetry points when type=path |
| | `xs_label(1:nxs)` (int) | label (G,X,M,K etc..) of the symmetry points when type=path |

| | | |
|---|---|---|
| | `nx` (int) | number of $k$ points when type=list. |
| | `x(1:nx,3)` (int) | coordinate of the $k$ points when type=list |

**b) PDOS**

`dos/in_dos.txt`

| namelist | Variable | Description |
|---|---|---|
| &dos | | |
| | `nen` (int) | number of energy points |
| | `na_dos` (int) | number of atomic sites on which the pdos will be projected |
| | `ia(1:na_dos)` (int) | index of the sites. |
| | `en_min` (real) | lower bound of energy window. |
| | `en_max` (real) | upper bound of energy window. |

`dos/in_energy.txt`

| namelist | Variable | Description |
|---|---|---|
| &energy | | |
| | `smearing` (char) | smearing type<br>'**mp**'→ Mathfessel Paxton,<br>'mv'→ Marzari Vanderbilt,<br>'fd'→ derivative of Fermi-Dirac.<br>'g'→ Gaussian. |

| | | |
|---|---|---|
| | `degauss` (real) | broadening |

`dos/in_mesh.txt`

In `dos/in_mesh.txt` all the options of `&mesh` are available however for PDOS one usually only use a MP k-point grid. Hence we have only listed below the most common parameters.

| namelist | Variable | Description |
|---|---|---|
| | `type` (char) | type of $k$ mesh<br>'**mp**'→ monkhorst pack mesh,<br>'path'→ path in k-space,<br>'list'→ list of $k$-vectors. |
| | `gx(3)` (int) | $gx = (n_a, n_b, n_c)$, $n_i$ integer, when type=mp. |
| | `dx(3)` (int) | $dx = (d_a, d_b, d_c)$ $d_i = 0, 1$ shift when type=mp. |

### c) MFT (magnetic force theorem)

The magnetic force theorem is used in two contexts: to evaluate the magnetocrystalline anisotropy or to compare the total energy of different magnetic configurations.

`mft/in_mft.txt`

| namelist | Variable | Description |
|---|---|---|
| &mft | | |
| | `calc` (char) | type of calculation<br>'**mae**'→ magnetic anisotropy calculation,<br>'mconfig'→ calculation of various magnetic non-collinear configurations, |

| | |
|---|---|
| `type` (char) | type of mesh in $(\theta, \phi)$<br>'mesh'$\rightarrow$ regular mesh over the full spherical coordinates,<br>'list'$\rightarrow$ list of several $(\theta, \phi)$ angles,<br>'path'$\rightarrow$ path between various $(\theta, \phi)$ angles, |
| `na_mft` (int) | number of site on which the energy is projected (default na_mft=0) |
| `ia(1:na_mfr)` (int) | index of the sites, if na_mft=0 no need to specify all the indices. |
| `nxa` (int) | • **calc=mae&type=mesh**: (`nxa`,`nxa`) mesh over the spherical coordinates,<br>• **calc=mae&type=path**: `nxa` is the number points between two angles,<br>• **calc=mae&ype=list**: `nxa` is the number of angles in the list,<br>• **calc=mfonfig**: `nxa` is the number of magnetic configurations. |
| `mconfig(na,nxa,3)` (real) | define explicitly the `nxa` magnetic configurations over the `na` atoms of system |
| `nangle` (int) | in case type=path; nangle is the number of angles ( 2) to generate the path. |
| `angle_xs(nxa,3)` (real) | list of angles in spherical coordinates |

`mft/in_energy.txt`

| namelist | Variable | Description |
|---|---|---|
| &energy | | |
| | `smearing` (char) | smearing type<br>'**mp**'→ Mathfessel Paxton,<br>'mv'→ Marzari Vanderbilt,<br>'fd'→ derivative of Fermi-Dirac.<br>'g'→ Gaussian. |
| | `degauss` (real) | broadening |

`mft/in_mesh.txt`

In `mesh/in_mesh.txt` all the options of `&mesh` are available however for MFT one only use a MP k-point grid. Hence we have only listed below the most common parameters.

| namelist | Variable | Description |
|---|---|---|
| | `type` (char) | type of $k$ mesh<br>'**mp**'→ monkhorst pack mesh,<br>'path'→ path in k-space,<br>'list'→ list of $k$-vectors. |
| | `gx(3)` (int) | $gx = (n_a, n_b, n_c)$, $n_i$ integer, when type=mp. |
| | `dx(3)` (int) | $dx = (d_a, d_b, d_c)$ $d_i = 0, 1$ shift when type=mp. |

## 5.2 output files

# Bibliography


[1] *Magnetism of iron: from the bulk to the monatomic wire* Gabriel Autès, Cyrille Barreteau, Daniel Spanjaard and Marie-Catherine Desjonquères J. Phys.: Condens. Matter **18** 6785-6813 (2006) .

[2] *Magnetocrystalline anisotropy energy of Fe(001) and Fe(110) slabs and nanoclusters: A detailed local analysis within a tight-binding model* D. Li, A. Smogunov, C. Barreteau, F. Ducastelle, and D. Spanjaard Phys. Rev. B **88** 214413 (2013).

[3] *An efficient magnetic tight-binding method for transition metals and alloys* C. Barreteau, D. Spanjaard, MC Desjonqueres Comptes Rendus Physique **17** 406-429 (2016).

[4] *Magnetocrystalline anisotropy of Fe, Co, and Ni slabs from density functional theory and tight-binding models* Ludovic Le Laurent, Cyrille Barreteau, and Troels Markussen Phys. Rev. B **100**, 174426 (2019).

[5] *Spin dynamics from a constrained magnetic tight-binding model* Ramon Cardias, Cyrille Barreteau, Pascal Thibaudeau, and Chu Chun Fu Phys. Rev. B **103**, 235436 (2021).