WIEN2WANNIER 1.0 User's Guide

From linearized augmented plane waves to maximally localized Wannier functions.

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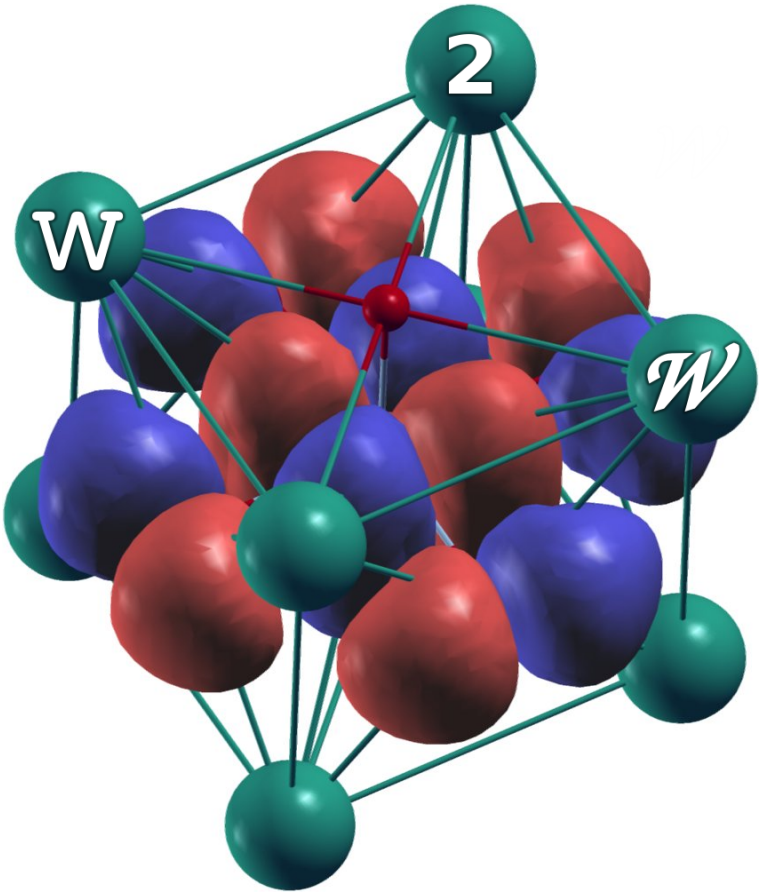

Contents

1 Introduction

In the solid state theorist's tool kit, algorithms based on density functional theory (DFT) represent the backbone applications. One of the more popular codes available is the WIEN2k package [2, 3]. It is based on dividing the real space unit cell into "muffin-tin" spheres centered on the ionic cores and an interstitial region. On the former, basis function with more or less atomic features are employed, while on the latter plain waves are used. The combined basis functions are called (linearized) augmented plane waves (LAPW).

While in WIEN2k a k-space representation of wave functions is convenient, there are many applications where a real-space picture is preferable: Determining transport properties (hopping parameters), visualization, and, especially, in codes relying on local orbital basis functions such as dynamical mean-field theory (DMFT [4]). One way to change to a real space representation is a Fourier transform of the Bloch states $\psi_{n\boldsymbol{k}}(\boldsymbol{r})$ from the DFT calculation, yielding

$$w_{m\boldsymbol{R}}(\boldsymbol{r}) = \frac{V}{(2\pi)^3} \int_{BZ} dk \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \left(\sum_n U^{(\boldsymbol{k})}_{nm} \psi_{n\boldsymbol{k}}(\boldsymbol{r}) \right) . \tag{1.1}$$

The resulting functions $w_{m\boldsymbol{R}}(\boldsymbol{r})$, parametrized by a direct lattice vector $\boldsymbol{R}$, are called Wannier functions. Due to the additional phase factors $U^{(\boldsymbol{k})}_{nm}$, which all lead to valid Wannier functions, there is considerable ambiguity in the choice of the real space basis set. This can be overcome by choosing Wannier orbitals $w_{m\boldsymbol{R}}(\boldsymbol{r})$ with minimal real-space extent (spread $\langle \Delta \boldsymbol{r}^2 \rangle$). These are known as maximally localized Wannier functions (MLWF). A popular program to compute the MLWF for a given set of Bloch functions is WANNIER90 [5, 6].

Unfortunately, the application of WANNIER90 to the LAPW basis set of WIEN2k is not as straightforward as for a pure plane wave basis. In this user's guide we describe the package WIEN2WANNIER which provides an interface between WIEN2k and WANNIER90. In any scientific publications arising from the use of WIEN2WANNIER, we ask that you cite cite Ref. [1]

> J. KUNEŠ, R. ARITA, P. WISSGOTT, A.TOSCHI, H. IKEDA, K. HELD,
> Comp. Phys. Commun. **181**, 1888 (2010), arXiv:1004.3934

to acknowledge your use of our code. When using WANNIER90, you should site Ref. [5]

> A.A. MOSTOFI, J.R. YATES, Y.-S. LEE, I. SOUZA, D. VANDERBILT, N. MARZARI,
> Comput. Phys. Commun. 178, 685 (2008), arXiv:0708.0650

independently of WIEN2WANNIER (cf. WANNIER90 user's guide [6]).

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2 Quickstart

Contents

This section outlines the procedure for a "standard" WIEN2WANNIER calculation. A detailed description of the individual programs can be found in Section 3. For a quick reference, see the plain-text file `CHEATSHEET`.

2.1 Preparatory steps

Before running WIEN2WANNIER, one needs a converged WIEN2k calculation. Additionally, during the setup for WIEN2WANNIER, the bands which are to be taken into account will have to be specified, and the main character (e.g., *d* bands on atom 2) of these bands should be known.

To obtain this information, a combination of partial DOS and bandstructure, or a "band character" plot is often expedient (e.g. `spaghetti`'s "fat bands" option, or `SpaghettiPrimavera` and `prima.py`, available in the *unsupported software* section of the WIEN2k website).

Copy Required Files

As a "zeroth" step before a Wannier projection, it is recommended to use the script

```
prepare_w2wdir subdir
```

to create the subdirectory *`subdir`* where the rest of the workflow will take place. Thus, one WIEN2k calculation can be the starting point of several WIEN2WANNIER runs.

2.2 Interface & Wannierization

Write Input Files

The script `init_w2w` takes the following steps:

`x kgen -fbz` generates the non-symmetrized k-mesh that WANNIER90 requires. The density of the mesh influences the quality of localization and visualization of the Wannier functions. Remark: The interface was only tested with unshifted k-meshes.

x findbands looks in *case*.output1 for bands in a given energy range $[E_{\text{min}}, E_{\text{max}}]$, and outputs the corresponding band indices $b_{\text{min}}, b_{\text{max}}$. To choose the energy window of interest, consult a (p)DOS and/or band structure plot.

write_inwf writes the main input file *case*.inwf for the interface. The band indices $b_{\text{min}}, b_{\text{max}}$ have to be specified, and initial projections A_{mn} may be given in terms of atomic sites and appropriate spherical harmonics.

write_win writes the input file for wannier90.x, *case*.win, on the basis of *case*.inwf and other files.

x wannier90 -pp reads the k-mesh in *case*.win and writes a list of nearest-neighbor k-points to *case*.nnkp.

Run Interface

After running init_w2w, one can proceed:

x lapw1 before the actual interface run, the eigenvectors and eigenvalues for the new (non-symmetrized) k-mesh have to be computed.

x w2w computes the overlaps M_{mn}, initial projections A_{mn} and eigenvalues E_n, and writes them to *case*.mmn, *case*.amn, and *case*.eig.

Run Wannierization

Finally,

x wannier90 computes the $U(\boldsymbol{k})$ by maximum localization. Output is stored in *case*.wout. The Wannier orbitals should be converged to a spread which is usually smaller than the unit cell of the structure.

2.3 Verification & Postprocessing

After a successful WANNIER90 run, one should check if the centers and spreads of the Wannier functions (printed in *case*.wout) are sensible. Another important consistency check is to compare the Wannier-interpolated bandstructure to the one computed by WIEN2k. WIEN2WANNIER also provides programs to create a real-space plot of the Wannier functions.

Compare Bandstructures

With the option hr_plot=T, WANNIER90 writes a bandstructure derived from the Wannier-interpolated Hamiltonian $H(\boldsymbol{k})$ to *case*_band.dat. To compare this to the bandstructure computed by spaghetti, e.g. in gnuplot, use the command (including a conversion from Bohr^{-1} to Ångström^{-1})

```
p 'case.spaghetti_ene' u ($4/0.53):5, 'case_band.dat' w l
```

Plot Wannier Functions

`write_inwplot` asks for a real-space grid on which the Wannier functions should be plotted, and writes *`case`*`.inwplot`.

`x wplot -wf `*`m` evaluates Wannier function number m on the real-space grid, and writes the density $|w_m(\boldsymbol{r})|^2$ to *`case_m`*`.psink` and the phase $\arg w_m(\boldsymbol{r})$ to *`case_m`*`.psiarg`.

`wplot2xsf` converts all *`case`*`*.psink` plus *`case`*`*.psiarg` files in the directory to `xsf` files which can be opened by XCrySDen.

`xcrysden --xsf `*`case_m`*`.xsf.gz` ; pick "Tools → Data Grid" from the menu and press OK. In the isosurface controls window choose an appropriate isovalue, e.g. 0.1, and check the "Render +/- isovalue" box.

3 Detailed description

Contents

This section lists the programs included in WIEN2WANNIER, along with brief descriptions and usage summaries. All programs have online help (`-h`), which may be more complete than the material here.

Programs that are described here include: the "main" WIEN2WANNIER programs `w2w` and `wplot`; several utility programs used in a typical WIEN2WANNIER run; and some programs that are needed in special cases, or grew out of WIEN2WANNIER development and are provided here in the hope that they will be useful, even if they are not needed in the context of WIEN2WANNIER.

3.1 W2W (compute overlaps)

This is the main program of the interface which provides the files *case*`.mmn`, *case*`.amn` and *case*`.eig` for WANNIER90 given the output of a WIEN2k run (most importantly, *case*`.vector`). `w2w` is based on `lapwdm`, since the main task, for the computation of the overlap matrices

$$M_{mn}^{(\boldsymbol{k},\boldsymbol{b})} \quad = \quad \langle \psi_{m\boldsymbol{k}} | \mathrm{e}^{-\mathrm{i}\boldsymbol{b}\cdot\boldsymbol{r}} | \psi_{n\boldsymbol{k}+\boldsymbol{b}} \rangle \tag{3.1}$$

that are stored in *case*`.mmn`, is to determine the basis functions $\psi_{n\boldsymbol{k}}(r)$ in the entire unit cell (using appropriate boundary conditions on the muffin-tin spheres).

In addition to standard WIEN2k files, a file *case*`.nnkp` is required which defines the $\boldsymbol{b}$ vectors for each $\boldsymbol{k}$ in Eq. (3.1). `wannier90.x` delivers this file when called with the flag `-pp`.

Execution

The program w2w is executed by invoking the command:

```
x w2w [-c -up|-dn -so -p] or
w2w w2w.def [#_of_proc] or w2wc w2w.def [#_of_proc]
```

While w2w itself is not parallelized, like x lapw2 -qtl, it accepts a -p switch (or #_of_proc) to read parallel vector and energy files.

With spin-orbit coupling (-so), w2w must be called separately for -up and -dn, producing *case*.mmn{up,dn}, *case*.amn{up,dn}, and *case*.eig{up,dn}. In a second step, the M_{mn} and A_{mn} must be added (and the eigenvalues copied) to produce *case*.mmn, *case*.amn, and *case*.eig, on which WANNIER90 may be run. This step is done by the program w2waddsp, which is automatically invoked by x wannier90-so.

Therefore, with SOC it is convenient to use a constrained spin-polarized calculation (runsp_c) instead of a non-spin-polarized one together WIEN2WANNIER. (Alternatively, one can "fake" the spin polarization by copying *case*.vsp and *case*.fermi to up and dn, and using *case*.vectorsodn and *case*.vectorso (for up.) Also, keep in mind that there are twice as many bands as for a calculation without SOC.

Input

A sample input file for WIEN2WANNIER is given below. It can be generated using write_inwf.

```
---------------------- top of file: case.inwf ----------------------
BOTH              # AMN, MMN, or BOTH
 21  23           # min band, max band
  3   3           # LJMAX in exp(ibr) expansion, #WF
2          # 2:d-t2g -> 2:dxy
 2 2 -2   0.00000000   0.70710678   # iat, l, m, Re(coeff), Im(coeff)
 2 2  2   0.00000000  -0.70710678
2          # 2:d-t2g -> 2:dxz
 2 2 -1   0.70710678   0.00000000
 2 2  1  -0.70710678   0.00000000
2          # 2:d-t2g -> 2:dyz
 2 2 -1   0.00000000   0.70710678
 2 2  1   0.00000000   0.70710678
--------------------------- bottom of file ---------------------------
```

Interpretive comments follow:

line 1: free format
switch

AMN	Only determine the initial orbital projections *case*.amn
MMN	Only determine the overlap matrices *case*.mmn
BOTH	Determine both the initial orbital projections and the overlap matrices

line 2: free format
Nmin Nmax

Nmin	the minimal Bloch band from the vector file to be taken into account, determining the lower edge of the (outer) energy window
Nmax	the maximal Bloch band

line 3: free format
LJmax Nproj

LJmax	the number of terms which are used in the spherical harmonics expansion to approximate $\exp(-\mathrm{i}\boldsymbol{kb})$, usually 3–4 is sufficient.
Nproj	the number of target Wannier functions

line 4: free format

Nent	the number of entries (Y_ℓ^m terms) for this initial projection

line 5: free format
IA L M X1 X2

IA	the atom where the entry is centered
L,M	the orbital and magnetic quantum numbers ℓ and m for this entry
X,Y	the complex coefficient multiplying Y_ℓ^m (real and imaginary part)

>>> **line 5** must be repeated for each Y_ℓ^m term (i.e., Nent times)

>>> **lines 4 and 5** must be repeated for each Wannier function (i.e., Nproj times).

If "switch" is MMN, the initial projections will have no effect. One can set Nproj=0 and omit them.

3.2 WPLOT (Wannier function plotter)

`wplot` evaluates the Wannier functions on a real-space grid. It reads the transformation matrices $U(\boldsymbol{k})$ from the file *case*`.chk` written by `wannier90.x` and thereby constructs the Wannier functions from the original WIEN2k Bloch states.

Execution

The program `wplot` is executed by invoking the command:

`x wplot [-up|-dn -c -so -p -wf` *m*`]` or
`wplot wplot.def [`*m* `[#_of_proc]]` or `wplotc wplot.def [`*m* `[#_of_proc]]`

`wplot` is not parallelized, but accepts a `-p` switch (or `#_of_proc`) to read parallel `vector` files. Moreover, as a crude form of parallelization, one can run several `wplot` instances in the same directory in parallel without interference (e.g. to plot several Wannier functions on fine grids).

The input file contains the index of the Wannier orbital to be plotted; *m* above overrides this. Output goes to *case_m*`.psink` ($|w(\boldsymbol{r})|^2$) and *case_m*`.psiarg` ($\arg w(\boldsymbol{r})$).

Input

`wplot` is based on `lapw7` and shares the general structure of the input file. A sample input file for `wplot` is given below. It can be generated via `write_inwplot`, or adapted from the template in `$WIENROOT/SRC_templates`.

```
-------------------- top of file: case.inwplot --------------------
3D ORTHO         # mode O(RTHOGONAL)|N(ON-ORTHOGONAL)
-1 -1 -1 1      #x, y, z, divisor of orig
 0 -1 -1 1      #x, y, z, divisor of x-end
-1  0 -1 1      #x, y, z, divisor of y-end
-1 -1  0 1      #x, y, z, divisor of z-end
 20 20 20 0 0 0 # grid points and echo increments
NO               # DEP(HASING)|NO (POST-PROCESSING)
WAN ANG LARGE    # switch ANG|ATU|AU LARGE|SMALL
1  1             # k-point, band index
------------------------ bottom of file -------------------------
```

Interpretive comments on this file are as follows:

line 1: A3, A1
mode flag

MODE	3D	a three-dimensional grid will be specified
	nD	with $n = 0, 1, 2$ exist in `lapw7`, but are untested with `wplot`
	ANY	read arbitrary grid from *`case`*`.grid` (untested)
flag	O	grid axes will be checked for mutual orthogonality
	N	axes may be non-orthogonal

line 2: free format

ix,iy,iz,idv	Coordinates of the origin of the grid, where x=ix/idv etc. in units of the *conventional* lattice vectors

line 3: free format

ix,iy,iz,idv	Coordinates of the end points of each grid axis

>>> **line 3** must be given for each direction (i.e., n times in total for an nD grid).

line 6: free format nx, ny, nz; N N N

nx,ny,nz	number of mesh points in each direction; the additional input on this line is unused

line 6: format(A3)

tool	DEP	"dephasing": each wave function is multiplied by a complex phase factor to align it (as far as possible) to the real axis
	NO	No post-processing

line 7: format(A3,1X,A3,1X,A5)
mode iunit whpsi

mode	WAN	the only option (other modes from `lapw7` deactivated)
iunit	ANG	Ångström units are used
	AU|ATU	Atomic units are used
whpsi	LARGE	the large relativistic component for each wave functions is evaluated
	SMALL	small relativistic component

line 8: free format
iskpt iswann

iskpt	this is an unused option
iswann	the index of the Wannier function to be plotted

Finding the right window for plotting can be tricky. WANNIER90 often yields orbitals that are not centered in the home unit cell; `wplot2xsf` can shift them later on, but in `wplot` one has to "hit" the orbitals as given by WANNIER90 (see section "Final State" in *case*`.wout`). Therefore, it is recommended to start with a coarse grid (for instance $10 \times 10 \times 10$), make sure the window is correct, and only then start a calculation with a finer grid.

3.3 prepare_w2wdir (copy required files)

A WIEN2k computation can be the starting point for various runs of WIEN2WANNIER. This script creates a new subfolder of a WIEN2k directory and is invoked by

```
prepare_w2wdir subdir
```

where `subdir` is the name of the subdirectory to be created.

3.4 init_w2w (prepare WIEN2WANNIER input files)

This script guides the user through the initialization of WIEN2WANNIER phase as described in Section 2.2.

```
init_w2w [-up|-dn] [-b [OPTIONS]]
```

In batch mode (`-b`), further options are available instead of interactive input.

3.5 findbands (get band indices inside energy interval)

This program reads *case*`.output1` to identify the bands which lie within a certain energy window. The program `findbands` is executed by issuing the command:

```
x findbands window [-up|-dn -so -hf -efermi EF] or
findbands findbands.def
```

window may be given as `-emin e -emax E` or `-all e E`. The energies are in eV with $E_F = 0$. The Fermi energy is read from *case*`.fermi` (written by `prepare_w2wdir`) unless given as `-efermi` (in Ry).

The output is given in *case*`.outputfind` and consists of the bands in the interval at each k-point, as well as which bands are contained in the interval across all k-points, and which bands cross the interval at any k-point.

3.6 write_inwf (prepare input file for W2W)

This program prepares the main input file *case*.inwf for w2w. It is executed by invoking the command

write_inwf (interactive) or
write_inwf -bands Nmin Nmax PROJ [PROJ ...] (noninteractive)

It will ask (in interactive mode) for a range of bands, which are all the bands to be taken into account by w2w (including those for disentanglement). Then, it will ask for "projection specifications" PROJ = SITE:ORB[:ZAXIS[:XAXIS]], which consist of colon- separated parts naming an atomic site, an orbital, and, optionally, rotated z- and x-axes. Please see write_inwf -h and write_inwf -H axes/sites/orbitals for further information on these. Interactively, you can also use tab completion to discover input options and command line history to recall past inputs.

The program will keep asking for projections until it has accumulated as many projections as bands were specified. However, one can stop early by pressing Ctrl-D (EOF); in this case, there will be fewer Wannier functions than bands (disentanglement).

3.7 write_win (prepare input file for wannier90.x)

This program reads *case*.inwf, *case*.klist, and some other files, and produces *case*.win, the input file for wannier90.x. It is executed by invoking the command

write_win [-fresh]

If *case*.win already exists, write_win updates it. Otherwise (or if -fresh is given), the template in $WIENROOT/SRC_templates is used.

3.8 wannier90 (wrapper for wannier90.x)

A wrapper script for wannier90.x is provided to take care of spin polarization and spin-orbit coupling. In the context of WIEN2WANNIER, wannier90.x is executed by invoking the command

x wannier90 [-up|-dn|-so|-pp] or wannier90 [-up|-dn|-so|-pp]

The wrapper script must be able to find the executable wannier90.x, i.e. you have to either have it in your $PATH, or edit the script wannier90_lapw to provide the location.

With -pp, wannier90.x will produce *case*.nnkp; with -so, w2waddsp will be called to add the spin channels together before running wannier90.x.

Extensive diagnostic output goes to *case*.wout, error messages to *case*.werr; the full results (in particular the $U(\boldsymbol{k})$ matrices) are stored in the binary file *case*.chk.

3.9 w2waddsp

In calculations including spin-orbit coupling, WANNIER90 has to be invoked on *case*.mmn and *case*.amn files which contain the sum of the overlaps / projections for the two spin channels.

(This procedure is needed also for non-spin-polarized cases, cf. Section 3.1.) To this end, `w2waddsp` reads *case*`.mmn{up,dn}`, *case*`.amn{up,dn}` and writes *case*`.mmn`, *case*`.amn`.

There is usually no need to call this program manually, it is run by `x wannier90-so`. If needed, it is executed by invoking the command

`x w2waddsp` or `w2waddsp w2waddsp.def`

after running `x w2w -up` and `-dn`.

3.10 write_inwplot (prepare input file for WPLOT)

This program may help in preparing the input file for `wplot`. (Alternatively, copy the template from `$WIENROOT/SRC_templates`.) It is executed by invoking the command

`write_inwplot` *case*

3.11 wplot2xsf

This program converts the files *case_m*`.psink` and *case_m*`.psiarg` produced by `wplot` to files *case_m*`.xsf` which can be opened, e.g., in XCrySDen [7] or VESTA [8].

Note that only real data can be represented in the `xsf` file. Therefore, $|w(\boldsymbol{r})|^2 \operatorname{sgn} \mathrm{Re}\, w(\boldsymbol{r})$ is saved by default. (In most cases the Wannier functions are real anyway.)

`wplot2xsf` has a number of options (see `wplot2xsf -h`), but usually it is executed by invoking the command

`wplot2xsf [-up|-dn]`

If all the required files have their standard names, this will convert all the plots in the current directory.

By default, `wplot2xsf` reads *case*`_centres.xyz`, and shifts the Wannier functions so that their centers have the coordinates given in that file. If `translate_home_cell` (and `write_xyz`) is set in *case*`.win`, this will result in a plot where the Wannier centers lie in the "home" unit cell.

3.12 convham (Fourier transform Wannier Hamiltonian)

This program Fourier transforms the WANNIER90 real space Hamiltonian $H(\boldsymbol{R})$ (*case*`_hr.dat`) to its k-space representation $H(\boldsymbol{k})$ (*case*`.ham_fine`) on the k-points given by *case*`.klist`. In this way, if the real-space Hamiltonian is sufficiently localized, $H(\boldsymbol{k})$ may be interpolated to arbitrarily fine k-grids. `convham` is executed by invoking the command

`x convham [-band]` or
`convham convham.def`

3.13 shifteig

w2w shifts the Fermi energy (as given in *case*.fermi in Ry) to zero in *case*.eig. If needed, this program can be used to apply an additional shift by DE (in eV). shifteig is executed by invoking the command

```
x shifteig [-up|-dn] -efermi DE or shifteig shifteig.def DE
```

3.14 rephase

Often, the plotted Wannier functions show a non-trivial phase. This program reads the psiarg files to determine the most probable phases of all Wannier functions. Then, the input for the interface file *case*.inwf is rewritten in a way that a subsequent run of WIEN2WANNIER and WANNIER90 leads to real Wannier orbitals (this does not work in all cases). The Fortran program rephase is invoked by the command

```
rephase case [-w] [-up/-dn] [-wf=idx_wann]
```

where the option -w means that *case*.inwf is automatically updated (future wien2wannier runs will then have a higher probability of producing real Wannier orbitals) and the option -w idx_wann indicates that the action is only applied for the Wannier function idx_wann.

3.15 joinvec (join parallel vector files)

This program joins together the partial vector and energy files from a parallel calculation into one *case*.vector and one *case*.energy. It is executed by invoking the command

```
x joinvec [-up|-dn -c -so]
```

All .vector_* files are merged into one .vector file containing the header of the first file .vector_1 (and correspondingly for the .energy files).

3.16 write_insp (write input file for SPAGHETTI)

This script is actually a utility script for WIEN2k use. It updates the Fermi energy read from *case*.scf2 in the input file for spaghetti, *case*.insp. It is invoked by

```
write_insp [-up/-dn]
```

4 Installation

This procedure assumes that WIEN2k is unpacked and configured (i.e. you have run `siteconfig`) in a directory `$WIENROOT`.

4.1 WIEN2WANNIER

Get the source from `http://www.ifp.tuwien.ac.at/forschung/arbeitsgruppen/cms/software-download/wien2wannier/` and unpack,

```
$ tar -xvf wien2wannier-X.Y.tar.gz
```

The directory `wien2wannier-X.Y/` has been created. Installation instructions are provided in the file `INSTALL`.

4.2 WANNIER90

WANNIER90 can be downloaded from `http://wannier.org`. It should be compiled with the same settings as WIEN2WANNIER, because `wplot` needs to read the binary `chk` file. You can find these settings in `$WIENROOT/{COMPILER,OPTIONS}`. Refer to the WANNIER90 documentation for furtherinstallation instructions.

5 Getting help

Additional information about all programs can be accessed via the help flag, `program -h`. Before asking the authors, please take a look at the FAQ section below which may answer the question.

The WIEN2WANNIER distribution also includes a file `CHEATSHEET`, which concisely summarizes the usual steps of a calculation.

5.1 FAQ

How does one choose the initial projections?

There is no general rule to choose the initial projections which have to be prepared in the `inwf` file. There are, however, some hints which usually help:

- In the energy interval of interest, identify the main atoms which contribute to the partial DOS. These atoms are usually good centers for the initial projections. The character of these atomic contributions can also be seen via the partial DOS. This usually leaves you with a clear idea which angular momentum quantum number combination is adequate.
- In problems with higher (e.g. octahedral) symmetry, crystal field splitting often separates originally degenerate manifolds in energy. Then the intuitive choice would be to take m_l combinations for the corresponding crystal field states, e.g. for t_{2g}.
- A glance at the bandstructure often helps to consider the multiplicity of equivalent WF and to identify certain hybridizations.
- It often helps to define the projections mutually orthogonal. In this case, the first step in WANNIER90, the orthogonalization is already taken into account at the level of wien2wannier.

The resulting Wannier orbitals are not localized

Several possible reasons (this list is not complete)

- mixing up Bohr/Angstrom units in the `.win` file at the unit cell definition.
- choosing non-optimal initial projections
- the number of k-points is too small (can be easily checked by increasing the number of k-points)

The bandstructure of WIEN2k and WANNIER90 does not match

In case of mismatch in terms of the x axis (k vectors), this usually traces back to a Bohr/Angstrom mismatch of WIEN2k and WANNIER90, which can be overcome by simply rescaling the x axis, eg. in gnuplot:

```
p 'case _band.dat' u ($1*0.5291):2 w l,'case.spaghetti_ene' u 4:5
```

If the x axis is fine and the bands themselves differ strongly, then one might have

- non-optimal initial projections
- too few k-points (can be easily checked by increasing the number of k-points)
- chosen the frozen energy window in WANNIER90 in a wrong way. This usually happens in cases with disentanglement where WANNIER90 has difficulties identifying the optimal subspace.

I obtained the error message "Eq. (B1) not satisfied" when starting WANNIER90

The default tolerance for the k mesh in WANNIER90 is quite small. Thus, it can happen that the k mesh from WIEN2k is correct but completeness relations in WANNIER90 are not fulfilled. There is an easy workaround, since WANNIER90 provides an input variable kmesh_tol which has to be inserted in the `.win` file and set to an appropriate value (eg. 0.0001).

When plotting a Wannier orbital in XCrySDen I can see nothing

One possible reason is that the WF centers do not have to be necessarily in the home unit cell at $[0\,0\,0]$. In the plotting workflow, the interface programs usually account for this by translating the WF to the home cell. However, the spatial mesh for `wplot` has to be defined with respect to the original centers which come out of WANNIER90. These centers can be found in the `.wout` file, and are automatically printed out when calling `write_inwplot` in order to write the input for `wplot`. Example: assume the WF is centered at $[-0.5\ -0.5\,;-0.5]$ in the basis of conventional unit vectors. Then, appropriate mesh vectors might be

```
-1 -1 -1 1     #x, y, z, divisor of orig
 0 -1 -1 1     #x, y, z, divisor of x-end
-1  0 -1 1     #x, y, z, divisor of y-end
-1 -1  0 1     #x, y, z, divisor of z-end
```

since this defines a cube centered at $[-0.5\ -0.5\ -0.5]$.

How can I access the Hamiltonian in the basis of Wannier functions?

The Hamiltonian $H(k)$ in the basis of Wannier orbitals is computed in WANNIER90 internally in the subroutine hamiltonian_get_hr() at `hamiltonian.F90`(WANNIER90 version 1.2).

My Wannier orbitals are not centered at the home unit cell when plotted with XCrySDen

Within WANNIER90 it happens quite frequently that a maximally localized Wannier function is not centered within the home unit cell, which is displayed by default by XCrySDen. The interface

program `write_win` automatically activates the option translate_home_cell in the WANNIER90 input file. Then, WANNIER90 should produce a file *case* `_centres.xyz`, where the vectors of all WF are stored which translate the orbital to the home unit cell. If this file cannot be located by `wplot2xsf` or the option –noshift is activated, no translation is conducted and the WF appear centered at their original position.
There is also a second, more peculiar, reason for the translation problem. WANNIER90 is very harsh when it comes to translating the centres of WF. If a Wannier orbital is centered only 1% outside of the home unit cell (which may happen easily due to numerical reasons) the WF is translated by a unit vector. In these cases, either manipulation of the *case* `_centres.xyz` file, or the WANNIER90 source code can help.

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