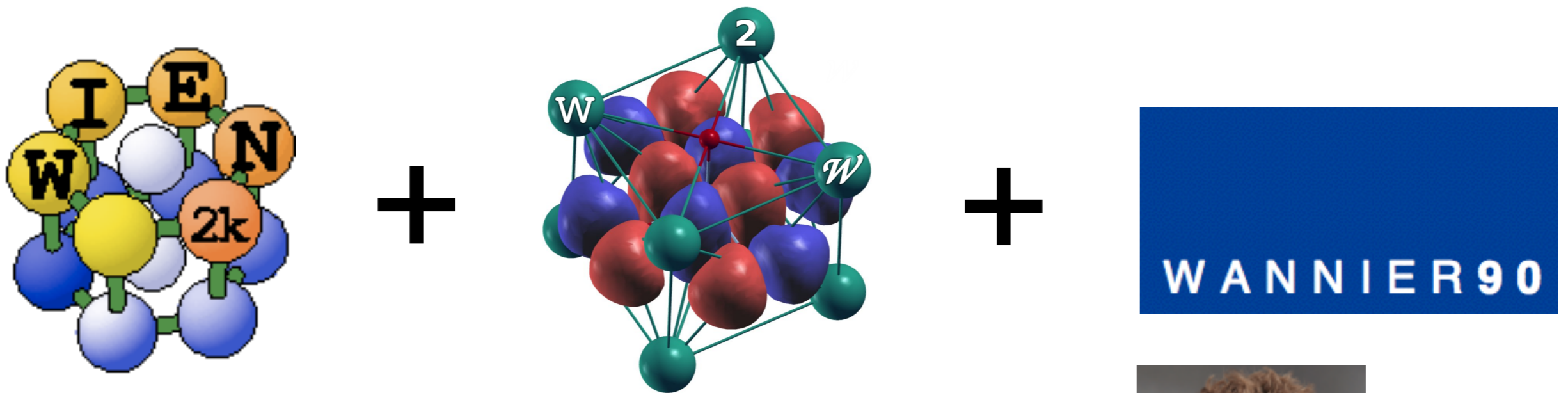


GaAs -- MLWF



Special thanks to Elias Assmann (TU Graz)
for the generous help in
preparation of this tutorial



YouTube video: <https://youtu.be/R4cIYHDh3GE>

I. Wien2k SCF

Create a tutorial directory, e.g.

```
$ mkdir .../exerciseIX/GaAs-MLWF
```

Create the structure file using the following parameters:

2 atoms per primitive unit cell (Ga,As)

Lattice "F" = f.c.c.

Lattice parameters $a_0 = b_0 = c_0 = 10.683$ Bohr

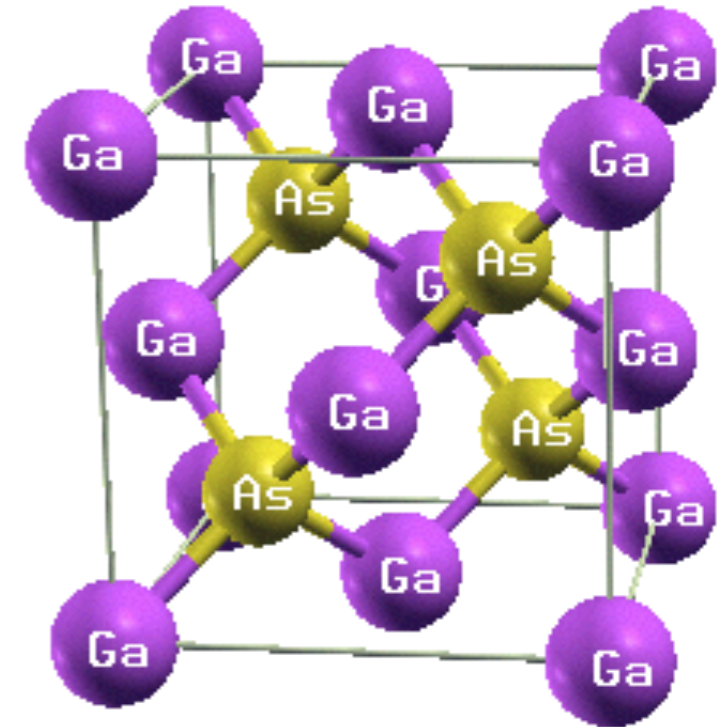
Positions: "0 0 0" for Ga and "1/4 1/4 1/4" for As; RMT's - automatic

You can use `xcrysden` to view the structure

```
$ xcrysden --wien_struct GaAs-MLWF.struct
```

Initialize Wien2k calculation (LDA, ~600 k-points \equiv 8x8x8 mesh)

```
$ init_lapw -b -vxc 5 -numk 600
```



Run regular SCF calculation using default convergence criteria

\$ run_lapw

After SCF cycle is completed (~8 iterations). We proceed with the band structure

Prepare the list of k-point to be used for the band structure plot (GaAs-MLWF.klist_band file) using xcrysden

xcrysden File > Open Wien2k

> Select k-path

Select points L(1/2 0 0), Γ (0 0 0), X(1/2 1/2 0), U(5/8 5/8 1/4), Γ

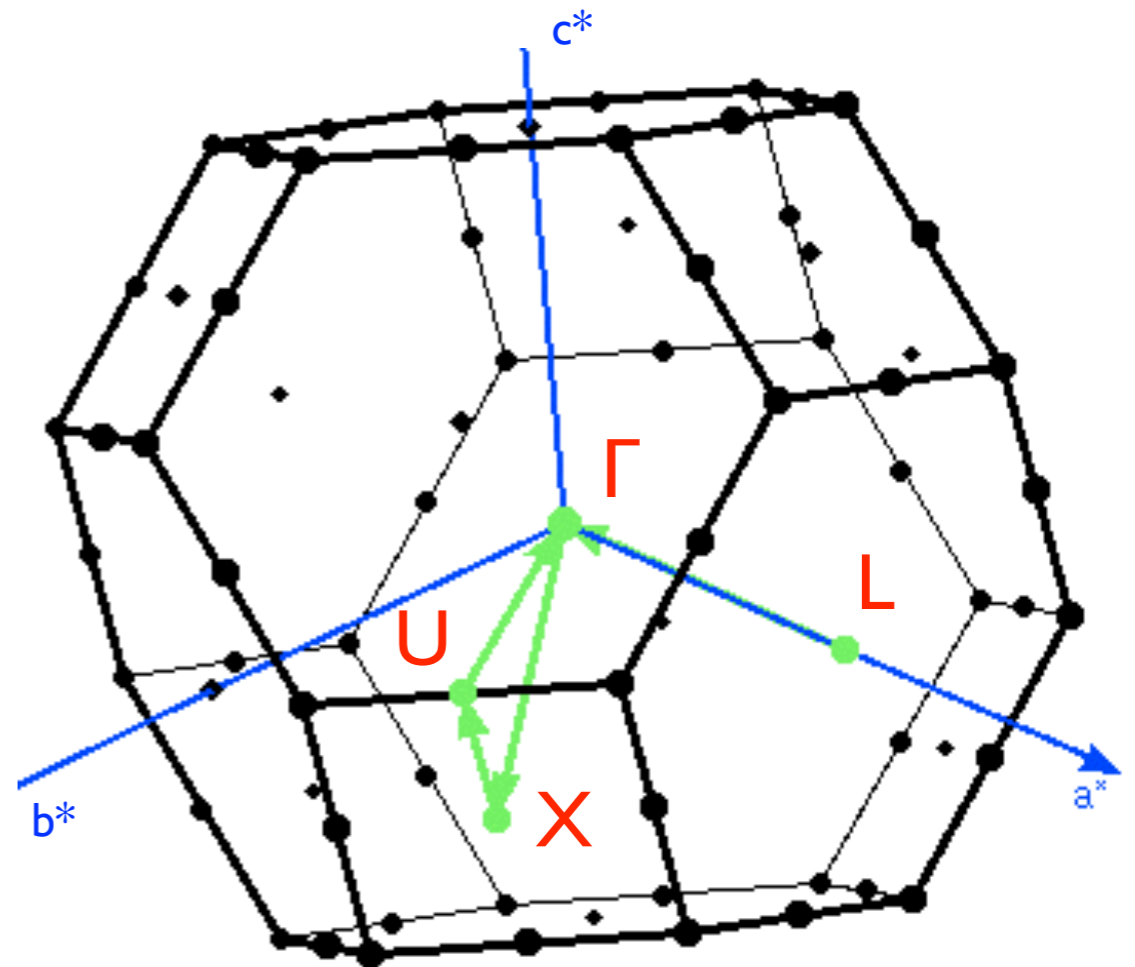
Set the total of 100 k-points along the path.

Save the list as

GaAs-MLWF.klist_band

Solve eigenproblem on the k-path

\$ x lapw1 -band



Get the Fermi energy

```
$ grep :FER *.scf
```

For the band structure plot we will use the web interface (w2web).
Create a new session and navigate to the current work directory.

```
w2web Tasks > Bandstructure
```

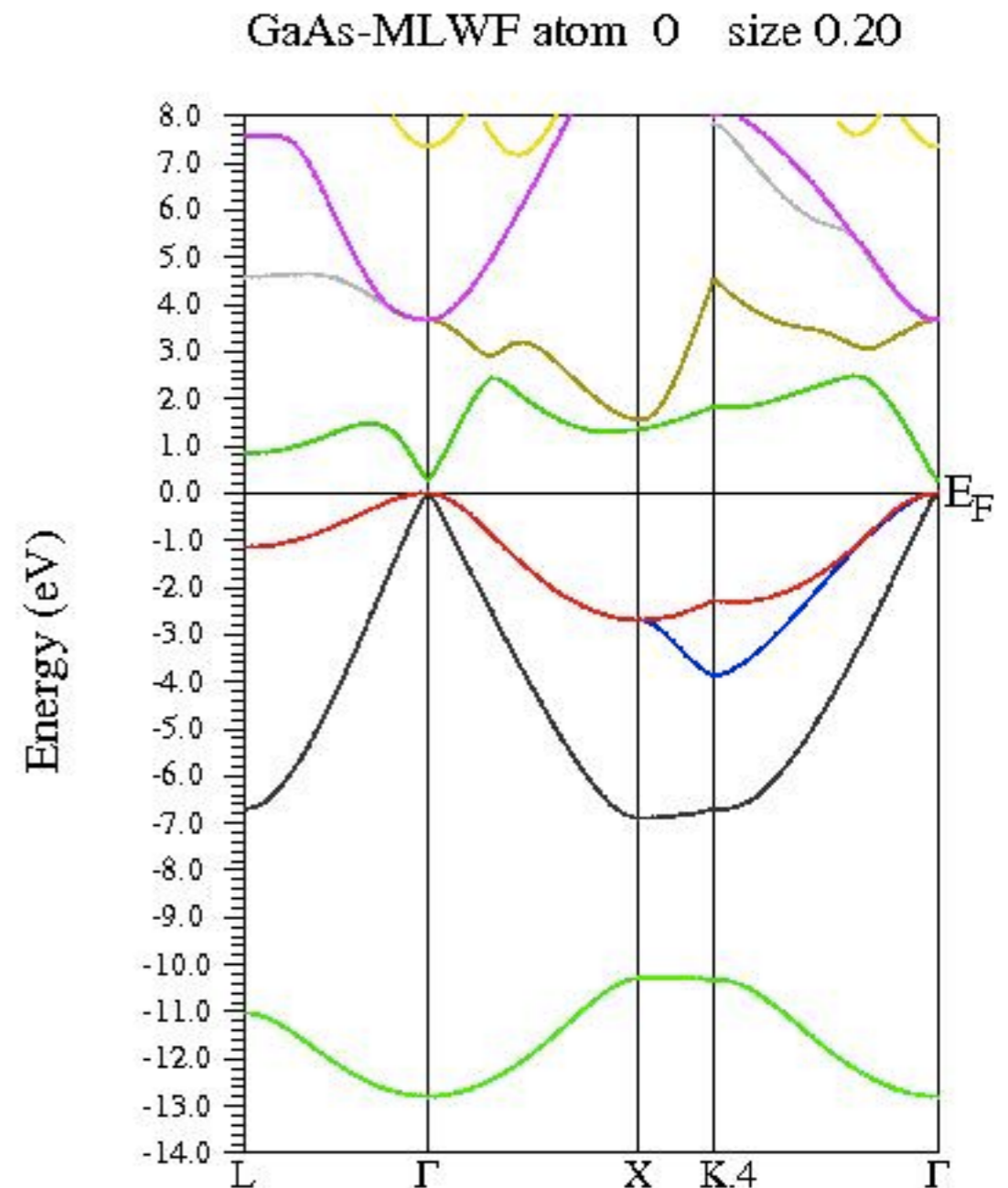
```
w2web Select
```

```
"Edit GaAs-MLWF.insp",  
insert the Fermi energy,  
save
```

```
w2web x spaghetti
```

```
w2web plot band structure
```

Your band structure will be similar to the one shown on the right.
Our aim is to construct Wannier functions that reproduce this band structure including valence and some conduction bands.



Before we proceed it is useful to determine the band indices for the region of interest

\$

grep :BAN *scf2

:BAN00004:	4	-2.243815	-2.243263	2.000000000
:BAN00005:	5	-2.243645	-2.243122	2.000000000
:BAN00006:	6	-0.757612	-0.748891	2.000000000
:BAN00007:	7	-0.748891	-0.745972	2.000000000
:BAN00008:	8	-0.748891	-0.745814	2.000000000
:BAN00009:	9	-0.744948	-0.742764	2.000000000
:BAN00010:	10	-0.743426	-0.742046	2.000000000
:BAN00011:	11	-0.597475	-0.409554	2.000000000
:BAN00012:	12	-0.163606	0.342616	2.000000000
:BAN00013:	13	0.056810	0.342616	2.000000000
:BAN00014:	14	0.094852	0.342616	2.000000000
:BAN00015:	15	0.362856	0.675520	0.000000000
:BAN00016:	16	0.456595	0.748030	0.000000000
:BAN00017:	17	0.612912	1.080595	0.000000000
:BAN00018:	18	0.612912	1.080595	0.000000000
:BAN00019:	19	0.881735	1.145545	0.000000000

} d-orb. of
| As and Ga
| (do not
| participate
| in bonding)
}

bonding +
antibonding
orbitals

↑
E_{min} (Ry)

↑
E_{max}

↑
occupancy

2. Construction of Wannier functions

Prepare a separate directory

```
$ prepare_w2wdir GaAs-MLWF GaAs-WANN
```

```
$ cd GaAs-WANN
```

Initialize Wien2Wannier

```
$ init_w2w
```

Select 8x8x8 k-mesh (unshifted);

energy range (eV) -13 10 (this is not very critical);

band indices [Nmin Nmax] 11 18 (see the previous page);

for the projection we choose “1:s,p” and “2:s,p” (1 = Ga, 2 = As)

Important: when editing “GaAs-MLWF.win” replace “hr_plot” by “write_hr”

Get the vector file on the full Brillouin zone mesh

\$ x lapw1

Compute matrix elements needed for Wannier90

\$ x w2w

Run Wannier90

\$ x wannier90

Verify the output

\$ less GaAs-WANN.wout

spread $\langle \Delta r^2 \rangle$
↓

...

Final State

WF centre and spread	1	(0.000000,	0.000000,	0.000000)	1.91743858
WF centre and spread	2	(0.000000,	0.000000,	0.000000)	5.85659132
WF centre and spread	3	(0.000000,	0.000000,	0.000000)	5.85659132
WF centre and spread	4	(0.000000,	0.000000,	0.000000)	5.85659105
WF centre and spread	5	(1.413312,	1.413312,	1.413312)	1.61146495
WF centre and spread	6	(1.413313,	1.413312,	1.413312)	3.82142578
WF centre and spread	7	(1.413312,	1.413312,	1.413312)	3.82142578
WF centre and spread	8	(1.413312,	1.413312,	1.413313)	3.82142553

...

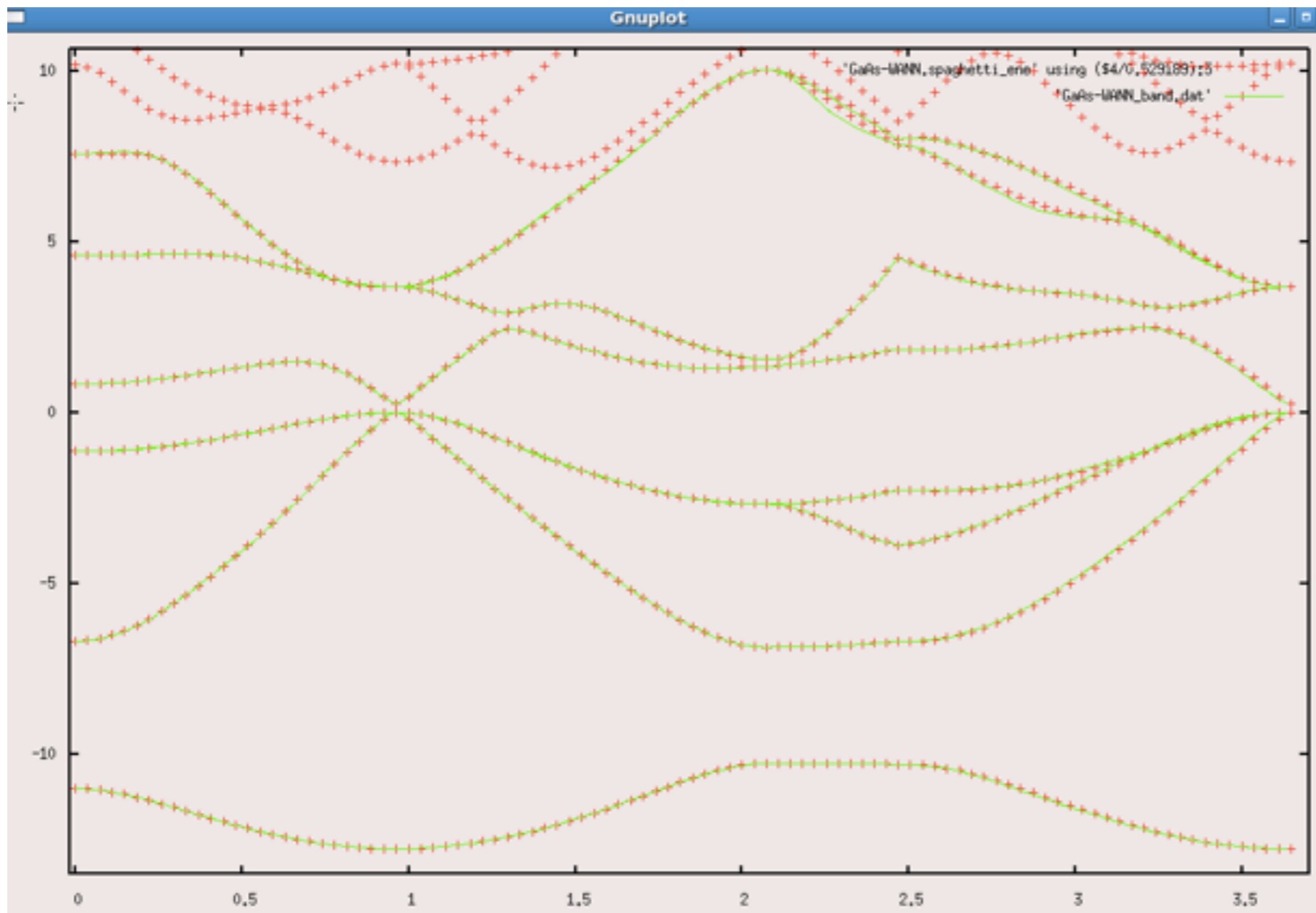
There you can see the position and spread of the WF's, how they changed in the course of convergence. WF's 1-4 are all positioned at the origin (atom 1), WF's 5-8 are centred at the 2nd atom (please check the coordinates)

3. Post-processing

Plot the band structure

\$ gnuplot

```
gnuplot> plot 'GaAs-WANN.spaghetti_ene' using ($4/0.529189):5, 'GaAs-WANN_band.dat' with lines
```



+ original Wien2k
band structure

— Band structure
computed from
Wannier functions

Plotting WF's (can take a while). Get the template of an input file

```
$ cp $WIENROOT/SRC_templates/case.inwplot  
GaAs-WANN.inwplot
```

Edit "GaAs-WANN.inwplot"

Select origin "-1 -1 -1 1" and axis x, y, z

" | -| -| |"

"-| | -| |"

"-| -| | |"

grid point mesh: 30 30 30

"1" for the Wannier function index

Compute the 1st Wannier function on the mesh chosen

```
$ x wplot -wf 1
```

If you need to plot any other WF's (2, 3, etc), just edit the option.

Convert the output of wplot into xcrysden format for plotting.

```
$ wplot2xsf
```

Visualize with xcrystden (instructions on the next page)

The screenshot displays the XCrystal software interface. The main window, titled "XCrySDen: GaAs-WANN_1.xsf", shows a 3D visualization of a crystal structure with atoms represented by purple spheres and bonds by green lines. A blue sphere is visible at the bottom of the structure. The interface includes a menu bar (File, Display, Modify, AdvGeom, Properties, Tools, Help) and a toolbar with various icons for file operations and visualization. On the right side, there are several control panels:

- Navigation and Translation:** Includes directional arrow keys, "Zoom +", "Zoom -", and "Translation Step" (set to 0.05).
- Rotation:** Includes "Rot +X", "Rot -X", "Rot +Y", "Rot -Y", "Rot +Z", "Rot -Z" buttons and a "Rotation Step" (set to 10).
- Isosurface/Property-plane Controls:** A detailed panel with tabs for "Isosurface", "Plane #1", "Plane #2", and "Plane #3". It includes options for "Display Isosurface", "Degree of triCubic Spline" (set to 2), "Isosurface tessellation type" (cubes or tetrahedrons), "Isosurface normals type" (gradient or triangles), "Minimum grid value" (-0.116683), "Maximum grid value" (0.198398), and "Isovalue" (set to 0.05). It also has checkboxes for "Render +/- isovalue" and "Expand Isosurface" (do not expand, to whole structure, or separately in each direction).
- Rendering Options:** Includes "Render isosurface as" (solid, wire, dot), "Isosurface's ShadeModel" (smooth, flat), "Two-sided lighting" (off, on), and "Transparency of isosurface" (off, on).
- Buttons:** Includes "Revert (+) Sides", "Revert (-) Sides", "Revert (+) normals", "Revert (-) normals", "Surface Smoothing", "Set COLOR parameters", and "Set TRANSPARENCY parameters".

At the bottom of the interface, there is a toolbar with buttons for "Atoms Info", "Distance", "Angle", "Dihedral", and "Stereo", along with "F", "Maxi", and "Exit" buttons.

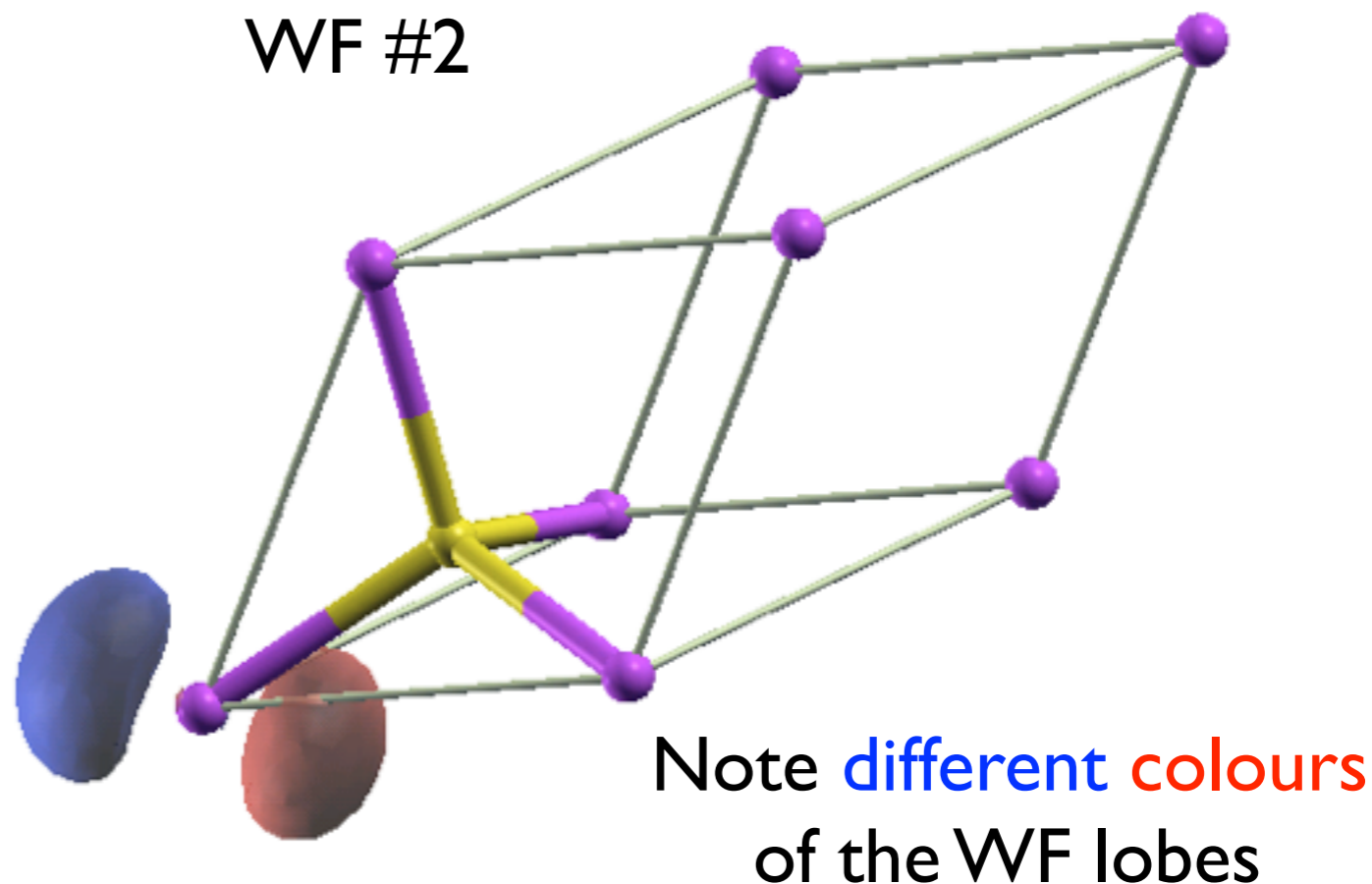
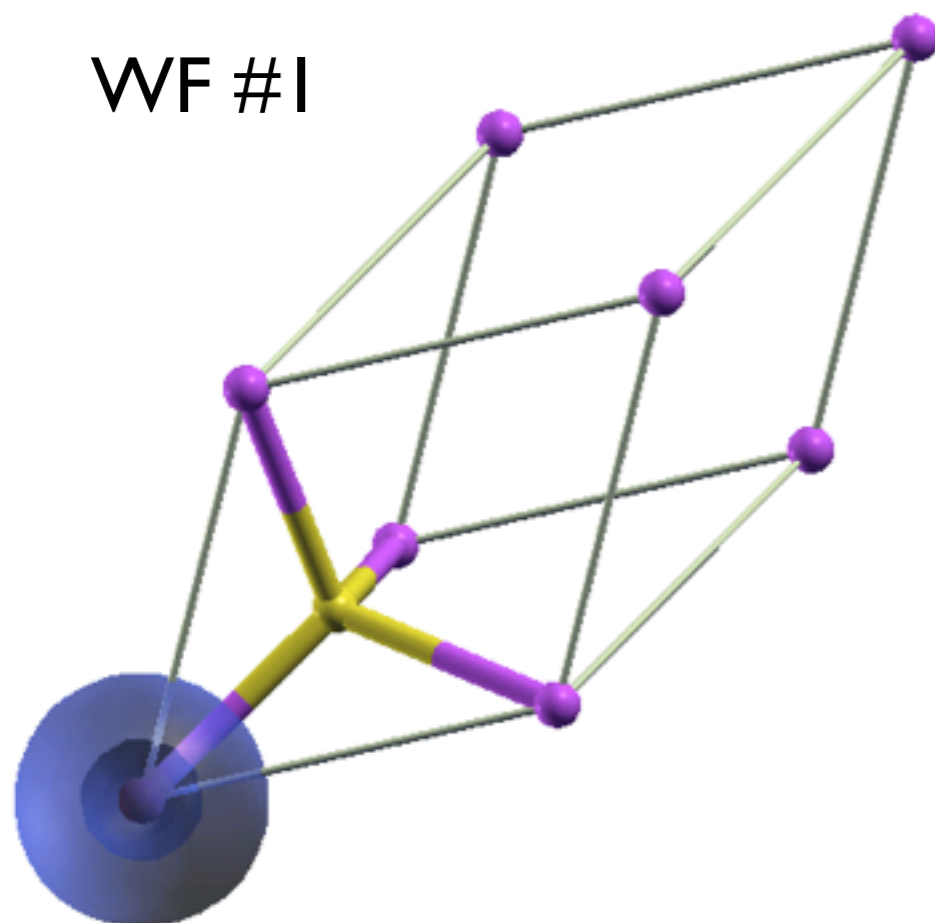
```
$ xcrysden --xsf GaAs-WANN_1.xsf
```

```
xcrysden Tools > Data Grid > OK
```

Check “render +/- isovalue”

Play with the settings. You will get a spherical (s-like) WF centred at the origin.

The second WF resamples p-orbital (you can get it by editing “GaAs-WANN.inwplot”, re-run “x wplot” and “wplot2xsf”). The new file should be called **GaAs-WANN_2.xsf**



Wannier Hamiltonian (similar to LCAO)

\$ less GaAs-WANN_hr.dat

...

0	0	0	1	1	-4.335108	0.000000
0	0	0	2	1	-0.000001	0.000000
0	0	0	3	1	0.000000	0.000000
0	0	0	4	1	-0.000001	0.000000
0	0	0	5	1	-1.472358	0.000000
0	0	0	6	1	-1.157088	0.000000
0	0	0	7	1	-1.157088	0.000000
0	0	0	8	1	-1.157088	0.000000

...

Home unit cell

$\langle s_i |$ $|s_i\rangle$

Matrix element (eV)
 $\langle s_i | H | s_i \rangle = E_{s_i}$

no imag. part of the matrix element

no on-site hopping between different orbitals

Determine on site energies E_s and E_p for Ga and As and compare them to those suggested by Harrison (note: only their relative differences are important)

From Harrison's solid state tables:

$$E_p(\text{Ga}) - E_s(\text{Ga}) = 5.9 \text{ eV}$$

$$E_p(\text{As}) - E_s(\text{As}) = 9.9 \text{ eV}$$

$$E_p(\text{Ga}) - E_p(\text{As}) = 3.3 \text{ eV}$$

Wannier Hamiltonian (cont.)

...

0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0

1	1
2	1
3	1
4	1
5	1
6	1
7	1
8	1

$\langle s_2 |$

-4.335108
-0.000001
0.000000
-0.000001
-1.472358
-1.157088
-1.157088
-1.157088
-0.001219

Matrix element (eV)

$\langle s_2 | H | s_1 \rangle = V_{ss\sigma}$

0.000000
0.000000
0.000000
0.000000
0.000000
0.000000
0.000000
0.000000
0.000000

...

0	0	1
---	---	---

Neighbour unit cell

WF are well localized
 \Rightarrow nearest-neighbour suffice

$\langle p_2 | H | s_1 \rangle = V_{sp}$

Table 2.25. Matrix for the eight *s* and *p* bands in the diamond structure within the tight binding approximation

	S1	S2	X1	Y1	Z1	X2	Y2	Z2
S1	$E_s - E_k$	$V_{ss}g_1$	0	0	0	$V_{sp}g_2$	$V_{sp}g_3$	$V_{sp}g_4$
S2	$V_{ss}g_1^*$	$E_s - E_k$	$-V_{sp}g_2^*$	$-V_{sp}g_3^*$	$-V_{sp}g_4^*$	0	0	0
X1	0	$-V_{sp}g_2$	$E_p - E_k$	0	0	$V_{xx}g_1$	$V_{xy}g_4$	$V_{xy}g_3$
Y1	0	$-V_{sp}g_3$	0	$E_p - E_k$	0	$V_{xy}g_4$	$V_{xx}g_1$	$V_{xy}g_2$
Z1	0	$-V_{sp}g_4$	0	0	$E_p - E_k$	$V_{xy}g_3$	$V_{xy}g_2$	$V_{xx}g_1$
X2	$V_{sp}g_2^*$	0	$V_{xx}g_1^*$	$V_{xy}g_4^*$	$V_{xy}g_3^*$	$E_p - E_k$	0	0
Y2	$V_{sp}g_3^*$	0	$V_{xy}g_4^*$	$V_{xx}g_1^*$	$V_{xy}g_2^*$	0	$E_p - E_k$	0
Z2	$V_{sp}g_4^*$	0	$V_{xy}g_3^*$	$V_{xy}g_2^*$	$V_{xx}g_1^*$	0	0	$E_p - E_k$

Now you have all information required to build your *ab initio* TB sp3 Hamiltonian (Yu & Cardona)