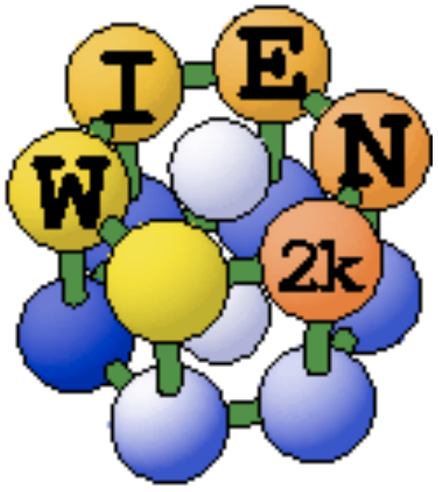
GaAs -- MLWF



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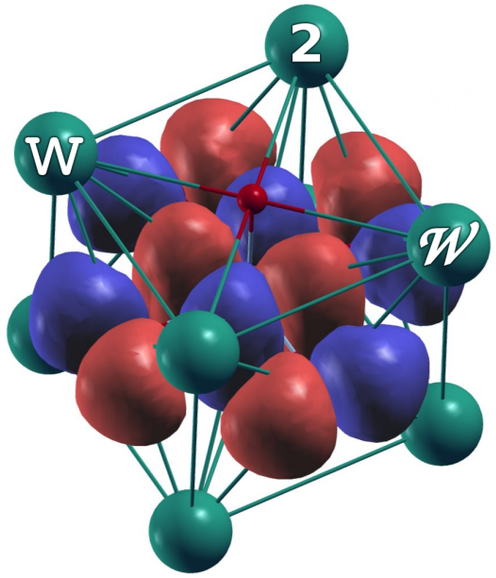

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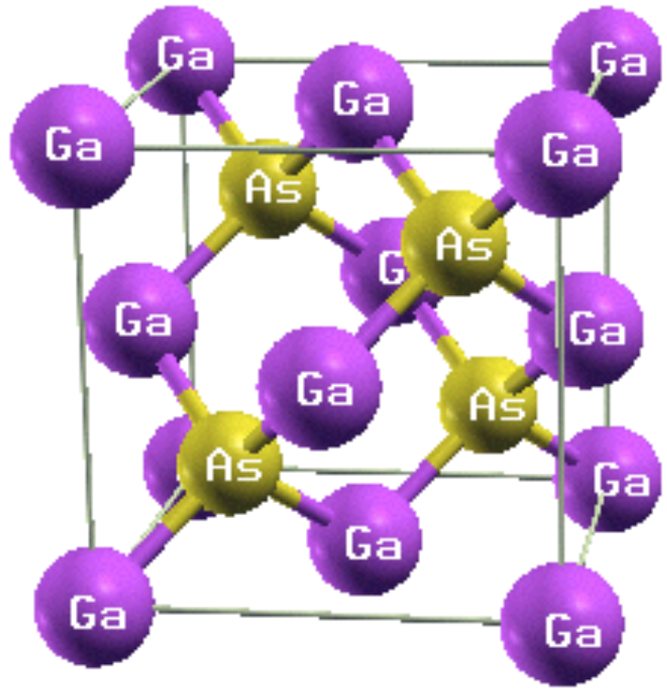
WANNIER90

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

YouTube video: https://youtu.be/R4c1YHDh3GE

1. 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 ≡ 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
```

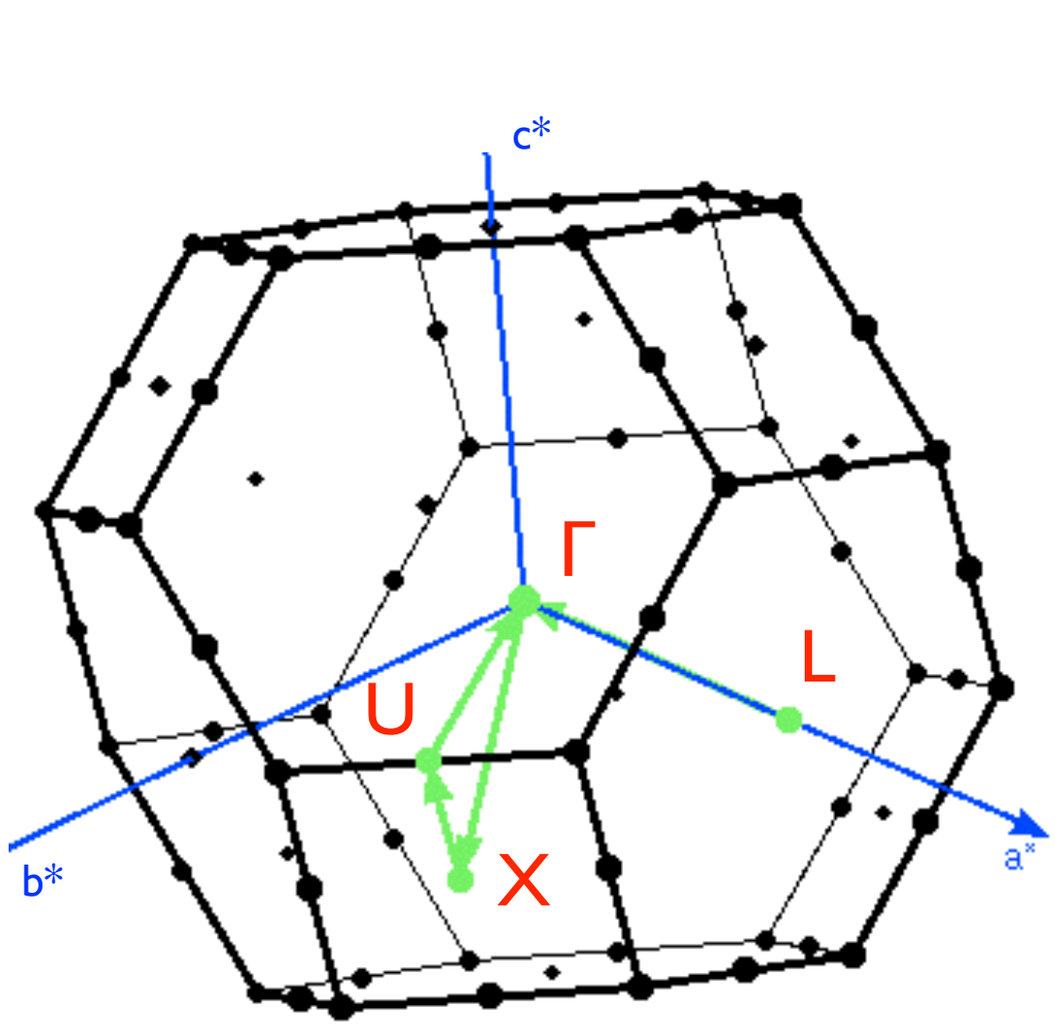
Select points L(1/2 0 0), Γ(0 0 0), X(1/2 1/2 0), U(5/8 5/8 1/4), Γ

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
```



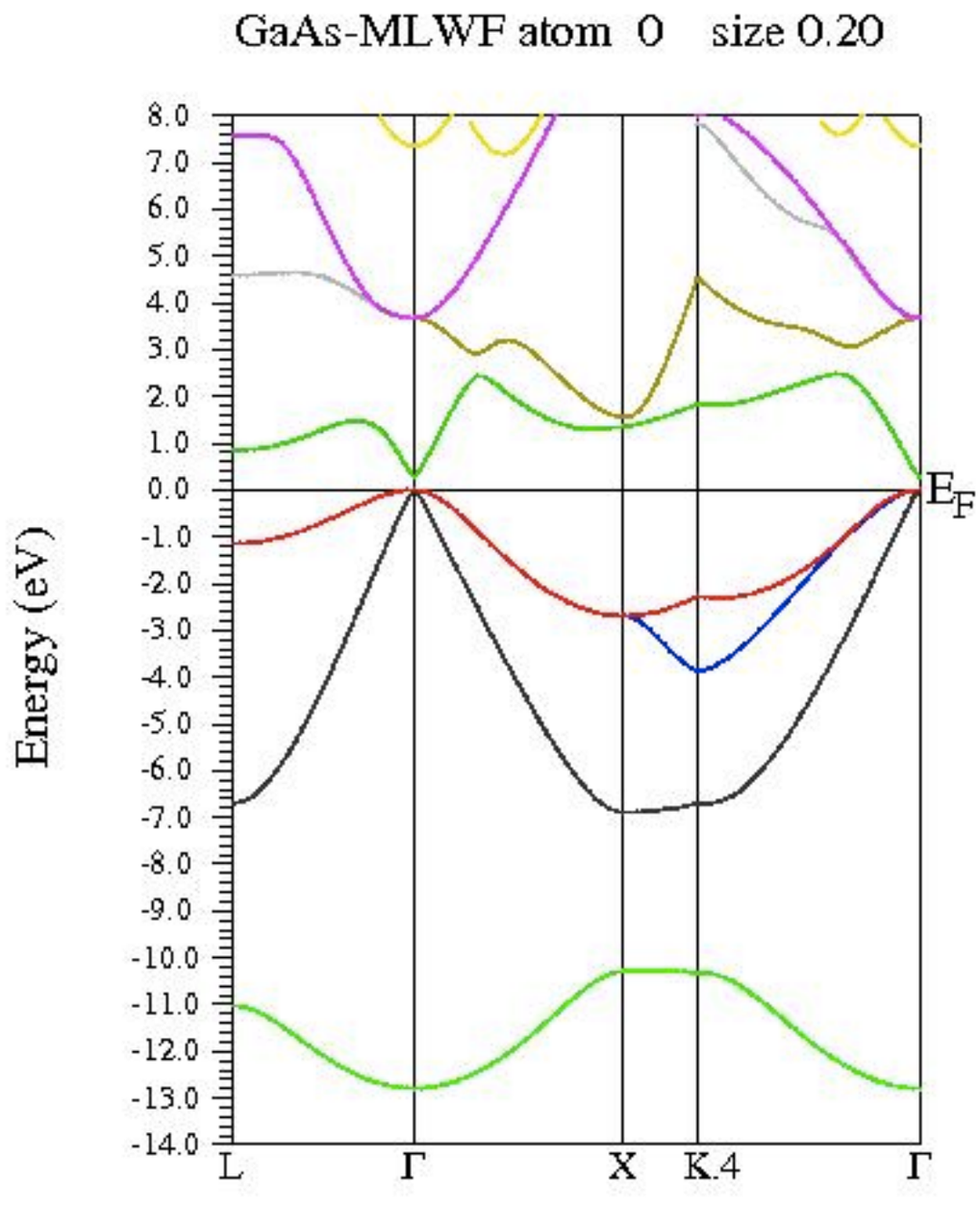
Get the Fermi energy

```
$  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   2.00000000
:BAN00005:    5    -2.243645    -2.243122   2.00000000
:BAN00006:    6    -0.757612    -0.748891   2.00000000
:BAN00007:    7    -0.748891    -0.745972   2.00000000
:BAN00008:    8    -0.748891    -0.745814   2.00000000
:BAN00009:    9    -0.744948    -0.742764   2.00000000
:BAN00010:   10    -0.743426    -0.742046   2.00000000
:BAN00011:   11    -0.597475    -0.409554   2.00000000
:BAN00012:   12    -0.163606     0.342616   2.00000000
:BAN00013:   13     0.056810     0.342616   2.00000000
:BAN00014:   14     0.094852     0.342616   2.00000000
:BAN00015:   15     0.362856     0.675520   0.00000000
:BAN00016:   16     0.456595     0.748030   0.00000000
:BAN00017:   17     0.612912     1.080595   0.00000000
:BAN00018:   18     0.612912     1.080595   0.00000000
:BAN00019:   19     0.881735     1.145545   0.00000000
```

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

bonding + antibonding orbitals

⇧ Emin (Ry)

⇧ Emax

⇧ 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 $\langle \Delta \mathbf{r}^2 \rangle$

$\Downarrow$

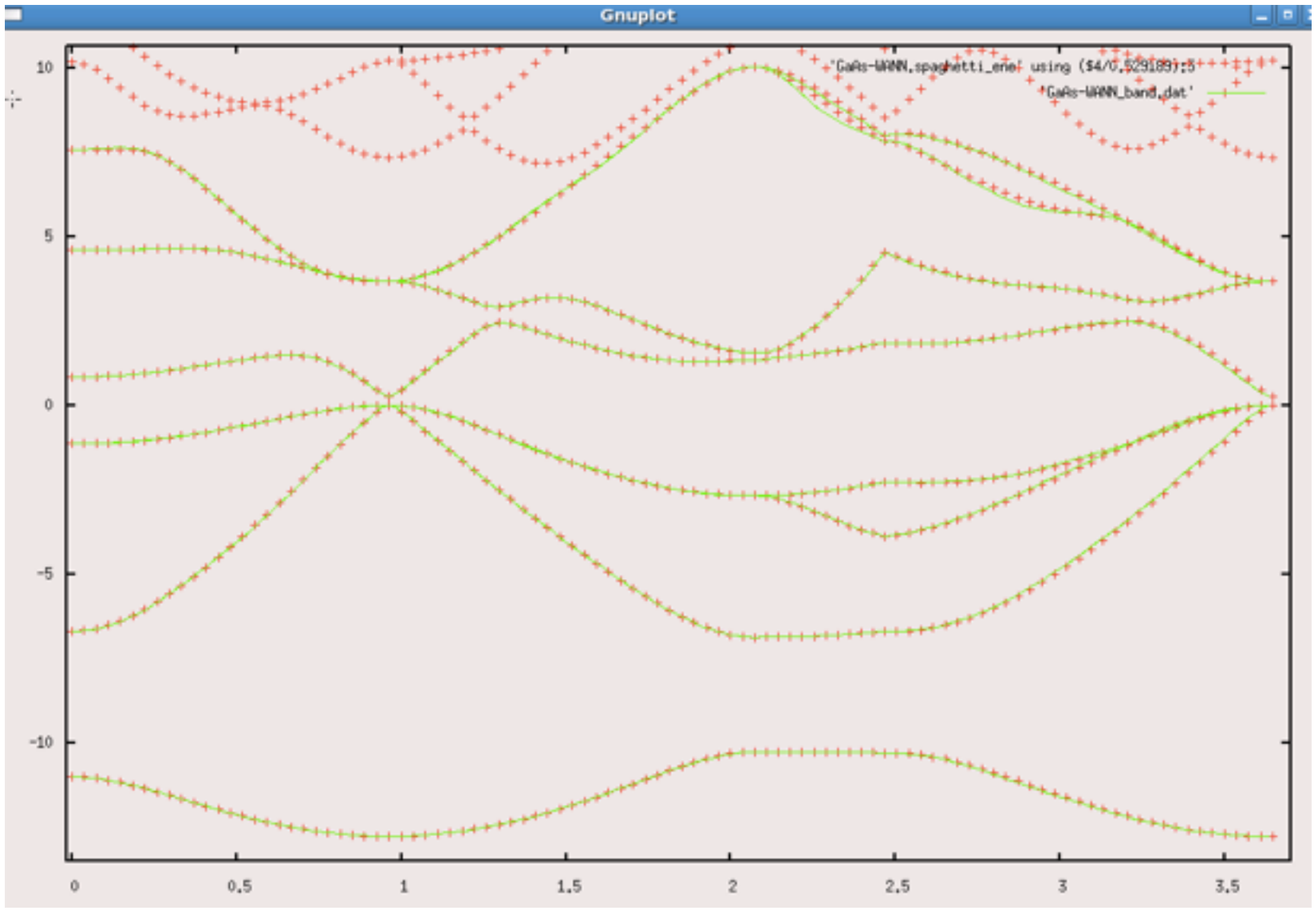
```
...
Final State
  WF centre and spread    1  (  0.000000,  0.000000,  0.000000 )     1.91743858
  WF centre and spread    2  (  0.000000,  0.000000,  0.000000 )     5.85659132
  WF centre and spread    3  (  0.000000,  0.000000,  0.000000 )     5.85659132
  WF centre and spread    4  (  0.000000,  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

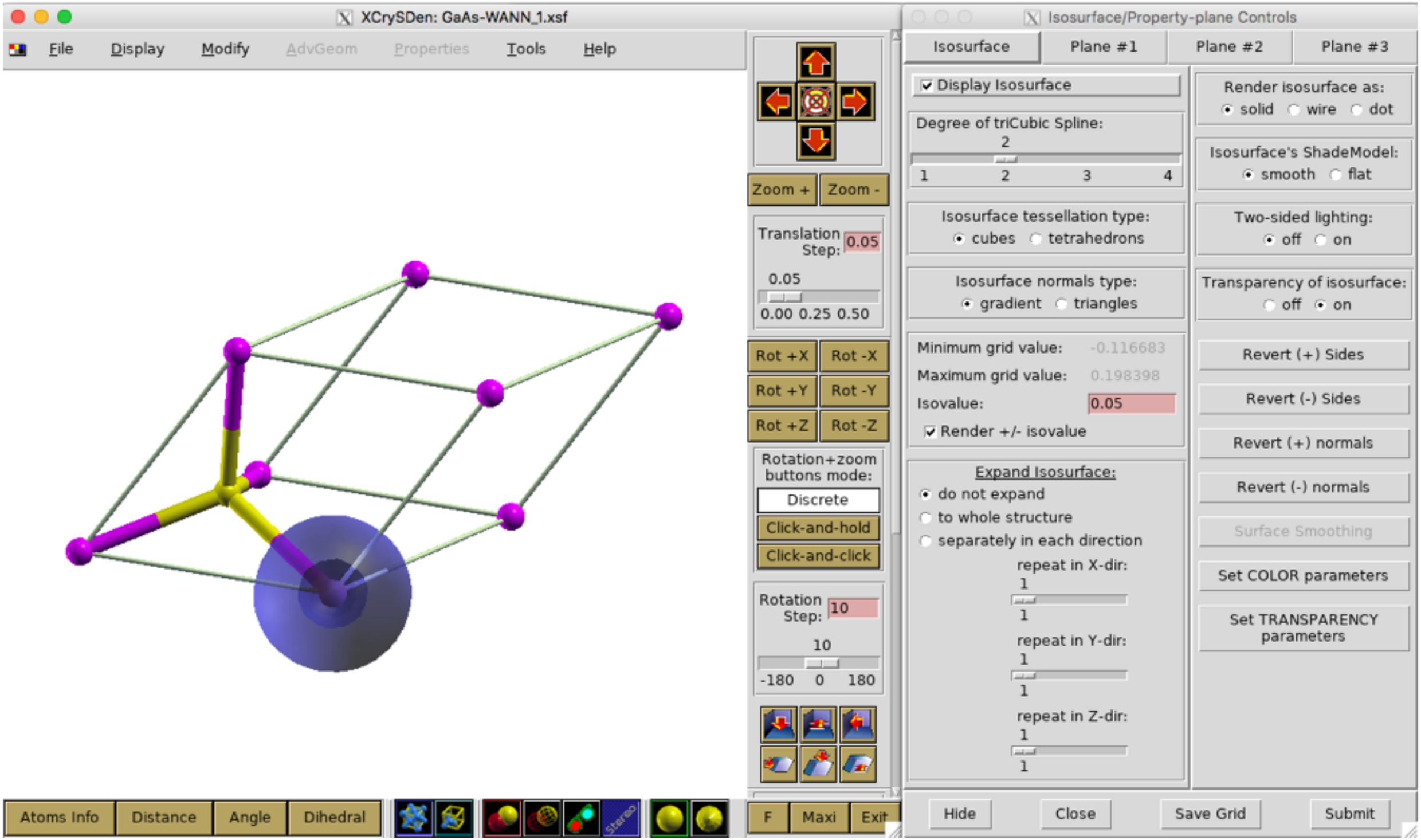
```
$ x wplot -wf 1
```

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 `xcrysden` (instructions on the next page)



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

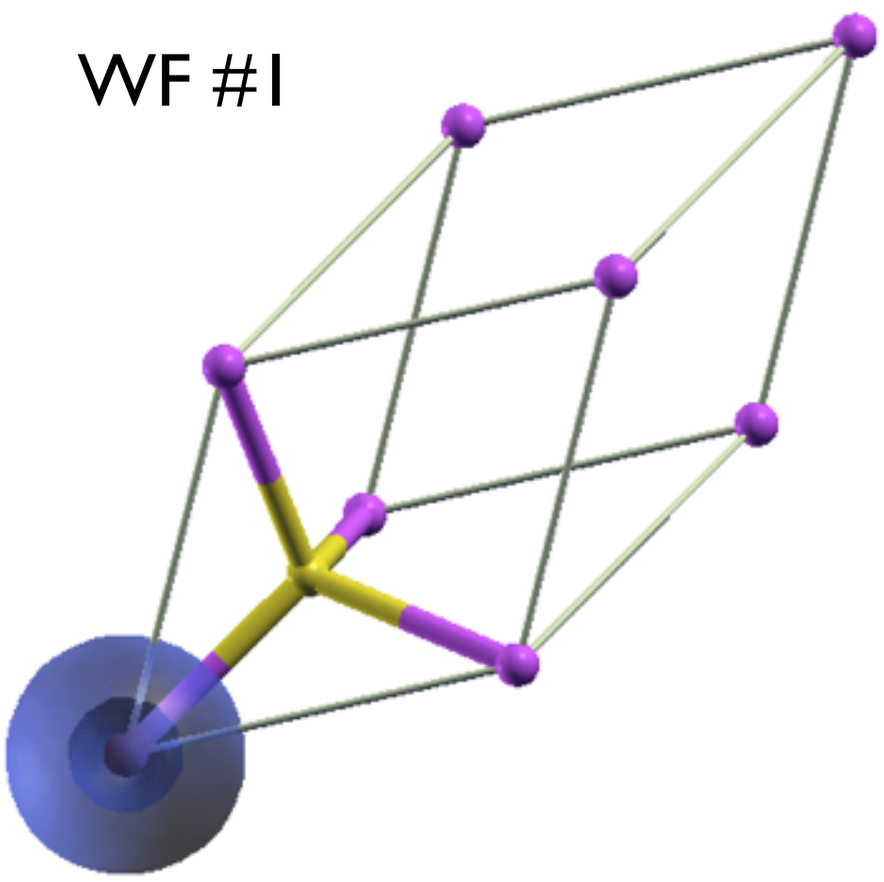
```
xcrysden Tools > Data Grid > OK
```

Check "render +/- isovalue"

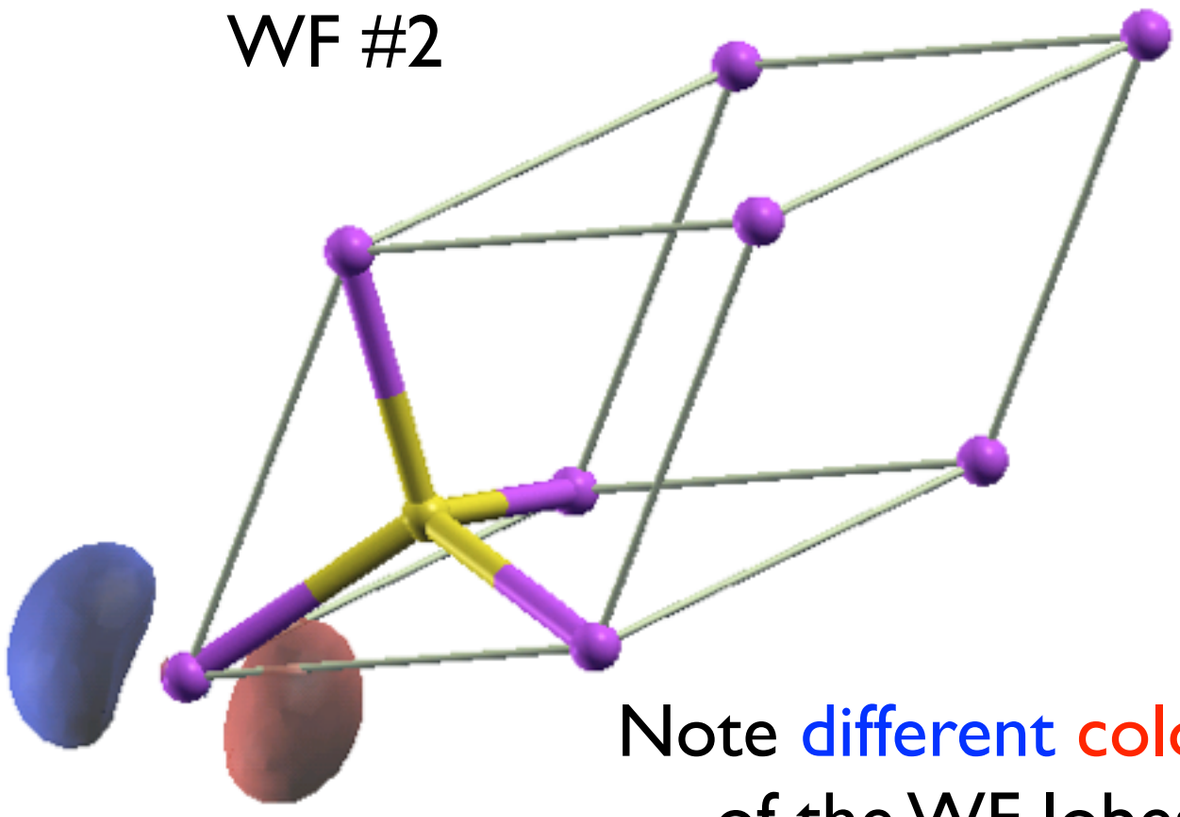
Play with the settings. You will get a spherical (s-like) WF centred at the origin.

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`**

WF #1



WF #2



Note different colours of the WF lobes

Wannier Hamiltonian (similar to LCAO)

$ **less GaAs-WANN_hr.dat**

...

			$\langle s_1 \vert$	$\vert s_1 \rangle$	Matrix element (eV) $\langle s_1 \vert H \vert s_1 \rangle = E_{s1}$	
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

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:

$E_p(Ga) - E_s(Ga) = 5.9$ eV

$E_p(As) - E_s(As) = 9.9$ eV

$E_p(Ga) - E_p(As) = 3.3$ eV

Wannier Hamiltonian (cont.)

Matrix element (eV)

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

```
...
     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
...
     0     0     1     1     1    -0.001219    0.000000
```

$\langle s_2|$

Neighbour unit cell

WF are well localized
⇒ nearest-neighbour suffice

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

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

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	$E_p - E_k$