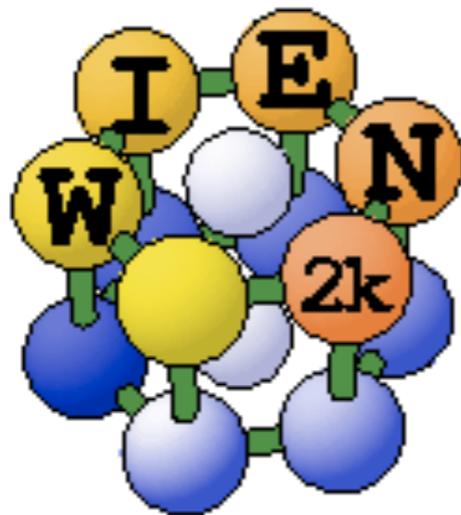


Effective band structure of $\text{Si}_{1-x}\text{Ge}_x$ alloy



+ fold2Bloch

YouTube video:

Instructions

w2web Construct a primitive lattice of Si

2-atoms per unit cell

Primitive lattice “P”, $\alpha = \beta = \gamma = 60^\circ$

Cell size (Bohr): $a = b = c = 3.870393 \text{ \AA}$

Coordinates:

Si (0 0 0)

Si (1/4 1/4 1/4)

RMTs = 2 Bohrs

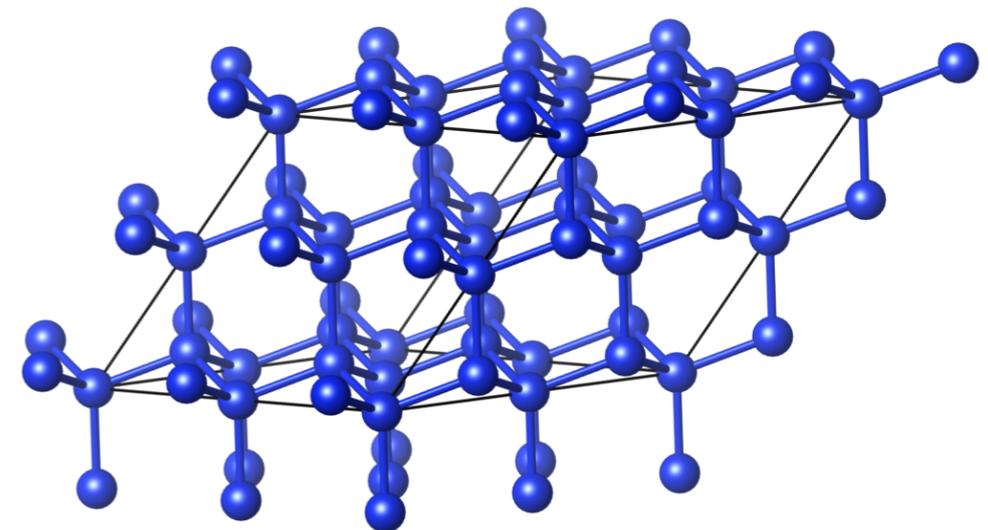
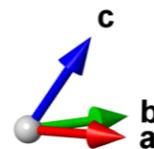
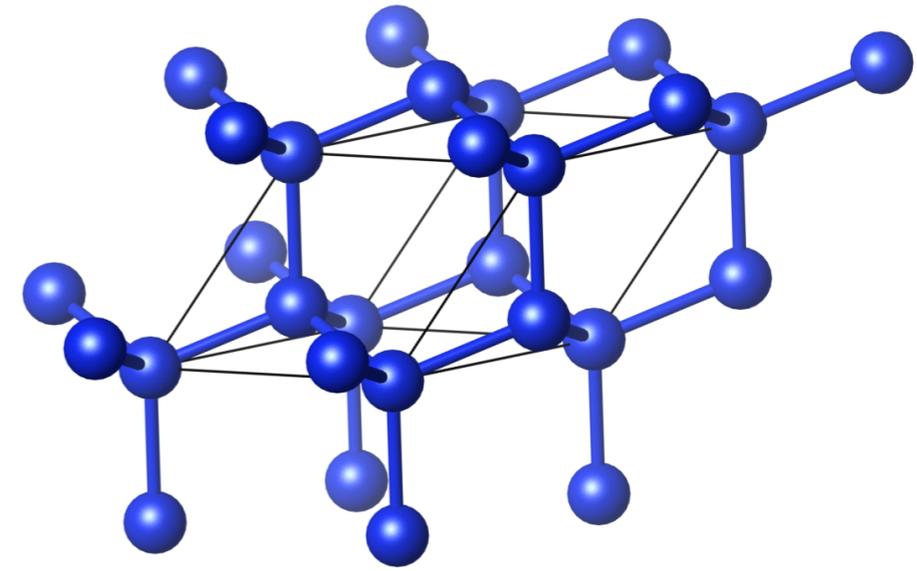
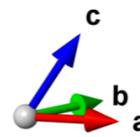
Do not initialize calculation.

Create a 2x2x2 supercell: no shifts, P-type lattice, no additional vacuum

\$ supercell

Rename “[case]_super.struct”
to “[case].struct”

The new supercell should have
16 Si-atoms (2 atoms x 2 x 2 x 2)



w2web Introduce Ge into the structure by switching 3 Si \rightarrow 3 Ge atoms
The Ge composition will be $3/16 = 0.1875$ (ca. 19%)

One possibility is to pick any 3 Si-atoms of your choice. But this choice will be “biased” and does not qualify as a random alloy.

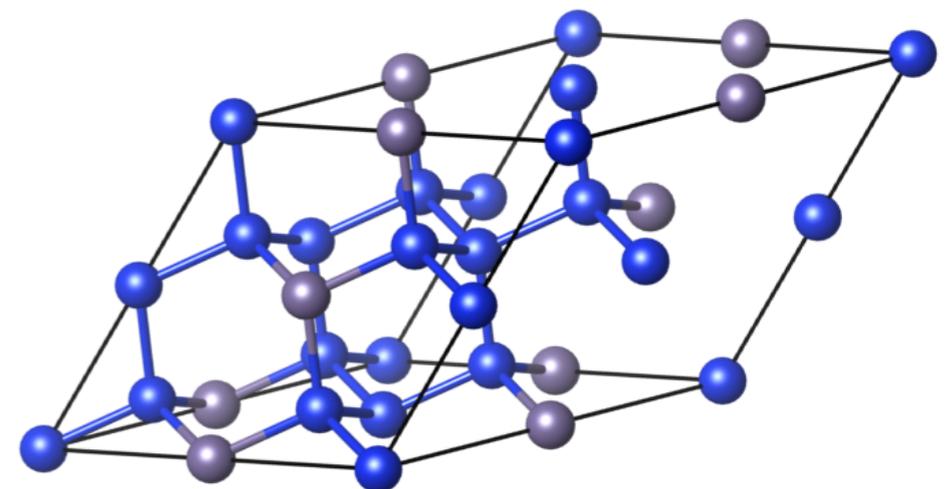
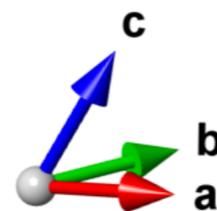
Alternatively, we can generate a randomized sequence of integers between 1 and 16 (total number of Si-atoms) using <https://www.random.org/sequences>

“3 2 6 9 13 4 7 16 12 1 5 10 15 14 11 8”

The first 3 numbers are labels of atoms to be switched. Of course every time you will get a different sequence. Thus arrangement of atoms is not unique.

More elegant solution involves the use of “Special Quasirandom Structures”, but it goes beyond this tutorial.

When substituting Si \rightarrow Ge using StructGen™, make sure to clear up Z value and label atoms as Ge 1, Ge 2, Ge 3, Si 1, Si 2, ...



Initialize SCF calculation: LDA, RKmax=6, 3x3x3 k-mesh (sifted)
(note: crude parameters are used for tutorial purposes)

\$ init_lapw -b ... or web interface

Run SCF calculation: iterative diagonalization, energy convergence 0.0001, charge convergence 0.001. It can be faster if you take advantage of OMP-parallelization (~10 mins on 4 cores)

\$ export OMP_NUM_THREADS=4

\$ run_lapw -ec ...

Save the calculation in "SCF" directory

\$ save_lapw ... or web interface

Copy L- Γ -X k-path template

\$ cp \$WIENROOT/LGX.klist_band [case].klist_band

Recalculate eigenvalues and wave functions for k-points on the L- Γ -X path

\$ x lapw1 -band

Copy [case].klist_band and [case].struct files to the scratch folder

```
$ cp ... $SCRATCH
```

Make sure that the scratch folder contains [case].klist_band, [case].struct, and [case].vector

```
$ cd $SCRATCH; ls
```

Perform unfolding of the vector file using 2:2:2 as a setting for the size of the supercell

```
$ fold2Bloch [case].vector 2:2:2
```

The newly created file [case].f2b contains 5 columns:
Unfolded KX, KY, KZ, Eigenvalue (Ry), Bloch spectral weight

Find the Fermi energy (typically 0.38-0.39 Ry) by examining sorted eigenvalues (4th column)

```
$ sort -n -k4,4 [case].f2b | less
```

Note values of the spectral weight (5th column) for the valence and conduction band edges. Which of them is more perturbed by the alloy disorder?

Copy plotting script to the Wien2k work directory

```
$ cp $WIENROOT/ubs_dots-w2k-octave.m .
```

Edit the plotting script:

KPATH = [1/2 0 0; 0 0 0; 1/2 1/2 0] corresponds to L- Γ -X;

FOLDS = [2 2 2] is our size of the supercell;

KLABEL = {'L'; 'G'; 'X'} are labels for k-points;

finpt = '[case].f2b' is the input file name;

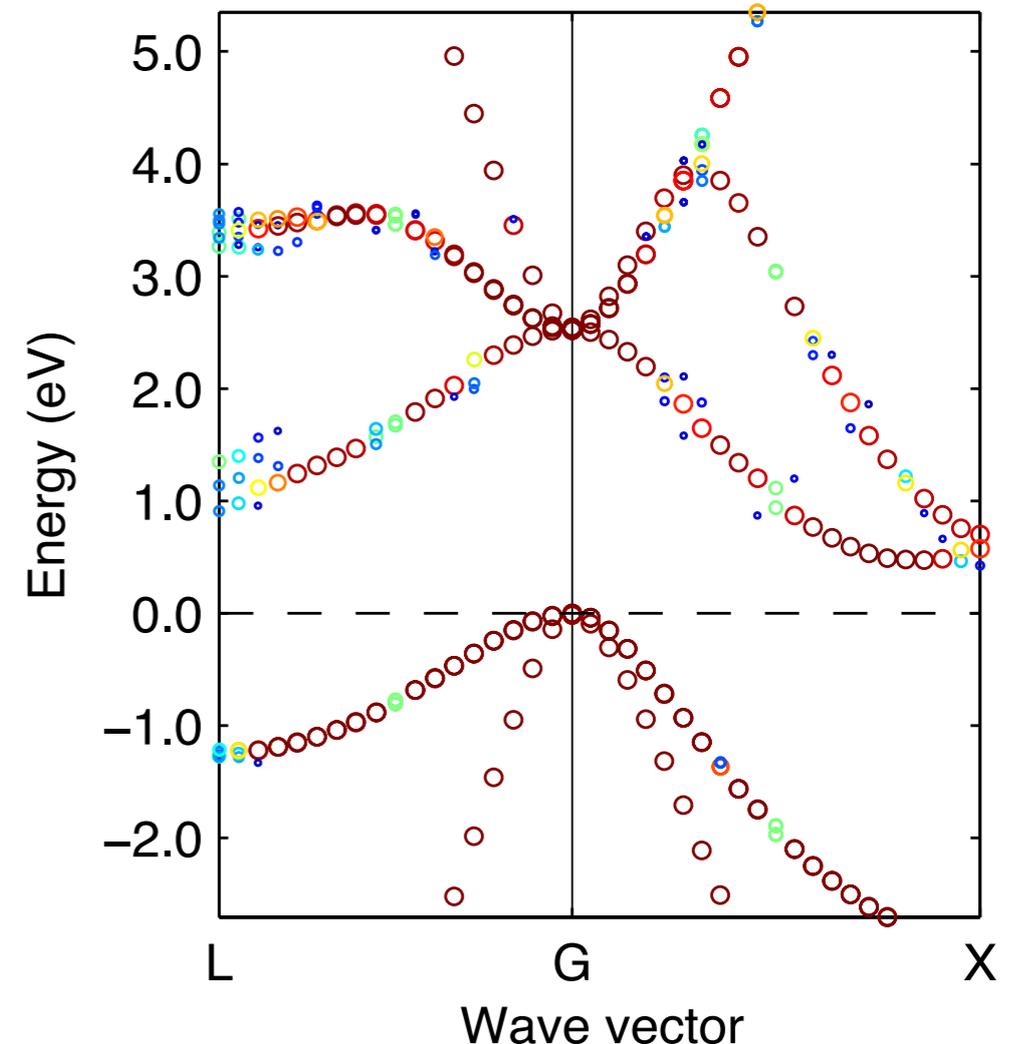
Ef = 0.385770 is the Fermi energy (Ry);

```
G = [ 0.083726 -0.027909 -0.027909;  
0.000000 0.078938 -0.039469;  
0.000000 0.000000 0.068362]
```

reciprocal lattice vectors from
[case].outputkgen;

Run plotting script and view the effective
alloy band structure

```
$ octave ubs_dots-w2k-octave.m
```



When you have time (requires 1-2 hrs)...

It should be noted that so far we ignored static atomic displacements that are present in alloys due to the size mismatch between the additive element (Ge) and the host (Si). Forces in our structure are of the order 15 mRy/Bohr that requires optimization of atomic positions.

The suggested procedure would be to build supercell, place alloying element, and perform optimization of atomic positions before undertaking infolding. The effective band structure with static atomic displacements included in calculation is shown below. Can you spot any changes?

