Manual

For the program "W2Auto" to work, the following software must be installed on your computer: `Python 3 with numpy, scipy` and `pandas` packages, `Wien2k, Wannier90, XTLS, Git` and `Gnuplot`.

Create a Python script (see Examples) and specify their parameters for launching Wien2k programs:

`SCFparams:`

`run` – whether to run the SCF stage

`struct_file` - name of structure file, this file could be *.struct* or *.cif.* We recommend to use `.struct` file, in this case you will avoid possible errors in `cif2struct` program. `.cif` files only for advanced users of Wien2k.

`runCommandPrefix` – prefix to run time consuming commands in parallel. For example: `'mpirun -np 16' or 'srun --ntasks=16'. Your parallel command should not finish execution before calculation ends, so do not use` *`sbatch`*.

`runParallel` – set it to `True` if your `runCommandPrefix` run command in parallel

`lapwParams` — parameters for `lapw` subprograms: `iterNum and ec`

`lstart_energy` — energy level (Ry) for `x lstart` command. If you set it in 0, will be used default value -9.0 Ry.

`Rkmax` — you can specify this value. This value will replace the default value of RKMax in `*.in1_st` file. If you set it in 0, will be used default value.

`efmod` — determines how E_F is determined. This parameter will replace the default value in `*.in2_st file`. Default value is `'TETRA'`

`ef_eval` - parameter that is different for different efmod values (see more in Wien2k User`s Guide)

`iqtlsave` - if you have some problems with the `lapw2` command, try to set this parameter in True. (see more in Wien2k User`s Guide)

DOSparams:

`run`

`runParallel`

`runCommandPrefix`

`xmin` - left border of energy on DOS plot. If you want to set it to default value (-10) set it to `None`.

BANDparams:

`run`

`runParallel`

`runCommandPrefix`

`klist_band` - name of file with klist bands

Wannierparams:

`run`

`runParallel`

`runCommandPrefix`

`wannierName` - name of directory for Wannier stage computation

XTLSparams:

`run`

`hopMatBorder` - min value of significant element in HopMat

`XTLSinput` - input file for XTLS program

`XTLS_path` – path to XTLS folder, which contains `/bin` and `/xc` folders.

common_params:

`dosInfo` - information gained from DOS analysis: `energyInterval`, `atomOrbitals`[1]

`kpoints` - number of kpoints, if 0 kpoints will be calculated automatically.

`debugMode` - if `True` save log of program execution

After setting parameters you need to call `runWien2k` function with `params` as argument, and run this Python script.

Directories for computations

Directory for launching program could have any name. Directories, in which calculations will be made, will be created automatically in `/w2webEmulator/caseBaseDir` path and will depend on name of structure file (`*.cif` or `*.struct` files). For example, for structure file `Fe3O4.struct` will be created following directories:

1. `w2webEmulator/caseBaseDir/Fe3O4` (path of computation of SCF stage)
2. `w2webEmulator/caseBaseDir/Fe3O4_DOS/Fe3O4` (path of computation of DOS stage and DOS graphs)

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[1] In `atomOrbitals` must be specified types of atoms from `*.struct` file. If in `*.struct` file there are several types of atoms with the same name, `w2auto` program will store them with postfix "_ATOM_(serial number)". In this case you need to specify names of these atoms corresponding their internal representation in program, i.e. with postfixes.

For example: In `*.struct` file there are several types(let it 5) of Oxigen atoms, all of them have the same name «O». Then if you need to specify them in `atomOrbitals` parameter, you need to do it like this: 'O_ATOM_1', 'O_ATOM_2', 'O_ATOM_3', 'O_ATOM_4', 'O_ATOM_5'.

Correct names of all types of atoms in `w2auto` program presented in `parse_log.txt` file in list with name `atomNamesList`. File `parse_log.txt` creates at the SCF stage in the same directory where configure script Fe3O4.py is.

3. `w2webEmulator/caseBaseDir/Fe3O4_Bandstructure/Fe3O4` (path of computation of Bandstructure stage and spaghetti graph)
4. `w2webEmulator/caseBaseDir/Fe3O4_Bandstructure/Fe3O4/wannierName` (path of computation of Wannier)
5. `w2webEmulator/caseBaseDir/Fe3O4_Bandstructure/Fe3O4/wannierName/XTLS` (path of computation of XTLS and spectra graphs)

All directories in `w2webEmulator/caseBaseDir` will be created **automatically.**

How to launch w2auto program

You can launch program by launching configure script Fe3O4.py in two ways:

1. `python3 -u Fe3O4.py`
2. Step 1: In the first line of configure script you should write shebang (symbols #!) and absolute path to Python interpretator, e.g. `#!/opt/anaconda/bin/python -u` or `#!/usr/bin/env python -u`

   Step 2: Make configure script executable: `chmod +x Fe3O4.py`

   Step 3: Now configure script could be launched as any executable file: `./Fe3O4.py`

Option `-u` for Python interpretator makes unbuffered binary `stdout` and `stderr`.