Notes on:
Automated Wannier Functions construction

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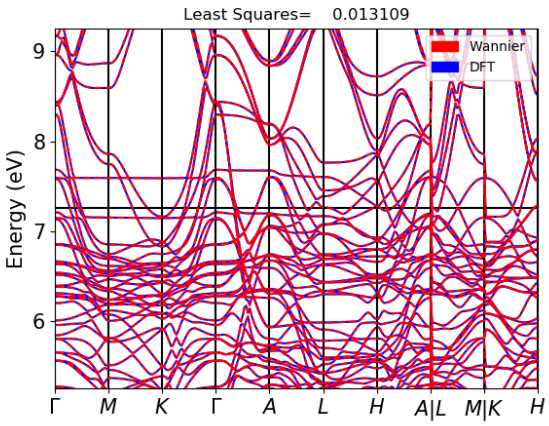
February 15, 2022



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The following colour code is used throughout the notes to make the distinction of items easier.

Colour	Explanation
green	File of the scheme
purple	Output file
red	External Software
blue	Variable in the code
orange	Function in the code

Table 1: Colour explanation throughout the notes

1 Basic idea

The main goal of the automated wannier functions construction scheme is to provide a general framework in order to compute the wannier functions of any 3D system (excluding f-block elements) automatically. This is achieved by combining the DFT package VASP [1, 2, 3, 4] and the wannier functions package Wannier90 [5].

The used methodology of constructing Wannier functions consists of the four calculation steps:

1. Self consistent calculations using VASP
2. Density of states calculations using VASP
3. Wannier functions construction using Wannier90
4. Band structure calculations using VASP

More details on the methodology are found in [6]

The framework targets at:

- generating the input files needed for VASP
- generating the input files needed for Wannier90
- plotting based on output

- identifying the missing parts due to errors in the procedure

The following external files and/or software are required to run the scheme:

- POSCAR
- VASP (tested in version: 5.2.12)
- Pseudopotentials for VASP
- Wannier90 (tested in version: 2.0.0)
- Python3
- Pymatgen

The scheme is based on several in-house developed scripts written in Python3, which include:

- vasp_input_hte_cif.py
  File to generate the input of VASP
- input_parameters.py
  The input file. Calculation parameters are defined here.
- highsymk.py
  File to generate the input of VASP
- autoconstruction.py
  File the generate the input file of Wannier90
- plotband.py
  File to plot the band structure obtained from VASP
- compareband.py
  File to plot the band structure obtained from VASP and Wannier90 in a single plot.

In the following, the reader can get familiar with the input file and practice the acquired knowledge following the detailed given examples.

2 Input

The input file of the automatic wannier functions construction scheme is called input_parameters.py. It consists of six python functions which are listed and explained in more detail below:

1. **Function calc_type()**

```
def calc_type():
        ## Type of Calculations you want to perform.

        SC = True      ## Self consistent
        DOS = True     ## Density of states
        WANN = True    ## Wannier functions construction
        BAND = True    ## Band structure

        SMART_SEARCH = False ## Searches and determines
    the progress of each directory. If set 'True', none of
     the previous tags is valid.

        CALCS = [SC,DOS,WANN,BAND]

        return CALCS, SMART_SEARCH
```

The variables of the calc_type() function and their meaning is summarised in Tab 2.

Variable	Type	Explanation
SC	boolean	Self consistent
DOS	boolean	Density of states
WANN	boolean	Wannier functions
BAND	boolean	Band structure
SMART_SEARCH	boolean	Switch between the two functionalities

Table 2: Variables in calc_type()

The code provides two different functionalities which are based on the choice of the tag SMART_SEARCH.

(a) SMART_SEARCH = FALSE
The code generates the input files of each of the steps their variables defined as TRUE.

(b) SMART_SEARCH = TRUE
The code ignores the rest variables and determines the progress of the calculation by reading the output files of VASP and wannier90. This functionality is used to automatically determine the missing steps of the procedure and only resubmit these parts.

2. **Function running_parameters()**

```
def running_parameters():
        cores = 24
        time = 24      ## in hours (always integer)
        memory = 0      ## in GB (if 0, it is set
    automatically)
        pr_id = ""     ## Project id (you can find it
    using csreport command)

        return cores, time, memory
```

The variables of the running_parameters() function and their meaning is summarised in Tab. 3.

Variable	Type	Explanation
cores	$n,\ n \in \mathbb{Z}^+$	number of cores
time	$n,\ n \in \mathbb{Z}^+$	time in hours
memory	$n,\ n \in \mathbb{Z}$	memory in GB
pr_id	string	project id

Table 3: Variables in running_parameters()

The code provides two different ways of defining the variable memory

(a) memory $\neq 0$
The code sets the memory based on the provided value (integer only)

(b) memory $= 0$
The code automatically determines the memory based on experience acquired from previous calculations (preferable for high throughput).

3. Function directories()

```
def directories():
        vasp_dir = ''   ## Path of VASP's executable
        wannier90_dir = '' ## Path of Wannier90's
    executable
        pseudopotentials_dir = ''  ## Path of
    pseudopotentials
        python_dir = '' ## Path of python#

        vasp_output = ''  ## Output file of VASP (only
    name, no path) eg. vasp.log
        wannier_output = ''  ## Output file of wannier90
    (only name, no path) eg. wannier90.wout

        return vasp_dir, wannier90_dir,
    pseudopotentials_dir, vasp_output, wannier_output
```

The variables of the directories() function and their meaning is summarised in Tab. 4.

Variable	Type	Explanation
vasp_dir	string	Path of VASP executable
wannier90_dir	string	Path of wannier90 executable
pseudopotentials_dir	string	Path of Pseudopotentials
python_dir	string	Path of python
vasp_output	string	Name of VASP output file
wannier_output	string	Name of wannier90 output file

Table 4: Variables in directories()

4. Function hte_tags()

```
def hte_tags():
        ## Input for INCAR and KPOINTS. Modify
    accordingly

        magnetism        = True   ## True if the system
    is magnetic, False otherwise
        non_collinearity = True   ## True if non-
    collinear system, False otherwise. It is set to False
    if magnetism is False
```

```
    SOC               = True   ## True if you want to include SOC, False otherwise. It is set to False if magnetism is False
    constraint        = False  ## True if you want to constrain along a certain direction. Set MAGMOM to specify the direction
    U_calc            = True   ## True if you want L(S)DA+U calculations, False otherwise

    ktype = "M"                ## M for Monkhorst Pack, G for Gamma

    kspace_density     = 50    ## KPOINTS
    kspace_density_wfs = 40    ## KPOINTS.wfs
    kspace_density_dos = 60    ## KPOINTS.dos

    ## NPAR is set automatically
    ## MAGMOM is parallel to x axis by default. Set it appropriately for different directions
    ## NBANDS is calculated automatically if it is not set (preferable for high throughput)
    ## ICHARG, LWANNIER90,  are set automatically

    incar_tags = {

    "prec" : "Accurate",
    "algo" : "NORMAL",
    "encut" : 500,
    "lorbit" : 10,
    "ediff" : 0.000001,
    "ediffg" : -0.001,
    "amix" : 0.001,
    "bmix" : 0.0001,
    "isym" : -1,
    "nelm" : 500,
    "istart" : 1,
    "ismear" : 1,
    "sigma" : 0.06,
    }

    return incar_tags, magnetism, non_collinearity, SOC, U_calc, kspace_density, kspace_density_wfs, kspace_density_dos
```

The variables of the hte_tags() function and their meaning is sum-

marised in Tab. 5

Variable	Type	Explanation
magnetism	boolean	Switches magnetism on and off
non_collinearity	boolean	Switches non_collinearity on and off
SOC	boolean	Switches SOC on and off
constraint	boolean	Switches constraint on and off
U_calc	boolean	Switches L(S)DA+U on and off
ktype	M or G	M for Monkhorst Pack, G for Gamma grid
kspace_density	$n,\ n \in \mathbb{Z}^+$	kspace density of the SC step
kspace_density_wfs	$n,\ n \in \mathbb{Z}^+$	kspace density of the WFS step
kspace_density_dos	$n,\ n \in \mathbb{Z}^+$	kspace density of the DOS step
incar_tags		See VASP documentation

Table 5: Variables in directories()

The dictionary incar_tags may contain all VASP tags available here However, certain limitations apply:

- Tag NPAR is computed automatically. Do not set.
- Tag MAGMOM is set as parallel to x-axis for every atom by default. If another magnetisation direction is the desired, please set it appropriately. Consider the length of the string based on the tags NON_COLLINEARITY and SOC.
- Tag NBANDS is set automatically if not defined. It is advised not to set it unless a specific reason exists.
- If constraint = True, MAGMOM should exist since it defines the constrained direction. Additionally, its length has to be consistent with the values of NON_COLLINEARITY and SOC. See section 6.1 of the Appendix for more details regarding constrained calculations.

5. Function pseudopotentials()

```
def pseudopotentials():
        pseudep = {
        "H" : "H", "He" : "He", ... , "Og" : "NA"
```

```
        }
        return pseudep
```

The pseudopotential of each atom in the pseudep dictionary is defined according to Tab. 6.

Input of dictionary pseudep		
Key → element	**Separator**	**Value → chosen pseudopotential**
"H"	:	"H"
"Sn"	:	"Sn_d"

Table 6: Input of pseudep dictionary

6. Function ldau_values()

This function is active only if U_calc = TRUE in hte_tags()

```
def ldau_values():
        u_val = {
        "La" : 9, "Ce" : 9, ... , "Lr" : 9
        }

        j_val = {
        "La" : 0.8, "Ce" : 0.8, ... , "Lr" : 0.8
        }

        l_val = {
        "La" : 2, "Ce" : 2, ... , "Lr" : 2
        }
        return u_val,j_val,l_val
```

The dictionaries u_val, j_val and l_val that correspond to the LDAU, LDAJ and LDAL tags in VASP for each chemical element are defined according to Tab. 7.

Input of dictionary u_val		
Key → element	**Separator**	**Value → LDAUU**
"Sm"	:	9
Input of dictionary j_val		
Key → element	**Separator**	**Value → LDAUJ**
"Sm"	:	0.8
Input of dictionary l_val		
Key → element	**Separator**	**Value → LDAUL**
"Sm"	:	2

Table 7: Input of u_val, j_val and l_val dictionaries

The code sets by default LDAUTYPE = 1 and LDAUPRINT = 2. Modification of these VASP tags is not possible from the input file but only from the source code file vasp_input_hte_cif.py. For more details see the Appendix in Section 6.2.

3 Output

The output files of the scheme depend on the variables set in the function calc_type of the input_parameters.py file. Tab. 8 summarises the output files obtained by running vasp_input_hte_cif.py and Tab. 9 the output of each of the rest files of the scheme.

Variable	Output files
Independent of variables	run.sh
If SC = True	INCAR, KPOINTS, POTCAR
If DOS = True	INCAR.dos, KPOINTS.dos, POTCAR
If WANN = True	INCAR.wfs, KPOINTS.wfs, POTCAR
If BAND = True	INCAR.band, POTCAR

Table 8: Output files of vasp_input_hte_cif.py

File of scheme	Output files
autoconstruction.py	wannier90.win
highsymk.py	KPOINTS.band
plotband.py	1.dat, ..., n.dat, band.png
compareband.py	wannband.png
input_parameters.py	No output

Table 9: Output files of the rest files of the scheme

All INCAR, all KPOINTS and POTCAR as well as the POSCAR are the input files of VASP. run.sh is the submission file (see section 6.3 of the Appendix for more details). wannier90.win is the input file of Wannier90, 1.dat,...,n.dat are supporting files needed for getting band.png which is the band structure along the chosen high symmetric kpath obtained using VASP. Finally, wannband.png displays the band structure from VASP and Wannier90 in a single plot.

4 The code in practice

All the required files are located within the folder auto_wann. The underlined folder contains a bash script temp-auto-wann.sh as well as the folder source_wann that contains the six source files of section 1 and the Examples folder. The suggested way to use the scheme is to create a template for easy use. Instructions to create the template (once) and to use the code is found in the step-by-step guide below.

4.1 Template

1. Navigate to your home directory, create a directory (template_wann) and paste the folder source_wann within the newly created directory.

```
$ cd
$ mkdir template_wann
$ cp -r ‘‘directory_of_source_wann’’/source_wann
  template_wann
```

2. Set the path of the created directory in the file temp-auto-wann.sh

3. Paste temp-auto-wann.sh in a convenient and easy to access directory (home)

```
$ cd
$ cp ``directory_of_temp-auto-wann.sh''/temp-auto-wann.
  sh .
```

4.2 Code

1. Create a directory and navigate within

```
$ mkdir my_dir
$ cd my_dir
```

2. Paste the necessary files and the template within the directory

```
$ cp ``directory_of_POSCAR_file''/POSCAR .
$ cp ~/temp-auto-wann.sh .
```

3. Run the script

```
$ sh temp-auto-wann.sh
```

5 Examples

1. **Self consistent calculation of $MnNi_2Ga$**
   Directory Example_1 contains the POSCAR file of $MnNi_2Ga$ as well as the six files of the scheme.

   Task: Create the input files of the self consistent calculation.

   Solution:

   (a) Set the input tags in calc_type() function of input_parameters.py as shown:

```
SC = True
DOS = False
WANN = False
BAND = False
SMART_SEARCH = False
```

   (b) Run the code

```
$ python3 vasp_input_hte_cif.py
```

Output: The files INCAR, POTCAR, KPOINTS and run.sh have been created.

2. **Density of States calculation of $MnNi_2Ga$**
   Directory Example_2 contains the POSCAR file of $MnNi_2Ga$ as well as the six files of the scheme.

   Task: Create the input files of the self consistent and density of states calculations.

   Solution:

   (a) Set the input tags in calc_type() function of input_parameters.py as shown:

```
SC = True
DOS = True
WANN = False
BAND = False
SMART_SEARCH = False
```

   (b) Run the code

```
$ python3 vasp_input_hte_cif.py
```

   Output: The files INCAR, INCAR.dos, POTCAR, KPOINTS, KPOINTS.dos and run.sh have been created.

3. **Input of all calculations**
   Directory Example_3 contains the POSCAR file of $MnNi_2Ga$ as well as the six files of the scheme.

   Task: Create the input files of the self consistent, density of states, wannier functions construction and band structure calculations.

   Solution:

   (a) Set the input tags in calc_type() function of input_parameters.py as shown:

```
SC = True
DOS = True
WANN = True
BAND = True
SMART_SEARCH = False
```

(b) Run the code

```
$ python3 vasp_input_hte_cif.py
```

Output: The files INCAR, INCAR.dos, INCAR.wfs, INCAR.band, POTCAR, KPOINTS, KPOINTS.dos, KPOINTS.wfs and run.sh have been created[1].

4. **Wannier90 input of YCo_2**
Directory Example_4 contains, among others, the POSCAR file of YCo_2, dos and wann directories which correspond to the density of states and the wannier functions construction respectively.

Task: Create the input file of wannier90 calculation.

Solution:
Navigate to the wann directory and run autoconstruction.py (dos/vasprun.xml file is needed).

```
$ cd  wann/
$ python3 autoconstruction.py
```

Output: The file wannier90.win has been created.

5. **Band structure calculation of YCo_2**
Directory Example_5 contains, among others, the POSCAR file of YCo_2, dos and wann and band directories which correspond to the density of states, the wannier functions construction and the band structure calculations respectively.

Task: Create KPOINTS used for the band structure calculations (KPOINTS.band).

[1]KPOINTS.band file is created with highsymk.py, see Example_5

Solution:
Navigate to the band directory and run highsymk.py

```
$ cd  band/
$ python3 highsymk.py
```

Output: The file KPOINTS has been created.

6. **SMART_SEARCH tag**
Directory Example_6 contains, among others, the POSCAR file of YCo_2, dos and wann directories which correspond to the density of states and the wannier functions construction respectively.

Task: All the necessary directories are present, however, something went wrong during the calculation and some parts are incomplete. Check the output files of each step to find out which part(s) is (are) incomplete. After finding the missing parts, use the code to resubmit only those. (Hint: Are all the directories present before and after running the code?)

Solution:

(a) Set the input tags in calc_type() function of input_parameters.py as shown:

```
SC = True
DOS = True
WANN = True
BAND = True
SMART_SEARCH = True
```

(b) Run the code
(vasp.out,dos/vasp.out,wann/vasp.out,band/vasp.out
and wann/wannier90.wout are needed).

```
$ python3 vasp_input_hte_cif.py
```

Output: Check the run.sh file to find the missing parts that are ready to submit.

7. **Band structure plot of YCo_2**
Directory Example_7 contains, among others, the POSCAR file of YCo_2,

dos and wann and band directories which correspond to the density of states, the wannier functions construction and the band structure calculations respectively.

Task: Visualise the band structure obtained from VASP

Solution:

(a) Navigate to the band directory and run plotband.py (band/PROCAR file is needed).

```
$ cd  band/
$ python3 plotband.py
```

(b) The file band.png has been created. Open it using

```
$ display band.png
```

8. **Band structure plot**
Directory Example_8 contains, among others, the POSCAR file of YCo_2, dos and wann and band directories which correspond to the density of states, the wannier functions construction and the band structure calculations respectively.

Task: Visualise the band structure obtained from VASP and the one obtained from Wannier90 in a single plot

Solution:

(a) Run compareband.py (band/1.dat,...,n.dat, band/PROCAR, wann/wannier90_hr.dat files are needed).

```
$ python3 compareband.py
```

(b) The file wannband.png has been created. Open it using

```
$ display wannband.png
```

6 Appendix

6.1 Constrained calculations

Modification of VASP tags I_CONSTRAINED_M and LAMBDA is only possible from the source code file vasp_input_hte_cif.py. Specifically, in function get_additional_tags() they are defined in the form:

```
incar_tags.append(['i_constrained_m'.upper(),1])
incar_tags.append(['lambda'.upper(),10])
```

6.2 LDA+U

Modification of VASP tags LDAUTYPE and LDAUPRINT is only possible from the source code file vasp_input_hte_cif.py. Specifically, in function get_additional_tags() they are defined in the form:

```
incar_tags.append(['ldautype'.upper(),1])
incar_tags.append(['ldauprint'.upper(),2])
```

6.3 Submission file

In case the calculations are not performed in the Lichtenberg High Performance Computer of TU Darmstadt (HRZ), please modify the generation of the submission file in the function get_run() (from line 345) of the source code file vasp_input_hte_cif.py

References

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[6] Z. Zhang, R.-W. Zhang, X. Li, K. Koepernik, Y. Yao, and H. Zhang, "High-throughput screening and automated processing toward novel topological insulators," The journal of physical chemistry letters, vol. 9, no. 21, pp. 6224–6231, 2018.