# orbvis: Installation and user guide

## orbvis is available on PyPI. Install it directly with pip as :

```
pip install orbvis
```

Or

```
git clone https://github.com/staradutt/orbvis.git
cd orbvis
pip install -e .
```

## Usage instructions:

**Step 1**: Generate and locate the required input files

- For orbital projected band structure:
  - PROCAR file from VASP is required
- For orbital projected DOS:
  - DOSCAR file from VASP is required

Make sure to identify the correct file path which will be required in step 2

**Step 2**: Write the config file
orbvis uses a VASP INCAR-style config file to control all plot settings

Sample config file for orbital projected bandstructure: sample_config.txt

```
# Required
MODE = band
PROCAR_PATH = ./PROCAR #provide full path to PROCAR file as identified in step 1
ISPIN = 2
SOC = false

# Orbital info format: [atom_list, "Element", orbital_list]
ORBITAL_INFO = [
    [[0,1,2], "Fe", [0,4,8]],    # s, d_xy, d_x^2-y^2 of Fe atoms 0-2
    [[3,4], "O", [1,2,3]]        # p_y, p_z, p_x orbitals of O atoms
]

# Optional customization
TITLE = Projected Bands
SAVEAS = feo_bands.png
EFERMI = 5.6
```

```
COLOR_SCHEME = 0
YMIN = -6
YMAX = 5
```

Sample config file for orbital projected dos:

```
#Required
MODE = dos
DOSCAR_PATH = ./DOSCAR #provide full path to DOSCAR file as identified in step 1
ISPIN = 1
ORBITAL_INFO = [[[0], "Ti", [0,1,2]]] # s,p_y,p_z of Ti atom 0 (start numbering from 0 in
POSCAR)
#optional
SIGMA = 0.2 #gaussian smearing
SHOW_TDOS = true
SAVEAS = dos_plot.png
```

More details on the config file is supplied in the config file syntax section.

**Step 3**: Run orbvis from the terminal. It will  generate the plot using the same filename specified in the config file.

orbvis sample_config.txt

**It is recommended to provide the full path to sample_config.txt*

## Config file syntax:

orbvis uses a configuration file to control all plotting behavior. The format is similar to a VASP-style INCAR file, with KEY = VALUE pairs. Comments begin with #

### Required Parameters:

| Parameter | Description | Mode | Example |
|---|---|---|---|
| MODE | Plot type: band or dos | both | MODE = band |
| ISPIN | Spin polarization: 1 (no spin), 2 (spin-polarized) | both | ISPIN = 1 |
| ORBITAL_INFO | Orbital projection info (see below) | both | ORBITAL_INFO = [[[0], "Fe", [0]]] |
| PROCAR_PATH | Path to PROCAR file | band only | PROCAR_PATH = ./PROCAR |
| DOSCAR_PATH | Path to DOSCAR file | dos only | DOSCAR_PATH = ./DOSCAR |

### Optional parameters:

These have default values, and can be omitted unless you want to override them.

| Parameter | Description | Default | Mode |
|---|---|---|---|
| SOC | Spin–orbit coupling: True or False | FALSE | both |
| EFERMI | Fermi level shift (float) | 0 | both |
| SAVEAS | Output file name (.png/.jpg) | output.png | both |
| TITLE | Plot title | "Orbvis" | both |
| COLOR_SCHEME | Colors used for orbitals (see below) | 0 | both |
| FIGSIZEX | Width of figure (in inches) | 10 | both |
| FIGSIZEY | Height of figure (in inches) | 6 | both |
| DPI | Output image resolution | 300 | both |
| YMIN / YMAX | y-axis limits (energy) | -5.0 / 5.0 | both |
| TRANSPARENCY | Orbital marker transparency (0–100) | 70 | both |
| LEGEND_LOC | Location of legend (matplotlib string) | None | both |

Band Mode Specific optional parameters:

| Parameter | Description | Default |
|---|---|---|
| BS_LINEWIDTH | Line width of band plot | 1.0 |
| SCALE | Orbital marker scale | 1.0 |
| PLOT_OPTION | Plot style (only 0 supported for scatter mode) | 0 |

XMIN / XMAX which set x axis limits are not allowed in band mode

DOS mode specific optional parameters:

| Parameter | Description | Default |
|---|---|---|
| TDOS_LINEWIDTH | Line width for total DOS | 1.0 |
| PDOS_LINEWIDTH | Line width for projected DOS | 1.0 |
| SIGMA | Gaussian broadening for DOS | 2.0 |
| XMIN / XMAX | Energy limits on x-axis | None |
| SHOW_TDOS | Show total DOS in PDOS plot | True |

## ORBITAL_INFO Format

ORBITAL_INFO is a list of items, each specifying:

```
[ [atom_indices], "Element", [orbital_indices] ]
```

- atom_indices: List of integers (0-based atom indices as they appear in POSCAR)
- element: String (used for label)
- orbital_indices: List of orbital indices (see below)

Example:

```
ORBITAL_INFO = [
    [[0, 1], "Fe", [0, 4, 5]],
    [[2], "O", [1, 2, 3]]
]
```

The first entry selects atoms 0 and 1, both of type “Fe”, and sums contributions from their s,d_xy and d_yz orbitals. The second entry selects atom 2, of the type “O”, and sums its contributions from p_y, p_z and p_x orbitals.

## Orbital Index Reference

| Index | Orbital |
|---|---|
| 0 | s |
| 1–3 | p_y, p_z, p_x |
| 4–8 | d_xy, d_yz, d_z^2, d_xz, d_x^2–y^2 |
| 9–15 | f orbitals |

## COLOR_SCHEME Options

| Value | Description |
|---|---|
| `0` | Auto assigns distinct colors (from `distinctipy`) |
| `1` | Auto assigns distinct Pastel colors (also `distinctipy`) |
| `["#FF0000", "#00FF00", "#0000FF"]` | Custom list of hex codes of colors such as those from coolors.co |
| `[“red”,”blue”,”green”` | Custom list of color names |
| `"tab10","tab20", “set10”` etc. | Matplotlib colormap name |

## Best Practices

- Use appropriate unicodes to label high symmetry points
- Always double-check file paths (e.g., `PROCAR_PATH`)
- Avoid using `SOC = True` with `ISPIN = 2`
- Use clear element labels in `ORBITAL_INFO`
- If unsure, omit optional parameters defaults are safe

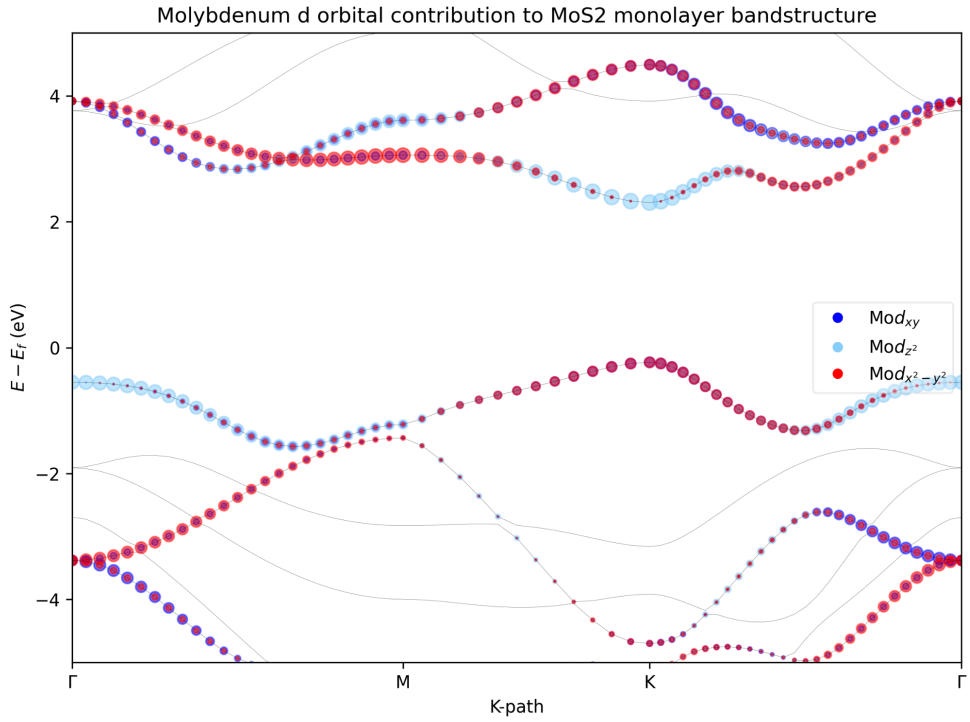
# Example config files to demonstrate usage

Examples for band mode

1. One orbital of one atom at a time, for ISPIN = 1 calculation
   MoS2 monolayer POSCAR. First atom Mo, second third atom S.
   Config file:

```
MODE = Band
TITLE = Molybdenum d orbital contribution to MoS2 monolayer bandstructure
PROCAR_PATH = MoS2_ispin1_hse/PROCAR
ISPIN = 1
ORBITAL_INFO = [[[0], "Mo", [4]], [[0], "Mo", [6]], [[0], "Mo", [8]]]
COLOR_SCHEME = ["blue","lightskyblue","red"]
PLOT_OPTION = 0
EFERMI = -2.9
SCALE = 100
TRANSPARENCY = 50
BS_LINEWIDTH = 0.1
FIGSIZEX = 8
FIGSIZEY = 6
LEGEND_LOC = center right
SAVEAS = Mo_d_MoS2_isp1.png
```

Generates:

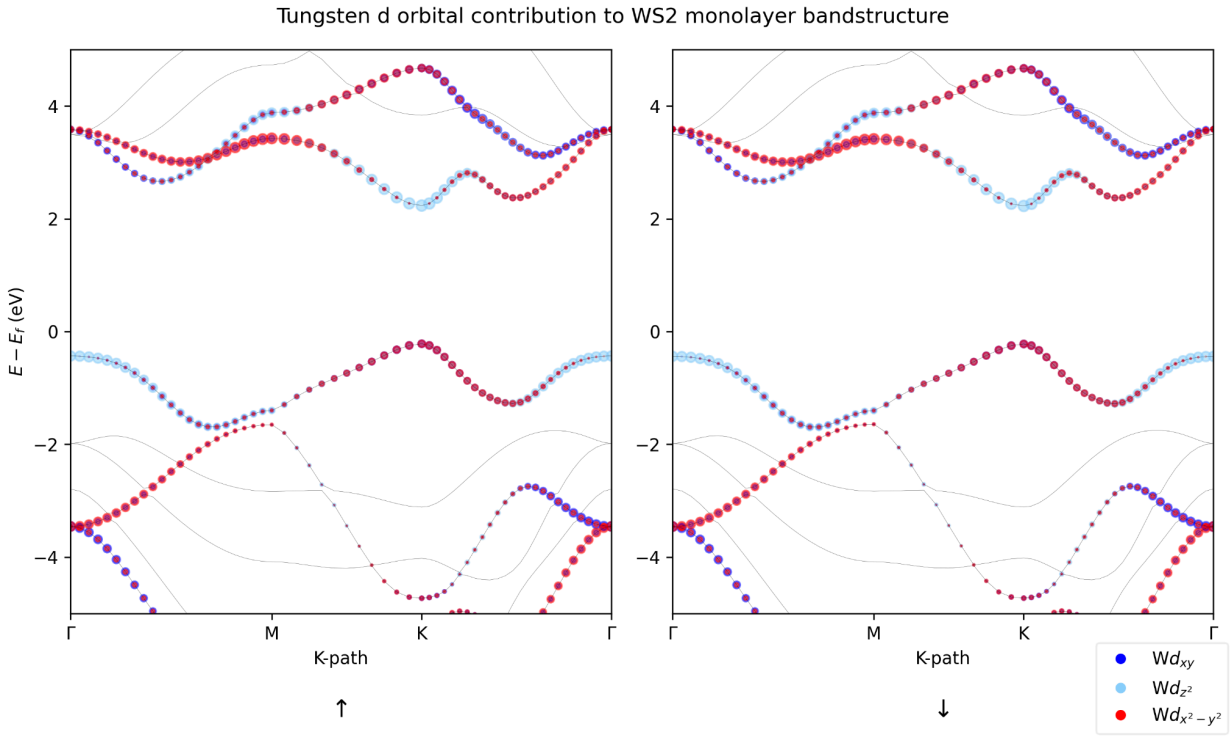



The above example produces similar results as [1] but with HSE.

2. One orbital of one atom at a time, for ISPIN = 2 calculation
   WS2 monolayer POSCAR. First atom W, second third atom S.
   Config file:

```
MODE = Band
TITLE = Tungsten d orbital contribution to WS2 monolayer bandstructure
PROCAR_PATH = WS2_ispin2_hse/PROCAR
ISPIN = 2
ORBITAL_INFO = [[[0], "W", [4]], [[0], "W", [6]], [[0], "W", [8]]]
COLOR_SCHEME = ["blue","lightskyblue","red"]
PLOT_OPTION = 0
EFERMI = -2.34
SCALE = 50
TRANSPARENCY = 50
BS_LINEWIDTH = 0.1
SAVEAS = WdWS2isp2.png
```

Generates:

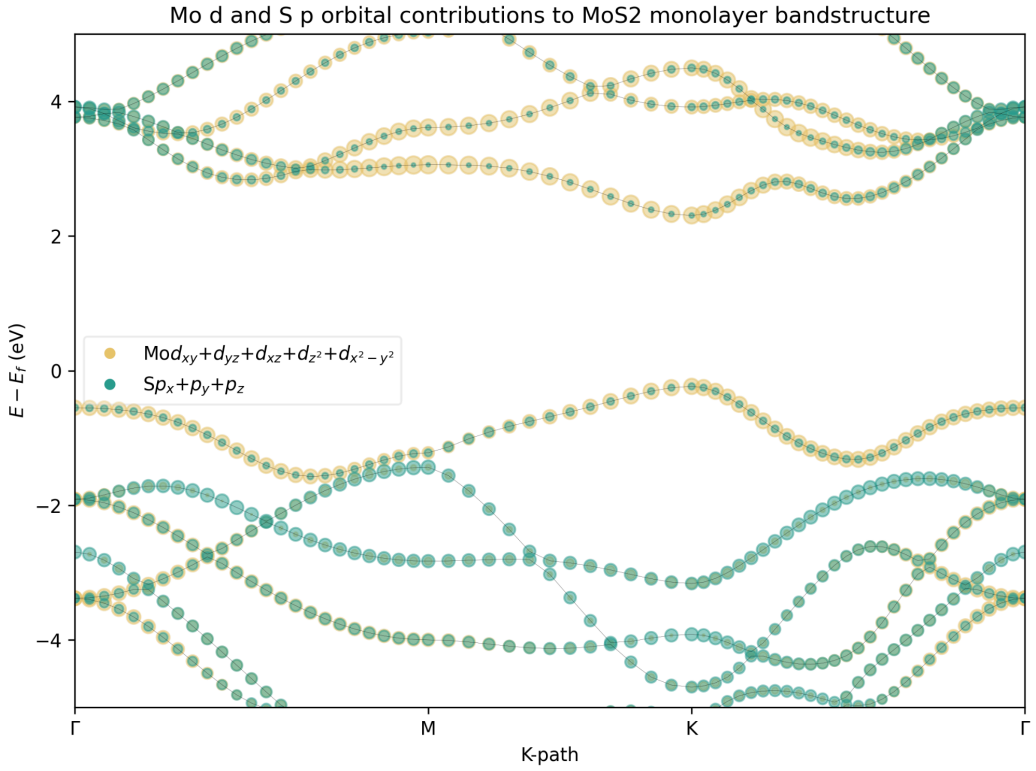



The above example produces similar results as [1] but with spin polarised HSE.

3. Many orbitals at a time, hex colors
   System: Three atom MoS2 monolayer POSCAR. First atom Mo, second third atom S.
   Config file:

```
MODE = Band
TITLE = Mo d and S p orbital contributions to MoS2 monolayer bandstructure
PROCAR_PATH = MoS2_ispin1_hse/PROCAR
ISPIN = 1
ORBITAL_INFO = [[[0], "Mo",[4,5,7,6,8]],[[1,2], "S", [3,1,2]]]
COLOR_SCHEME = ["e9c46a","2a9d8f"]
PLOT_OPTION = 0
EFERMI = -2.9
SCALE = 100
TRANSPARENCY = 50
BS_LINEWIDTH = 0.1
FIGSIZEX = 8
FIGSIZEY = 6
LEGEND_LOC = best
SAVEAS = Sp_Mod_MoS2_isp1.png
```

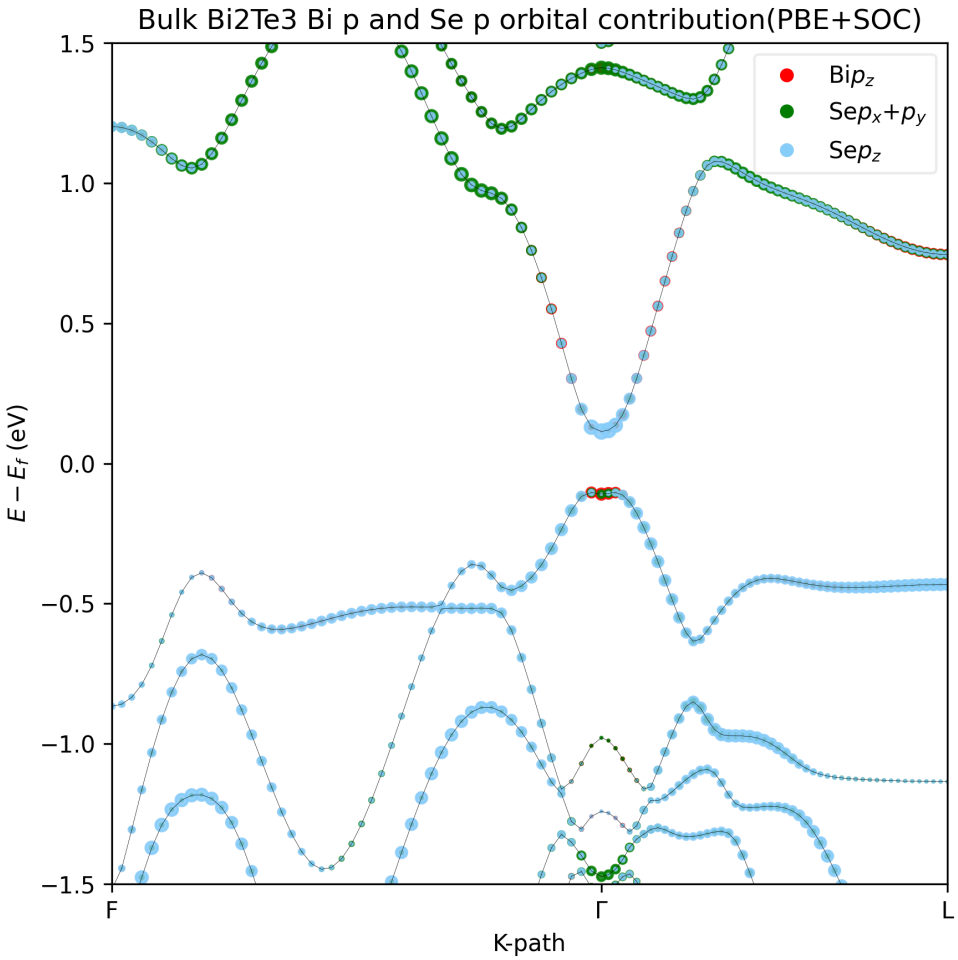
Generates:




The above example produces similar results as [1] but with HSE.

4. For SOC  calculation
   Bulk Bi2Se3 POSCAR. First two atoms Bi, next three atoms Se.

```
MODE = Band
TITLE = Bulk Bi2Te3 Bi p and Se p orbital contribution(PBE+SOC)
PROCAR_PATH = PROCAR
SOC = true
ORBITAL_INFO = [[[0,1], "Bi",[2]],[[0,1], "Se", [3,1]],[[2,3,4],"Se",[2]]]
COLOR_SCHEME = ["red","green","lightskyblue"]
PLOT_OPTION = 0
EFERMI = 4.33
SCALE = 75
TRANSPARENCY = 60
BS_LINEWIDTH = 0.1
FIGSIZEX = 6
FIGSIZEY = 6
LEGEND_LOC = best
YMAX = 1.5
YMIN = -1.5
SAVEAS = Bi2Se3bulk.png
```



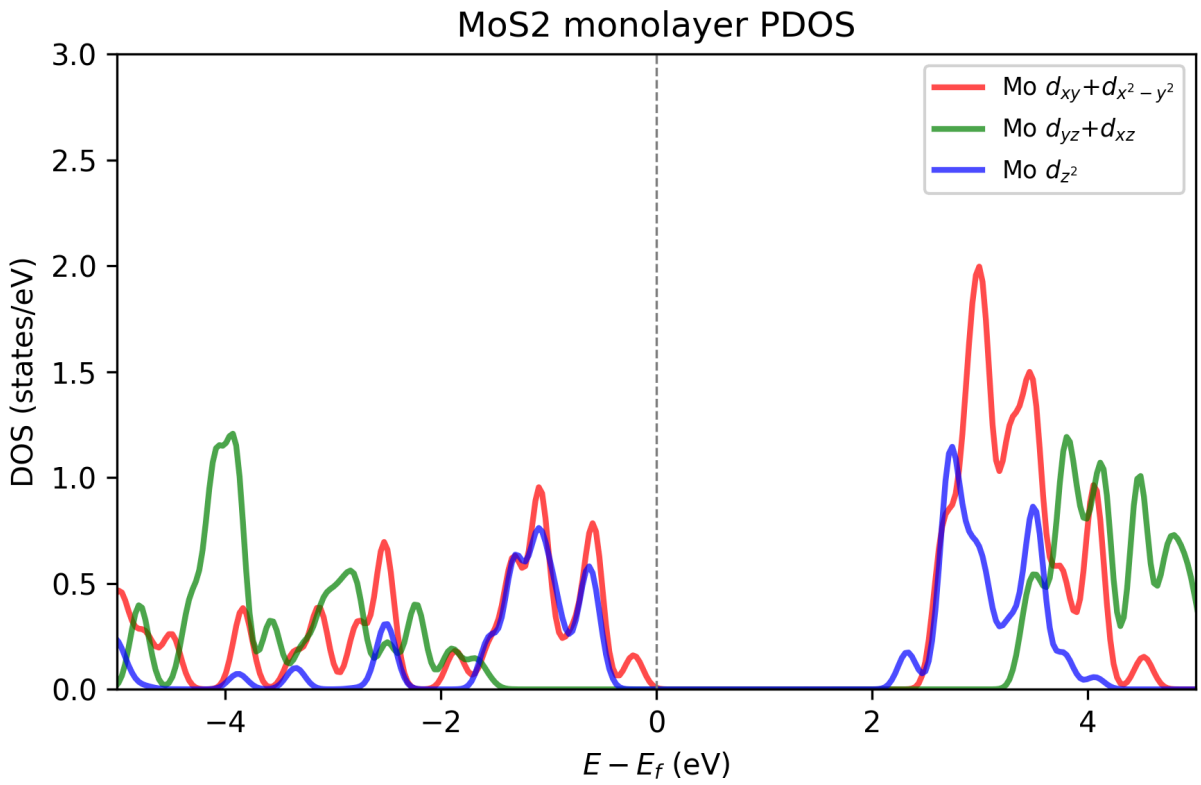

Generates results similar to [2]

## DOS mode:

1.Many orbitals of one atom at a time, for ISPIN = 2 calculation.
System: three atom MoS2 monolayer. First atom Mo, second third atom S.

```
MODE = dos
DOSCAR_PATH =/Examples/MoS2_ispin1_hse/DOSCAR
ORBITAL_INFO = [[[0], "Mo ", [4,8]],[[0], "Mo ", [5,7]],[[0], "Mo ", [6]]]
ISPIN = 1
COLOR_SCHEME = ["red","green","blue"]
SIGMA = 2.5
PDOS_LINEWIDTH = 2
SAVEAS = mos2_isp1_dos_hse.png
YMIN = 0
YMAX = 3
XMAX = 5
XMIN = -5
```

```
SHOW_TDOS = False
FIGSIZEX = 6
FIGSIZEY = 4
TITLE = MoS2 monolayer PDOS
```




Generates results similar to [1] but with HSE.

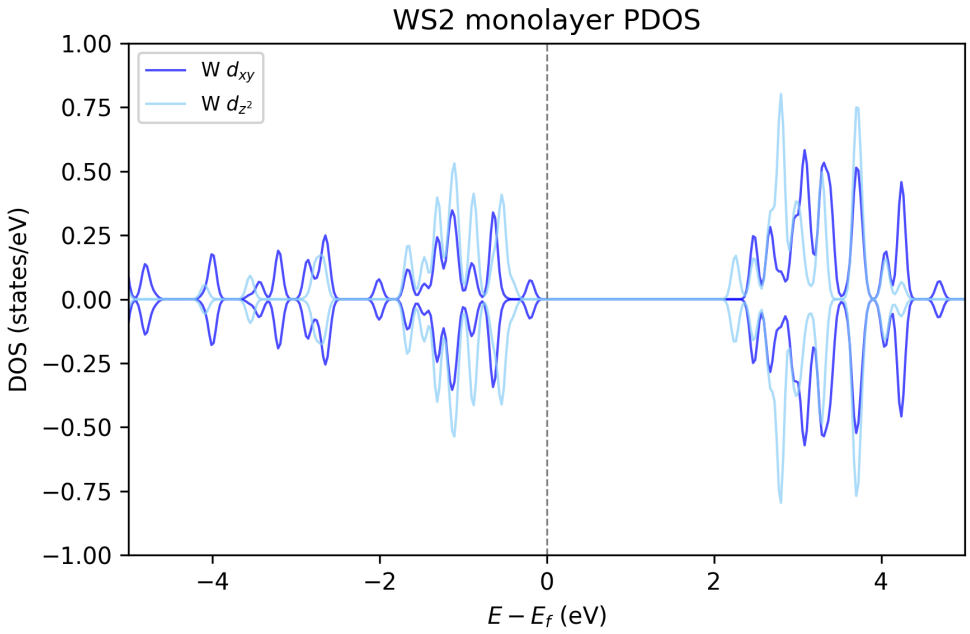
2.One orbital of one atom at a time, for ISPIN = 2 calculation.
System: WS2 monolayer DOSCAR. First atom W, second third atom S.

Config file:

```
DOSCAR_PATH = WS2_ispin2_hse/DOSCAR
ORBITAL_INFO = [[[0], "W ", [4]],[[0], "W ", [6]]]
ISPIN = 2
COLOR_SCHEME = ["blue","lightskyblue"]
SIGMA = 1.0
PDOS_LINEWIDTH = 1
SAVEAS = ws2_isp2_dos_test.png
YMIN = -1
YMAX = 1
XMAX = 5
```

```
XMIN = -5
SHOW_TDOS = False
FIGSIZEX = 6
FIGSIZEY = 4
TITLE = WS2 monolayer PDOS
```

Generates results similar to [1] but with spin polarized HSE:




References:

[1] C.-H. Chang, X. Fan, S.-H. Lin, and J.-L. Kuo, “Orbital analysis of electronic structure and phonon dispersion in MoS2, MoSe2, WS2, and WSe2,” *Physical Review B*, vol. 88, no. 19, Nov. 2013, doi: 10.1103/physrevb.88.195420.

[2] Acosta, C. M., Lima, M. P., da Silva, A. J. R., Fazzio, A., & Lewenkopf, C. H. (2018). Tight-binding model for the band dispersion in rhombohedral topological insulators over the whole Brillouin zone. *Physical Review B*, *98*(3). https://doi.org/10.1103/physrevb.98.035106