

# Wannier90

## A brief overview of the code

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# Features

## wannier90 v1.0.2

- MLWF for isolated and entangled bands
- Plotting of WF
- Band structures via Wannier Interpolation
- Fermi surface plots via Wannier Interpolation

# Wannier90 Files

Generated from PWSCF (pw2wannier90.x)

silicon.mmn ← Bloch overlaps  
silicon.amn ← Projections  
silicon.eig ← eigenvalues

Wannier90 Input file

silicon.win

<seedname>.win

# <seedname>.win

```
! these are
% all
# comments

keyword = 1.0
keyword : 1.0
keyword 1.0 !all work

iprint = 1 !normal

iprint = 3 !debugging
          !level output
```

# The System

Unit Cell

```
begin unit_cell_cart  
bohr  
-3.411 0.000 3.411  
 0.000 3.411 3.411  
-3.411 3.411 0.000  
end unit_cell_cart
```

← default Angstroms

Atomic Positions

```
begin atoms_frac  
Cu 0.00 0.00 0.00  
end atoms_frac
```

← also atoms\_cart

# Projections: A starting guess

```
begin projections
Cu:d
f=0.25,0.25,0.25:s
f=-0.25,-0.25,-0.25:s
end projections
```

'd' orbitals on Cu atoms  
+ 2 interstitial 's'

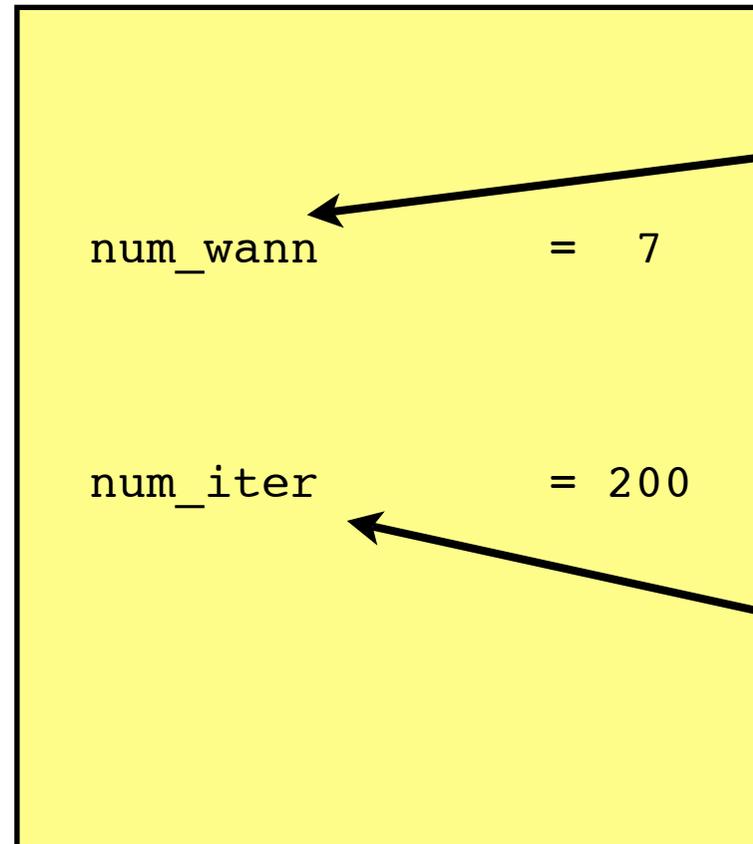
```
begin projections
Si:sp3
end projections
```

sp3 orbitals on Si

```
use_bloch_phases : T
```

no initial guess

# Controlling the minimisation -1



Number of WF

Number of steps to  
minimise spread

# Controlling the minimisation - 2

```
num_bands      = 12
```

```
dis_win_max    = 38.0
```

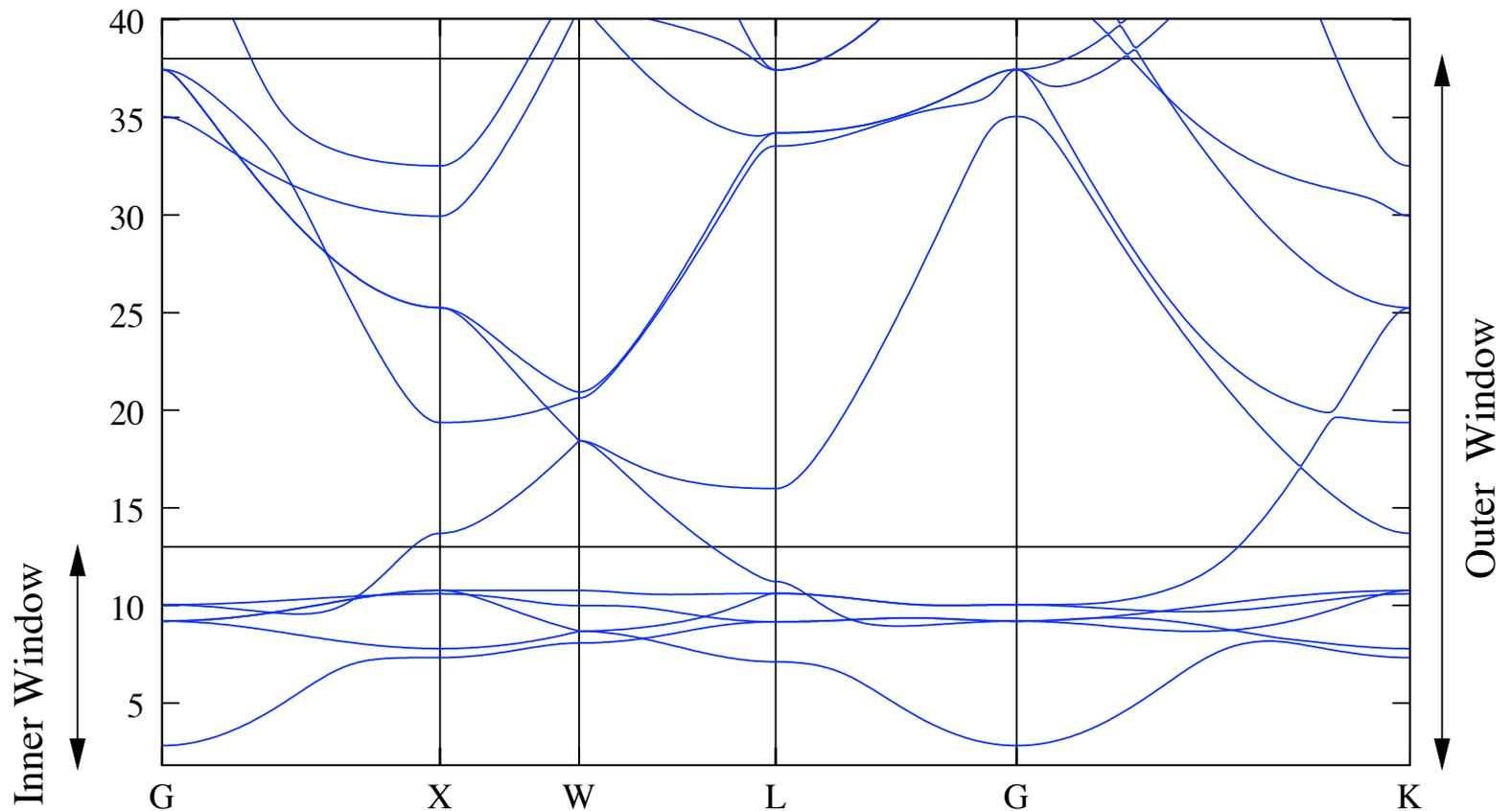
```
dis_froz_max   = 13.0
```

```
dis_num_iter   = 60
```

Number of bands

Top of outer window

Top of inner window



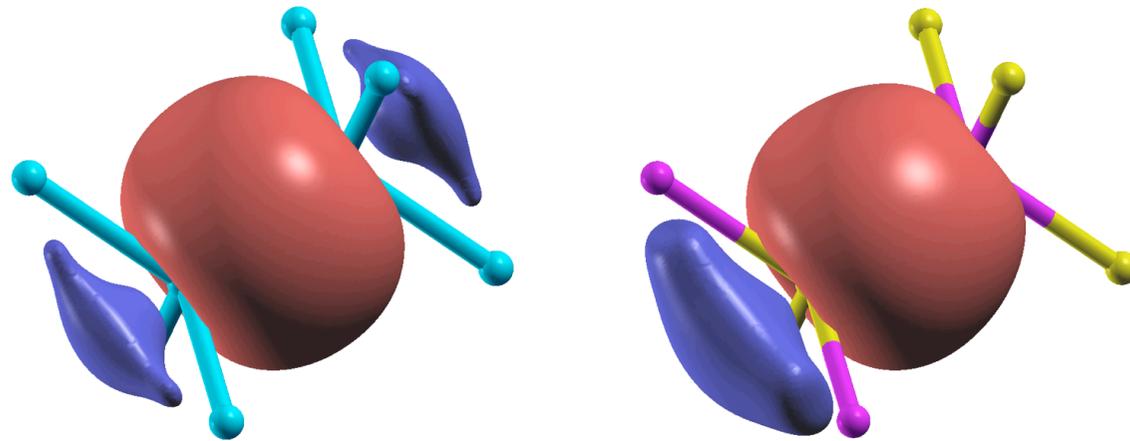
# Job Control

```
restart = wannierise  
restart = plot  
  
num_dump_cycles = 100
```

# Plotting WF

```
wannier_plot = T  
wannier_plot_supercell = 3  
  
wannier_plot_list = 1,4,8  
wannier_plot_list = 1:4,6
```

# Plotting WF



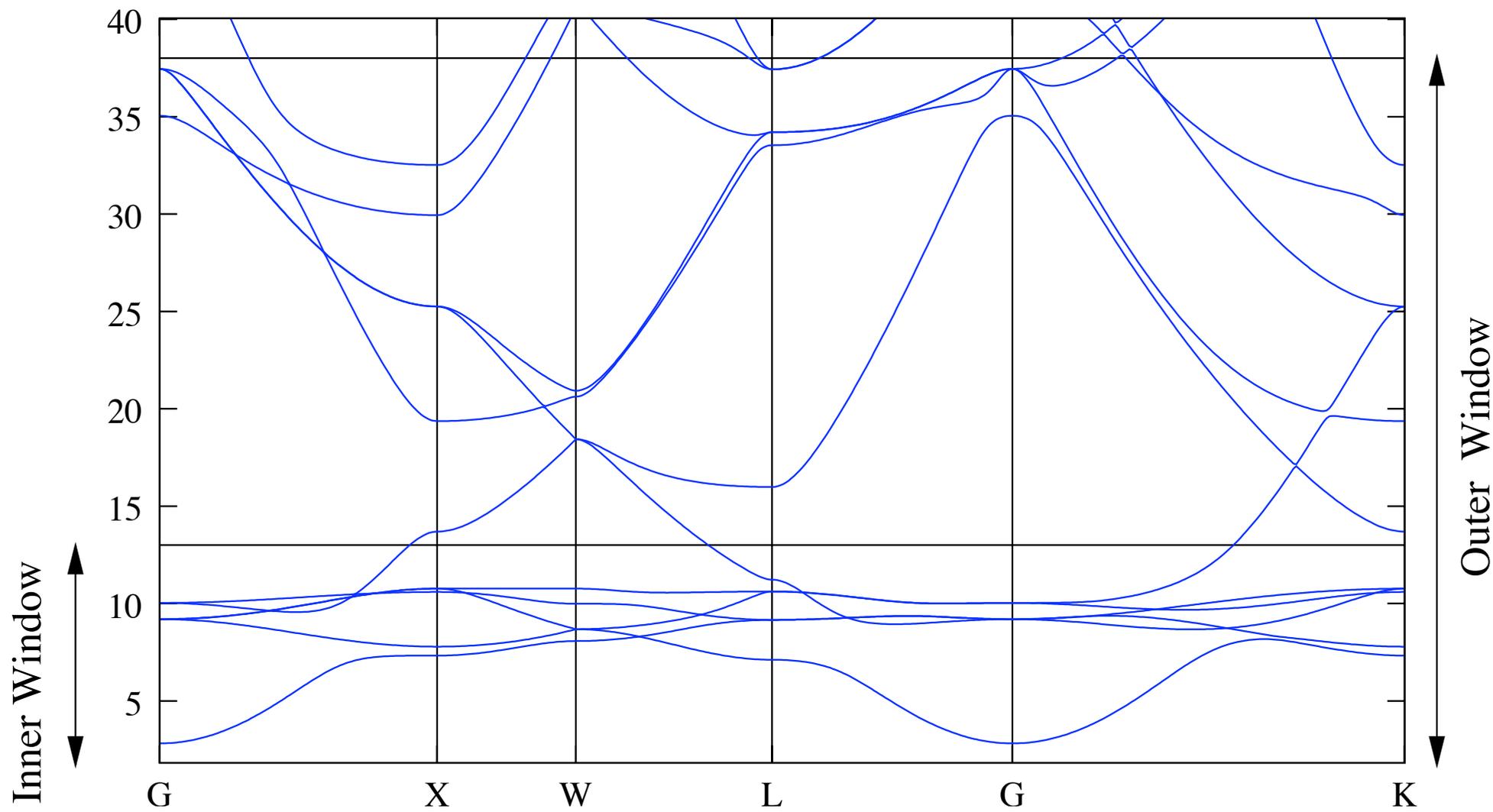
[www.Xcrysden.org](http://www.Xcrysden.org)

# Plotting bands

```
bands_plot = T
bands_num_points = 50

begin kpoint_path
G 0.00 0.00 0.00      X 0.50 0.50 0.00
X 0.50 0.50 0.00      W 0.50 0.75 0.25
W 0.50 0.75 0.25      L 0.00 0.50 0.00
L 0.00 0.50 0.00      G 0.00 0.00 0.00
G 0.00 0.00 0.00      K 0.00 0.50 -0.50
end kpoint_path
```

# Plotting bands



# Do I believe the results?

- Spread well converged ( $<10^{-5}$  Ang<sup>2</sup>)
- Individual Spreads small ( $<5$  Ang<sup>2</sup> ?)
- MLWF real (plot them)
- For disentanglement plot interpolated bands

# (new) Features

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## Next release

- Efficient Gamma-point routines
- Improved plotting
- Transport
- DOS plots
- Spinor WF

# Help and Advice

- [www.wannier.org](http://www.wannier.org)
- User Guide
- Read the source code!
- Wannier90 mailing list (sign up on website)