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`
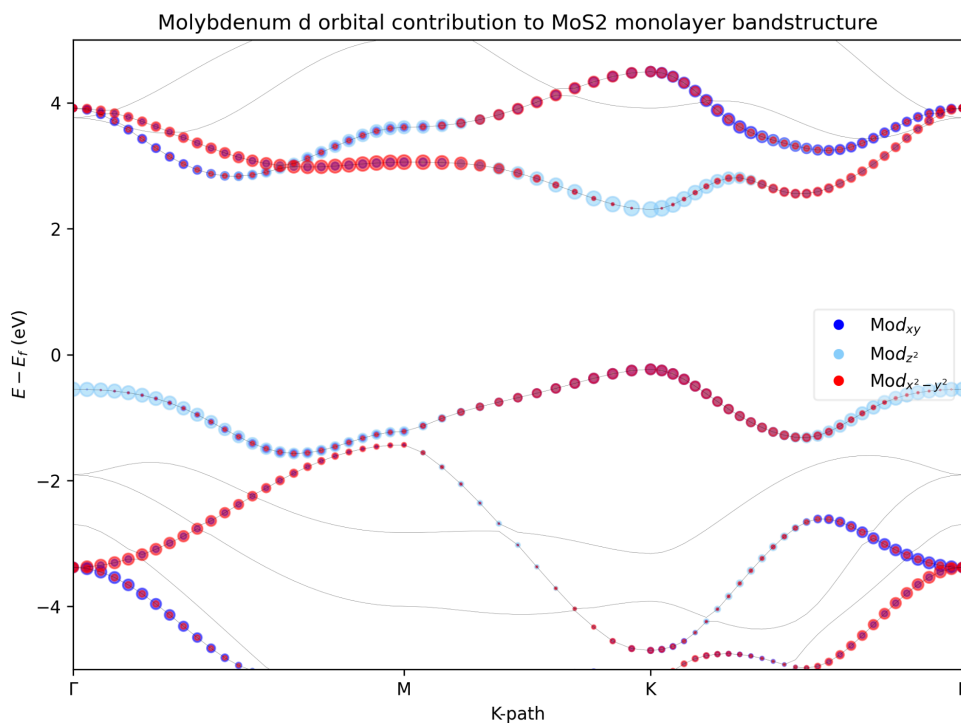- If unsure, omit optional parameters defaults are safe

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:

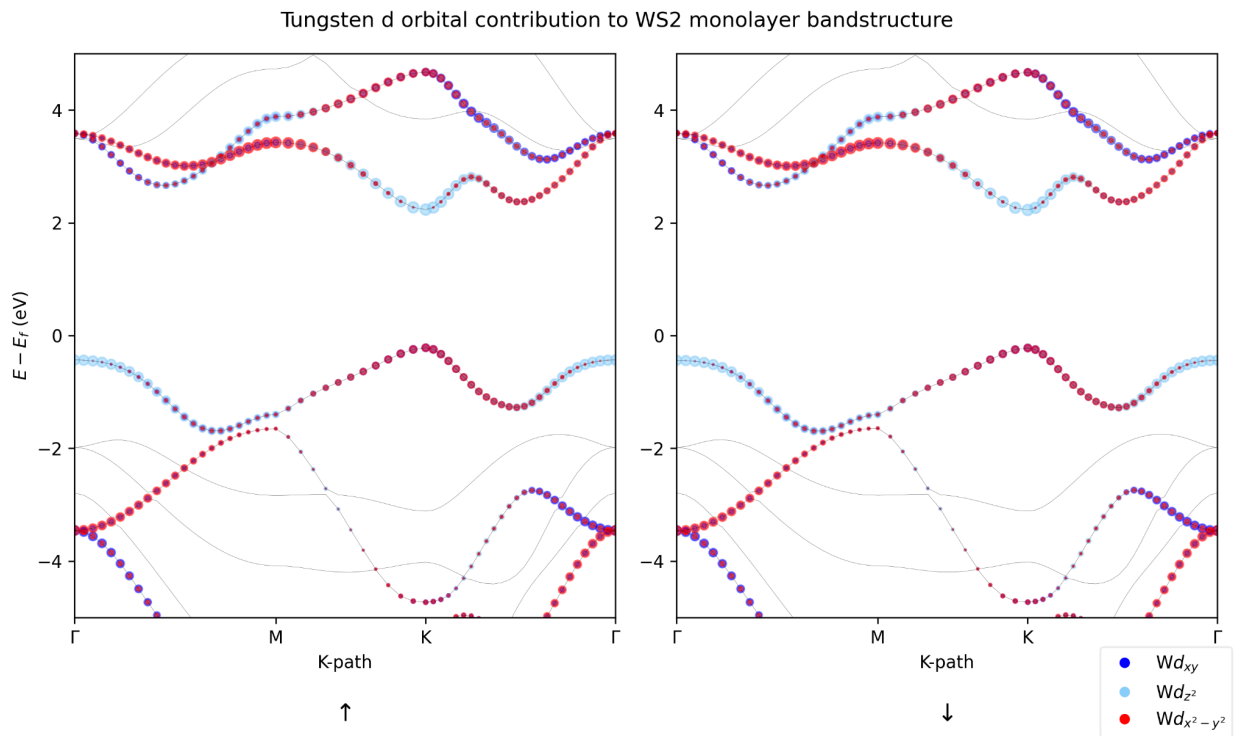The above example produces similar results as [1] but with HSE.

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:

Tungsten d orbital contribution to WS2 monolayer bandstructure

The above example produces similar results as [1] but with spin polarised HSE.
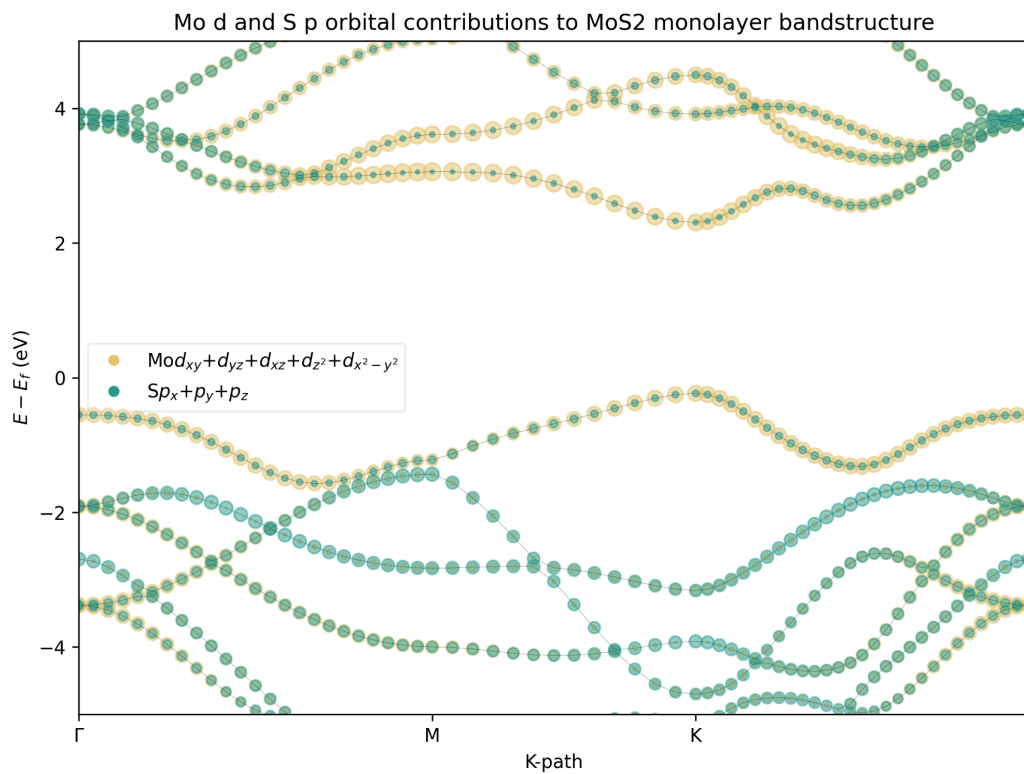
3. Many orbitals at a time, hex colors
   System: Three atom MoS2 monolayer POSCAR. First atom Mo, second third atom S.
   Config file:

```
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
```
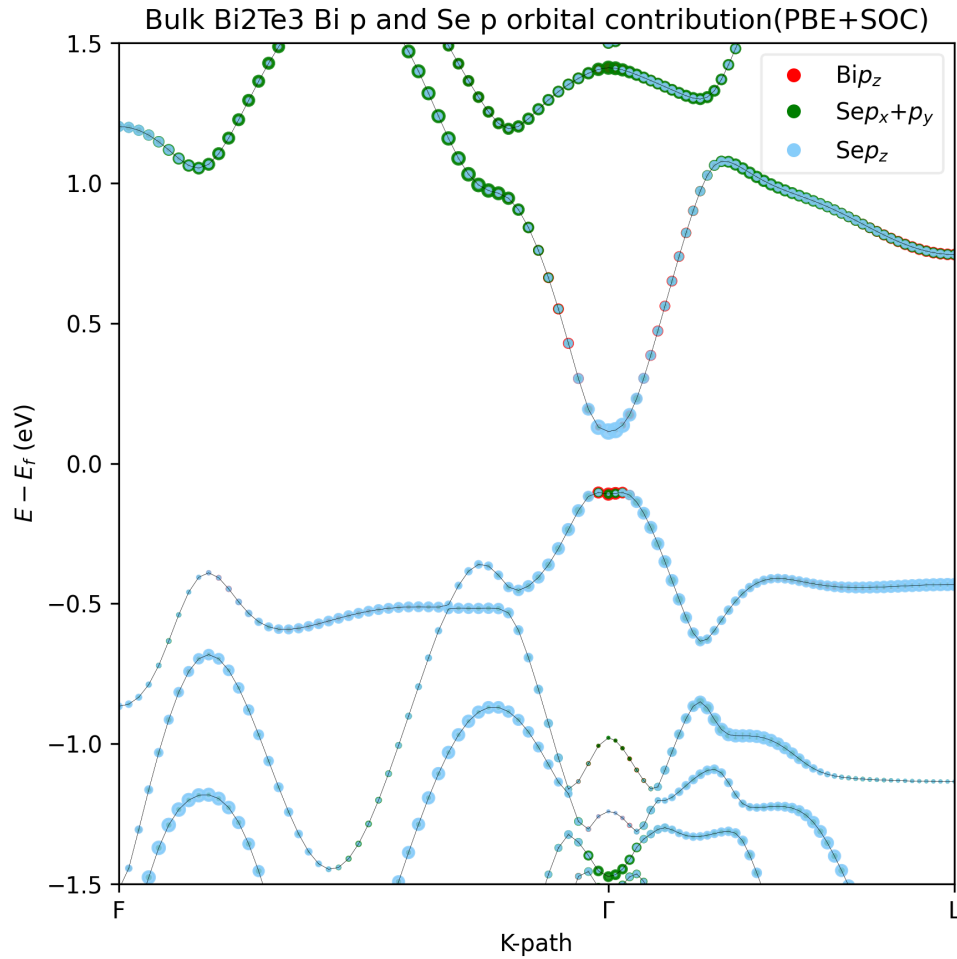
Generates:

Mo d and S p orbital contributions to MoS2 monolayer bandstructure

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
```

Bulk Bi2Te3 Bi p and Se p orbital contribution(PBE+SOC)

Legend:
- Bip_z (red)
- Sep_x+p_y (green)
- Sep_z (light blue)

Y-axis: $E - E_f$ (eV)
X-axis: K-path (F, Γ, L)

Generates results similar to [2]

5. For Disjoint K-path
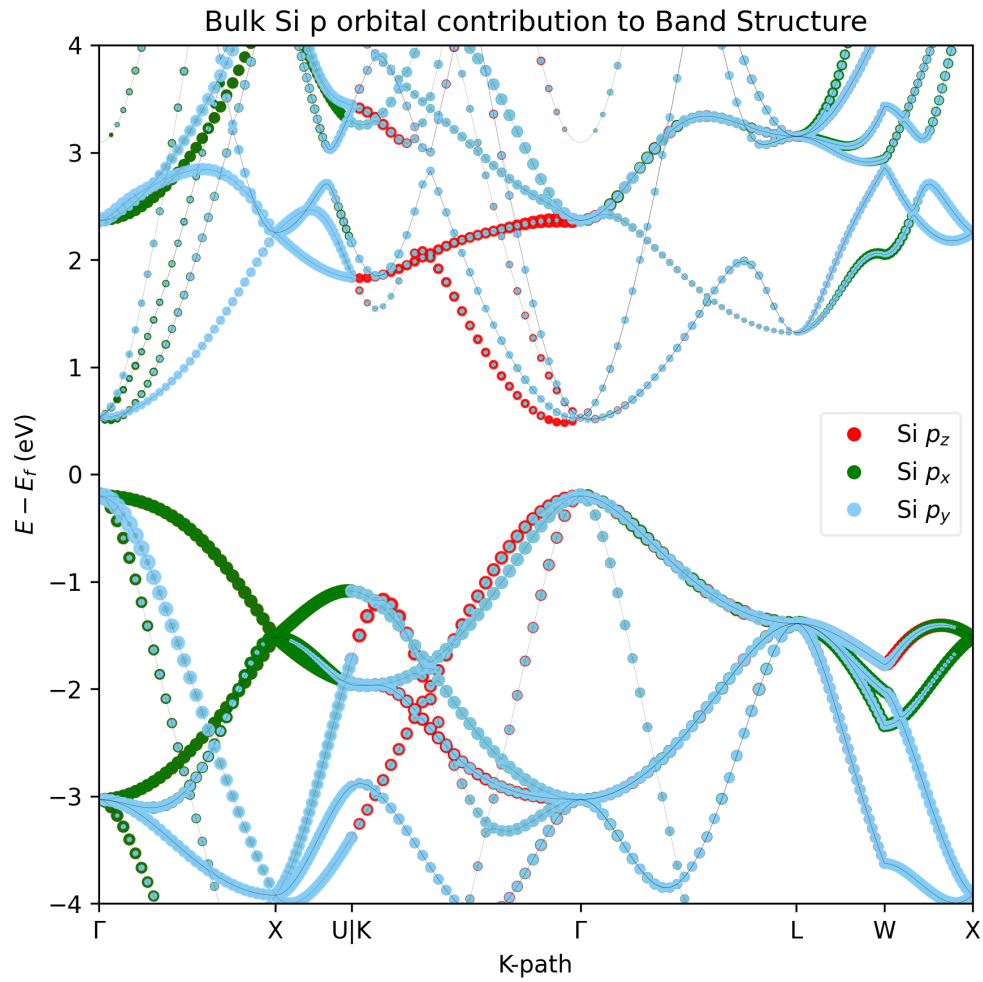   Bulk Si POSCAR. 8 Si Atoms. KPATH: Γ-X-U | K-Γ-L-W-X
    Bandconfig:

```
MODE = Band
TITLE = Bulk Si p orbital contribution to Band Structure
PROCAR_PATH = PROCAR
ISPIN = 1
ORBITAL_INFO = [[[0,1,2,3,4,5,6,7], "Si ",[2]],[[0,1,2,3,4,5,6,7], "Si ",
[3]],[[0,1,2,3,4,5,6,7],"Si ",[1]]]
COLOR_SCHEME = ["red","green","lightskyblue"]
PLOT_OPTION = 0
EFERMI = 5.955
SCALE = 100
TRANSPARENCY = 85
```

```
BS_LINEWIDTH = 0.05
FIGSIZEX = 6
FIGSIZEY = 6
LEGEND_LOC = best
YMAX = 4
YMIN = -4
SAVEAS = Si_OrbBs.png
```

Output:
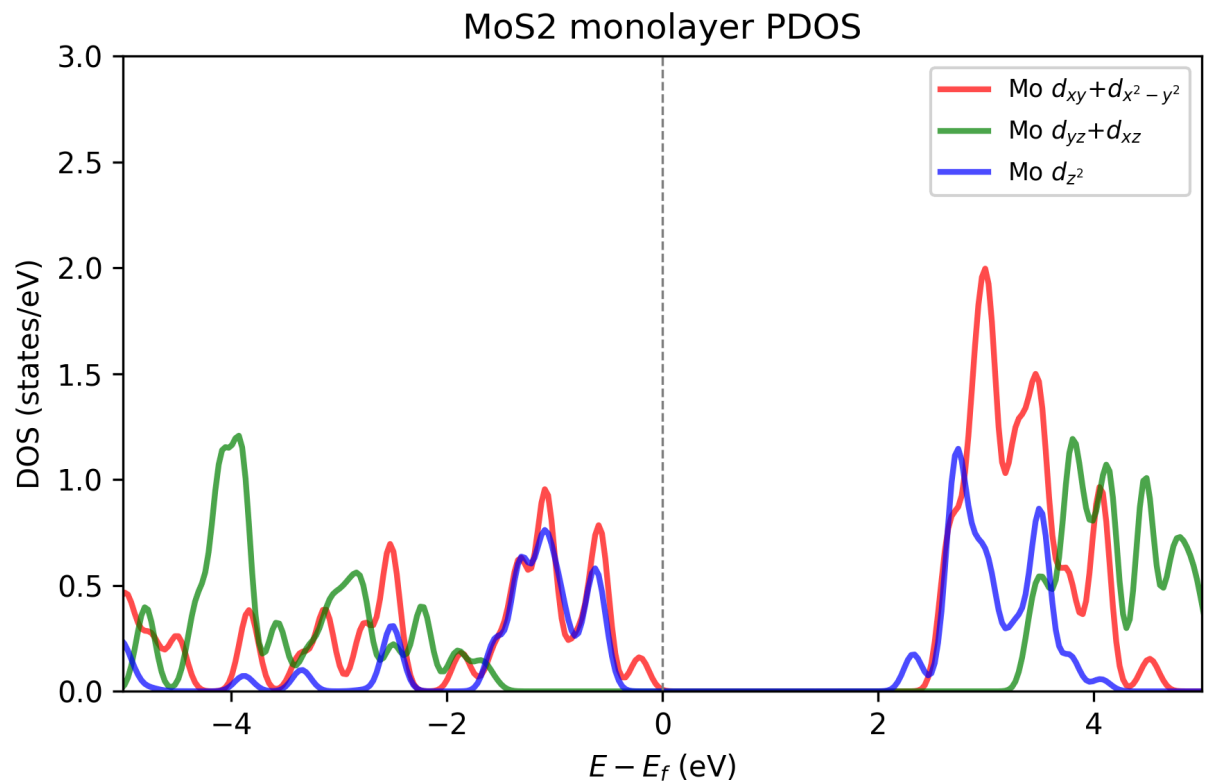

Bulk Si p orbital contribution to Band Structure

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.
Config file:

```
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
```


MoS2 monolayer PDOS

Legend: Mo $d_{xy}+d_{x^2-y^2}$ (red), Mo $d_{yz}+d_{xz}$ (green), Mo d_{z^2} (blue)

Y-axis: DOS (states/eV)
X-axis: $E - E_f$ (eV)
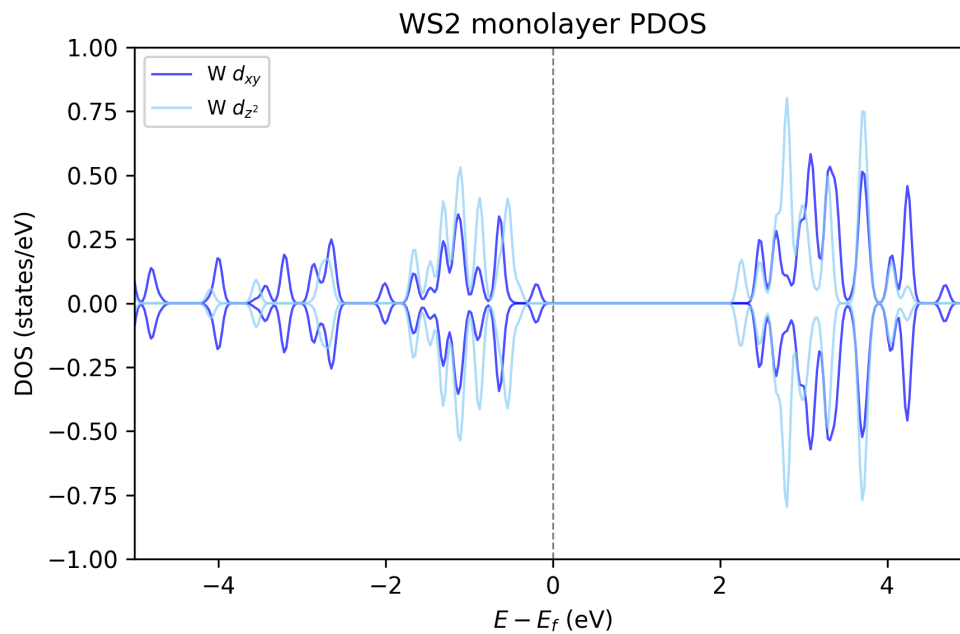
Generates results similar to [1] but with HSE.

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