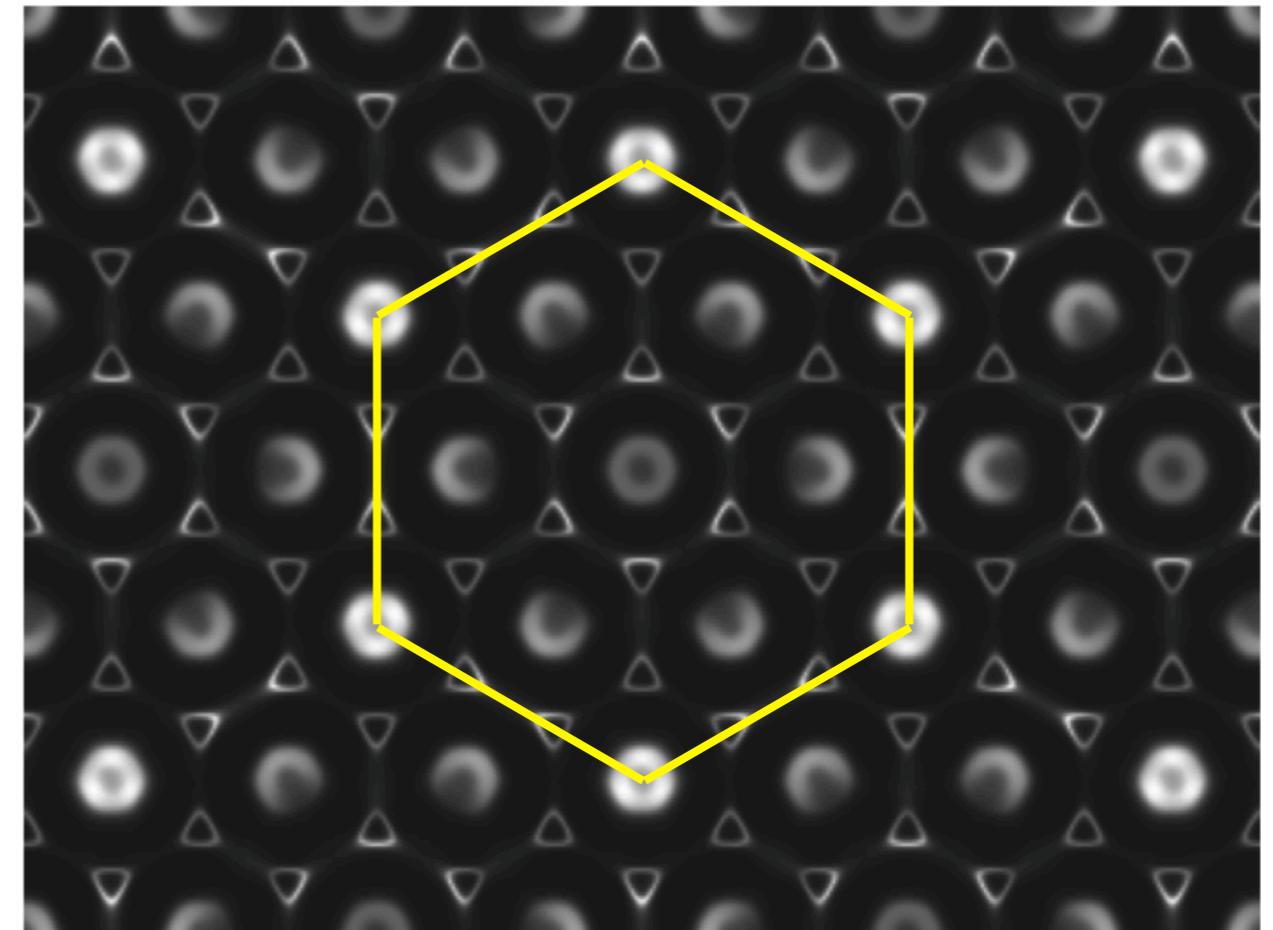
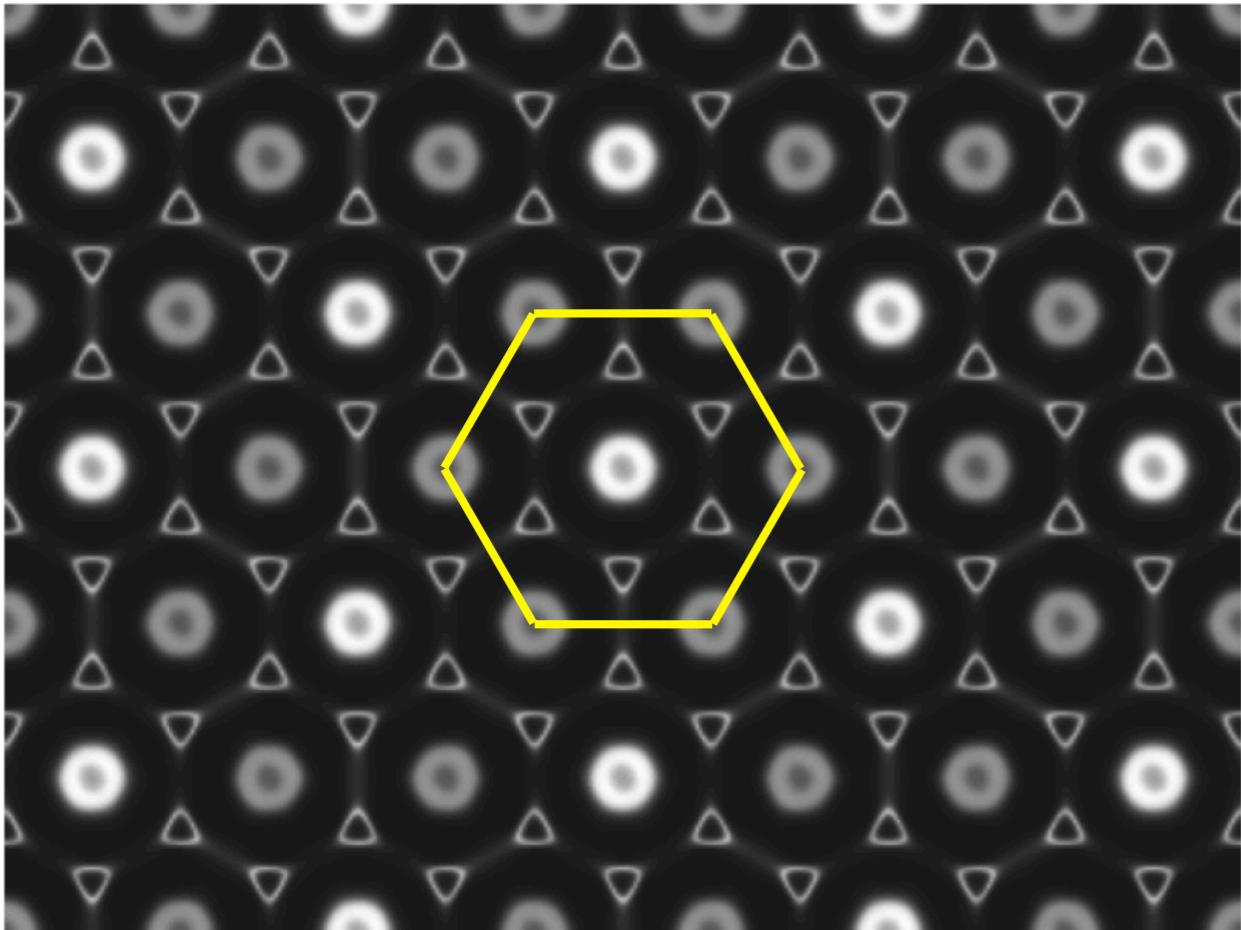


# Unfolding band structure into a conceptual Brillouin zone



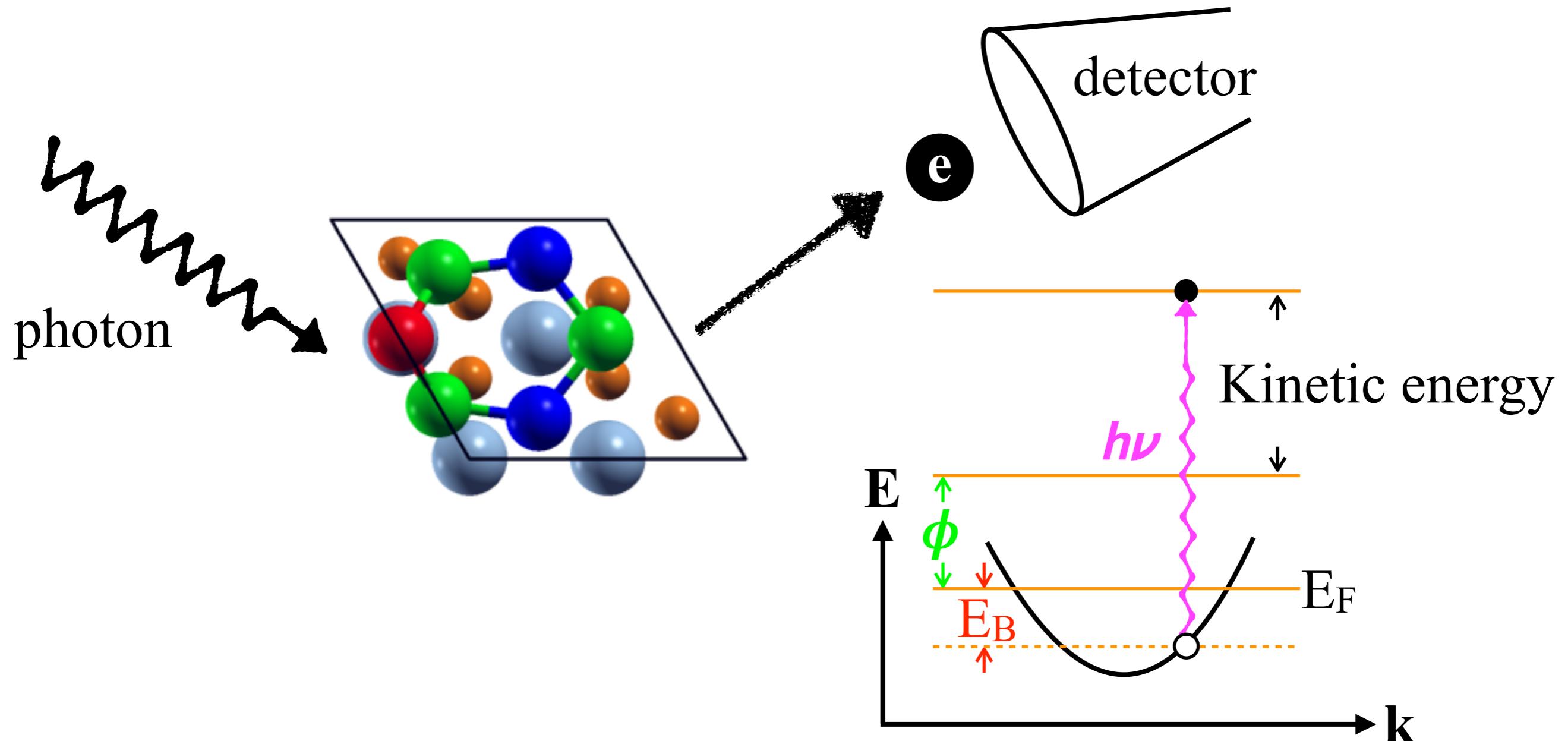
Chi-Cheng Lee

*Institute for Solid State Physics, The University of Tokyo, Japan*

OpenMX hands-on workshop, Nov. 23, 2016

# What is Band Structure?

# Angle-Resolved Photoelectron Spectroscopy (ARPES)



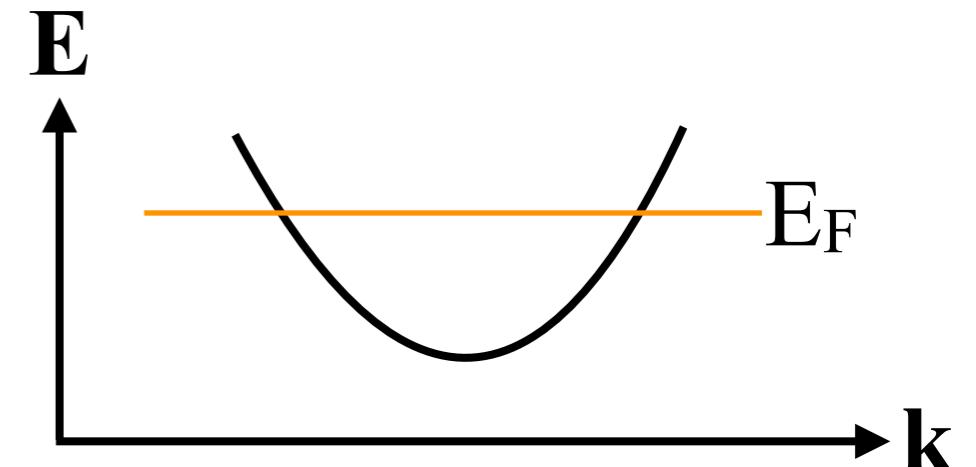
- ARPES experiment can directly measure the kinetic energy and momentum of an emitted electron. From that the relationship between binding energies and momenta of the electrons can be plotted as the **band structure**.

# Bloch theory and Kohn-Sham Hamiltonian

$$\hat{H}\psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + U(r)\right)\psi = \varepsilon\psi$$

$$U(r+R) = U(r)$$

$\psi_{nk}(r) = e^{ikr} u_{nk}(r)$  with eigenvalue  $\varepsilon_{nk}$

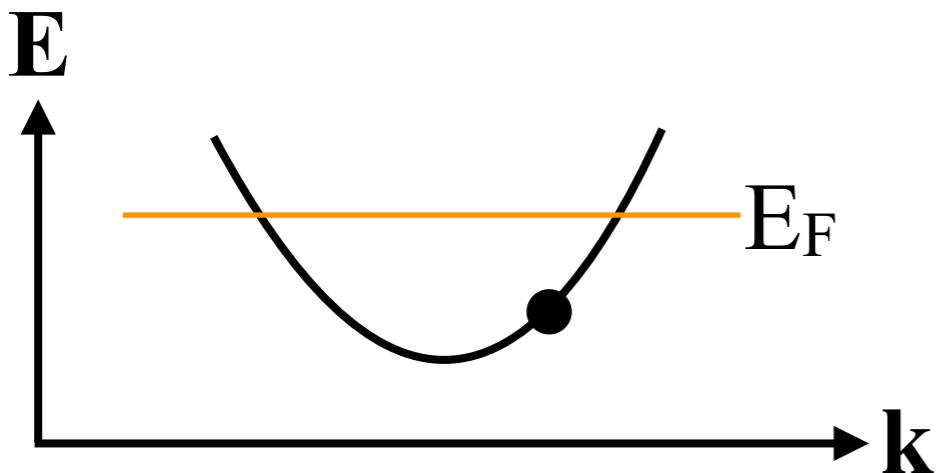


This is called  
**Band Structure**

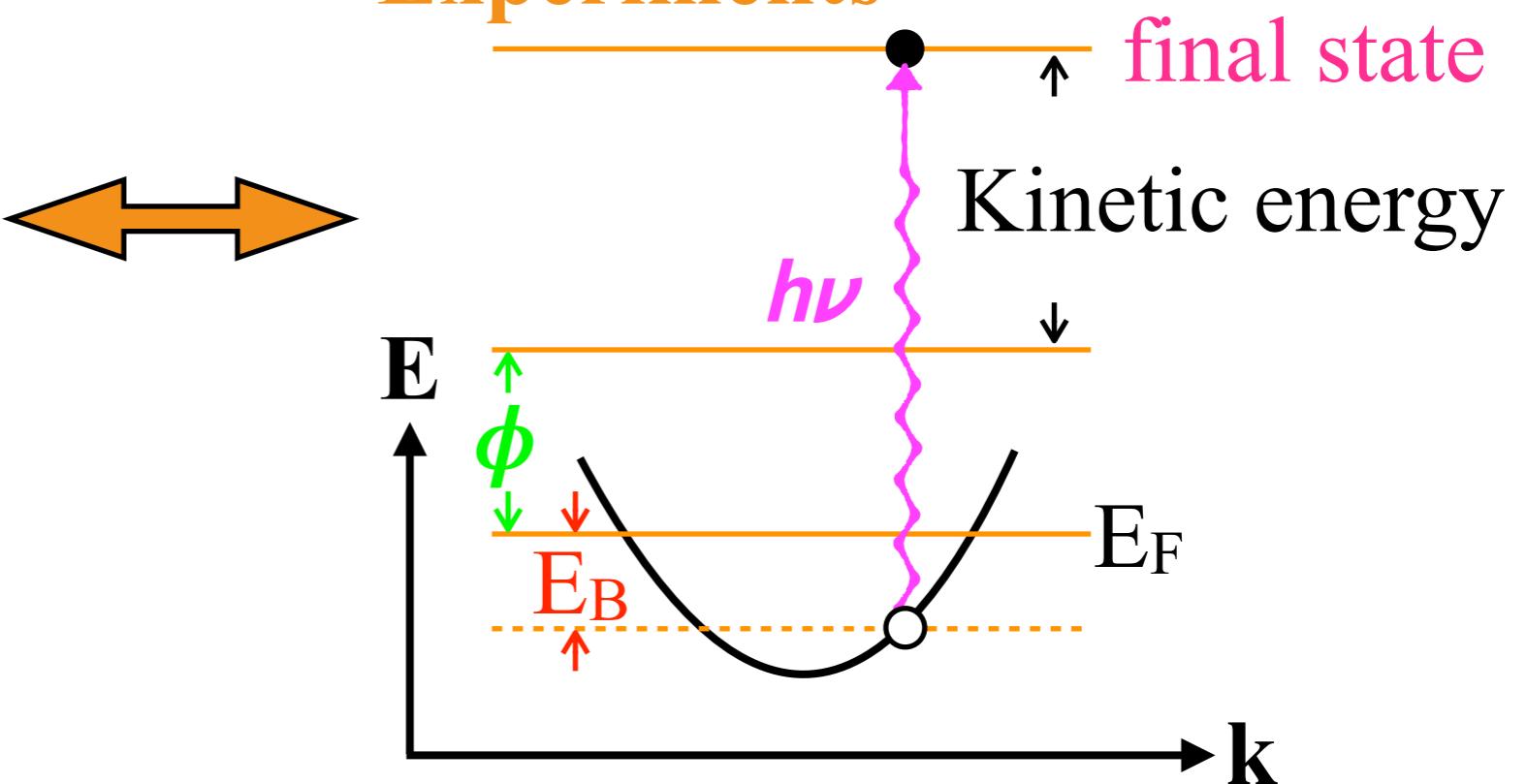
- Within the independent-electron picture, the eigenstates of single-particle Hamiltonian can be compared with the electrons that were measured by experiments that record the single-particle properties, such as ARPES experiments.
- Note that Kohn-Sham Hamiltonian that we learned in previous lectures falls into this category. (This interpretation might not be always valid!)

# Agreement on Band structures?

## Theoretical calculations



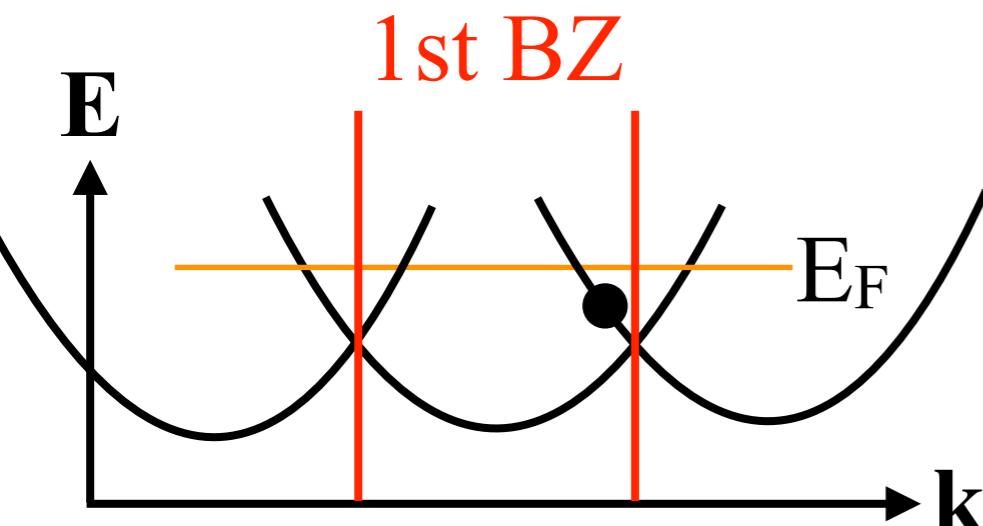
## Experiments



- To capture the single-particle properties from the theoretical calculation is relatively simple since we can obtain the eigenstates of the system under the assumption that the band theory works. (Recall that we have independent electrons experiencing the many-body interactions in the mean-field level through a one-body potential.)
- To understand the relation between experiment and theory is actually a tough task since the real situation involves the knowledge of final states in the bulk, surface properties, plane waves in vacuum, ... Or even beyond. (three-step model, one-step model, photon properties, ...)

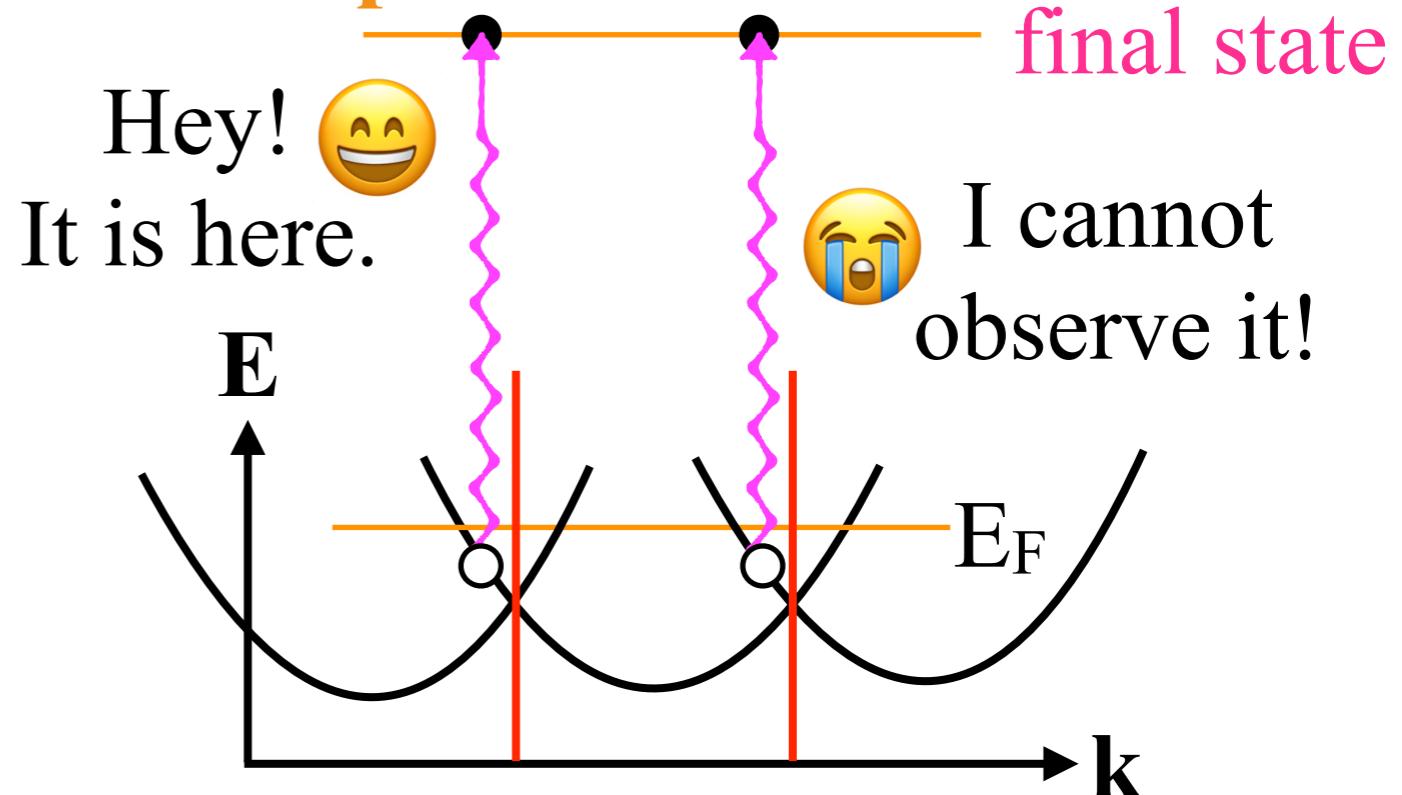
# An issue about band folding due to periodicity

## Periodic-zone representation



you might see  
gap-opening at  
zone boundary

## Experiments

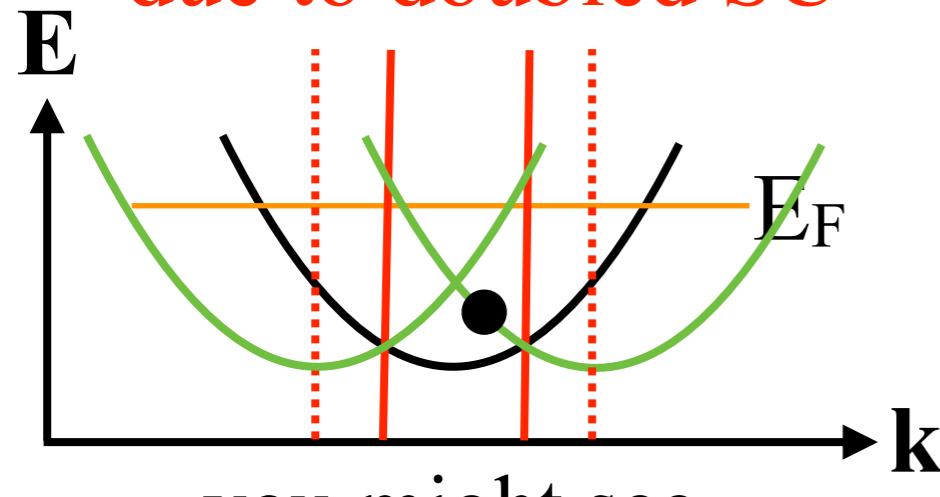


- In DFT calculations, there is no difference between the eigenstates inside and outside the BZ as long as they differ by a  $G$  vector since we have periodicity. However, ARPES cannot observe all the states.
- Which state can be observed can be analyzed by carefully considering the matrix elements between the relevant initial and final states.

# Another case: Band folding due to supercell

## Periodic-zone representation

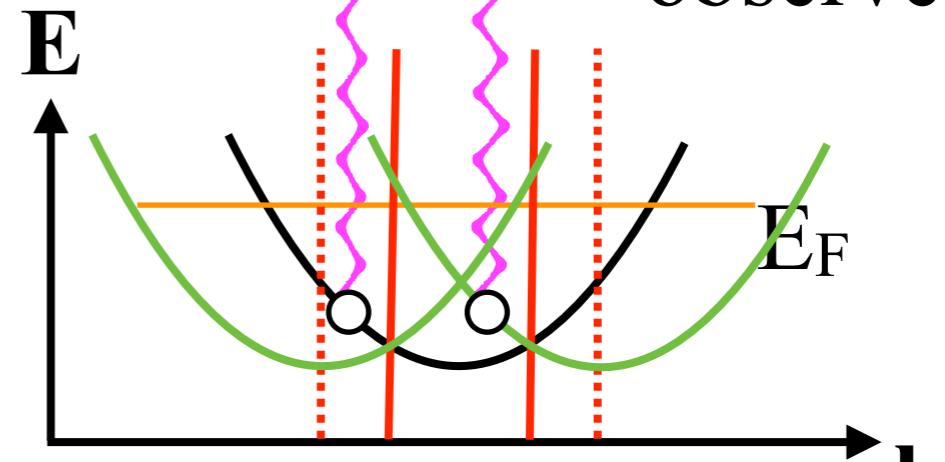
1st BZ shrinks  
due to doubled SC



you might see  
gap-opening at  
zone boundary

## Experiments

Hey! 😊 It is here.  
I cannot observe it!

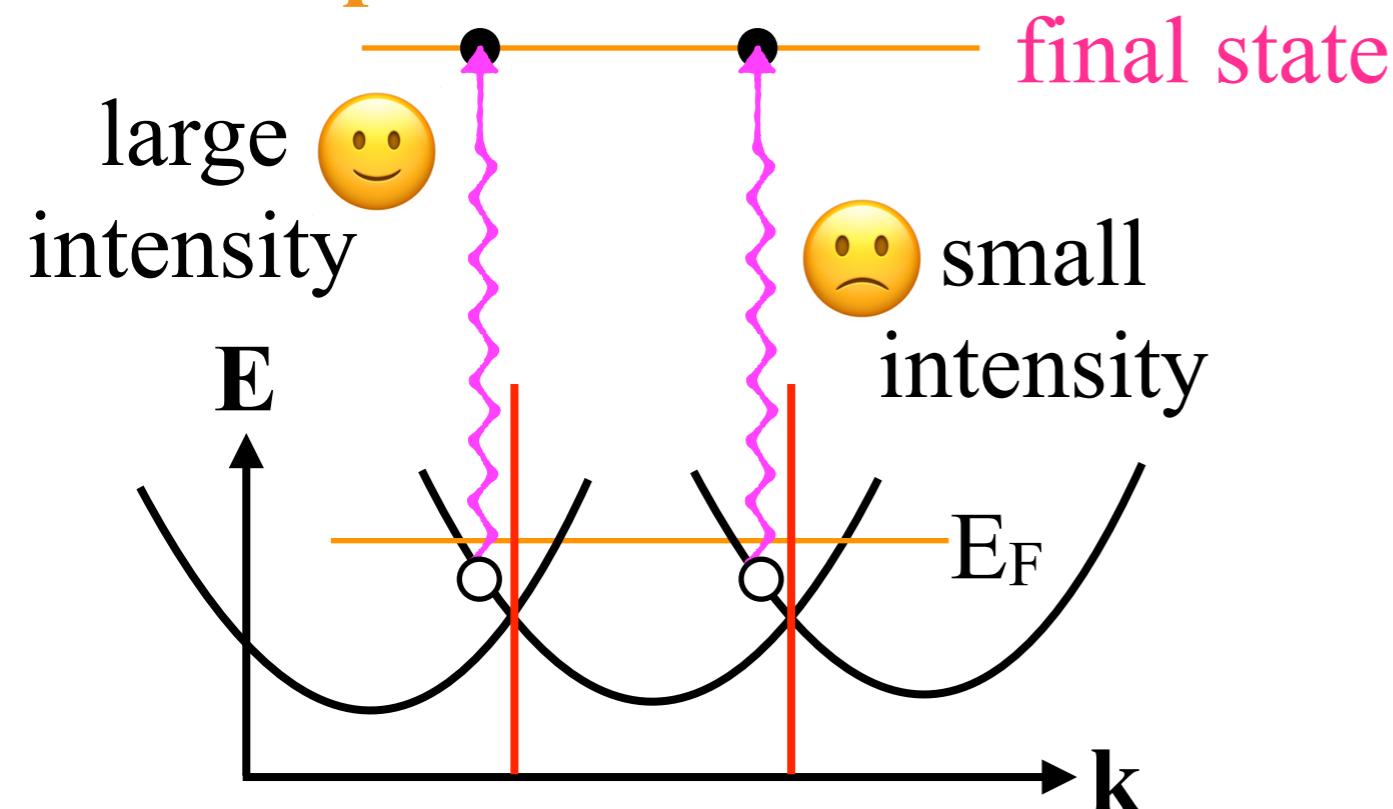


ARPES sometimes prefers the extended-zone representation

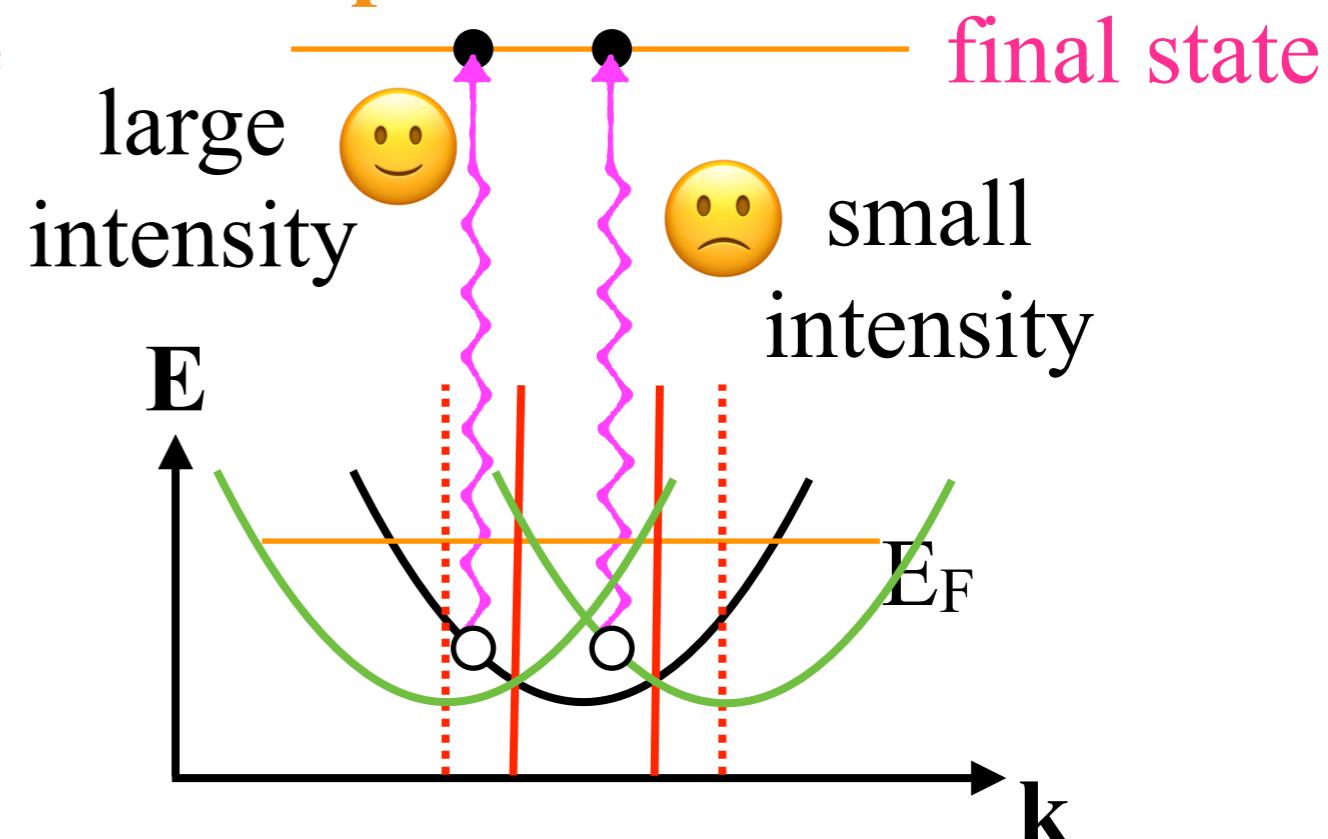
- Measured band structure cannot be suddenly changed by a small perturbation where we need to perform a supercell calculation.
- It is quite common that we need to perform supercell calculations to study the effects of imperfections and/or new orders, such as impurities, dislocations, orbital order, and magnetic order.

# More realistic situation

## Example 1

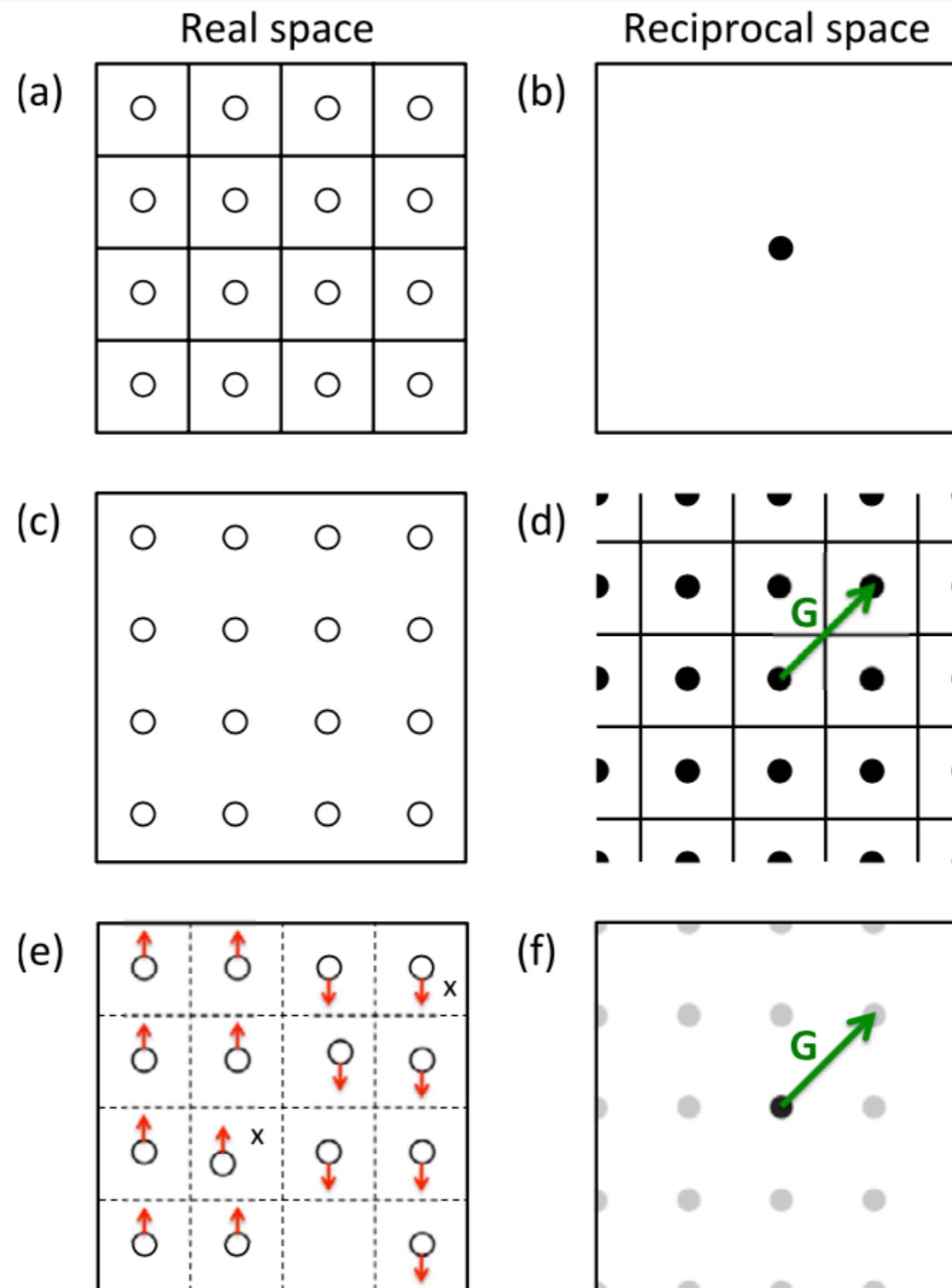


## Example 2



- The states differ by a  $G$  vector could carry different spectral weights, which correspond to different lifetimes. Zero lifetime cannot be measured by experiments. For example, the folded bands generated by a perfect supercell calculation should not be measured by ARPES.
- Since the matrix elements in ARPES are complicated, it is desired to have a way to analyze the band structure, for example, unfolding the band structure before calculating the matrix elements. In most cases, unfolded bands already have enough information for comparison with experiments (zero is zero) and for theoretical interests.

# An example for Fermi point



# How to Unfold Band Structure

# Changing basis from $|KJ\rangle$ to $|kj\rangle$ in real space

The idea for performing unfolding is to represent the spectral weight by a reference  $|kj\rangle$  or  $|kn\rangle$  basis, where  $|kj\rangle$  denotes the eigenstate of a conceptual system and  $|kn\rangle$  the Wannier function or LCAO orbital. To make the implementation practical, the supercell eigenstates  $|KJ\rangle$  is inserted to eliminate “ $|kj\rangle$ ”. Note that from  $|KJ\rangle$  to  $|kj\rangle$  is exactly the “unfolding procedure” where  $k$  belongs to the BZ of the conceptual cell.

**Wannier function**  $A_{kn,kn}(\omega) = \sum_{\substack{KJ \\ \text{rn RM}}} \langle kn | KJ \rangle \langle KJ | A(\omega) | KJ \rangle \langle KJ | kn \rangle$

**LCAO orbital**  $A_{kj,kj} = \sum_{mnK} S_{nm}^{-1}(k) \langle km | KJ \rangle A_{KJ,KJ} \langle KJ | kn \rangle$

100% spectral weight at SC  $\varepsilon_{KJ}$

$$A_{kj,kj}(\omega) = \frac{L}{l} \sum_{KG} \delta_{k-G,K} W_{KJ} A_{KJ,KJ}(\omega)$$

Overlap matrix elements for  
non-orthogonal basis set

$$W_{KJ} = \sum_{MNr} e^{ik(r-r'(M))} C_M^{KJ} C_N^{KJ*} S_{0N,rm(M)}$$

Wei Ku *et al.*, Phys. Rev. Lett. **104**, 216401 (2010).

Chi-Cheng Lee *et al.*, J. Phys.: Condens. Matter **25**, 345501 (2013).

hands-on workshop

# Changing basis from $|KJ\rangle$ to $|kj\rangle$ in real space

**LCAO orbital**  $A_{kj,kj} = \sum_{mnK} S_{nm}^{-1}(k) \langle km|KJ\rangle A_{KJ,KJ} \langle KJ|kn\rangle$

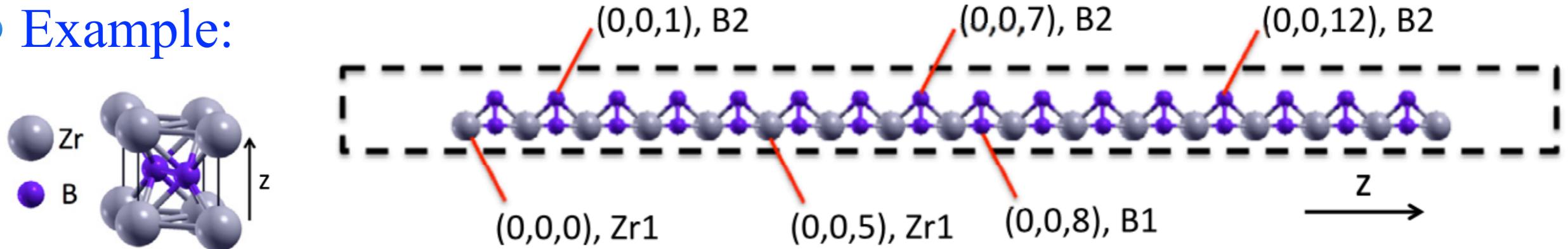
$$A_{kj,kj}(\omega) = \frac{L}{l} \sum_{KG} \delta_{k-G,K} W_{KJ} A_{KJ,KJ}(\omega)$$

$$W_{KJ} = \sum_{MNr} e^{ik(r-r'(M))} C_M^{KJ} C_N^{KJ*} S_{0N,rm(M)}$$

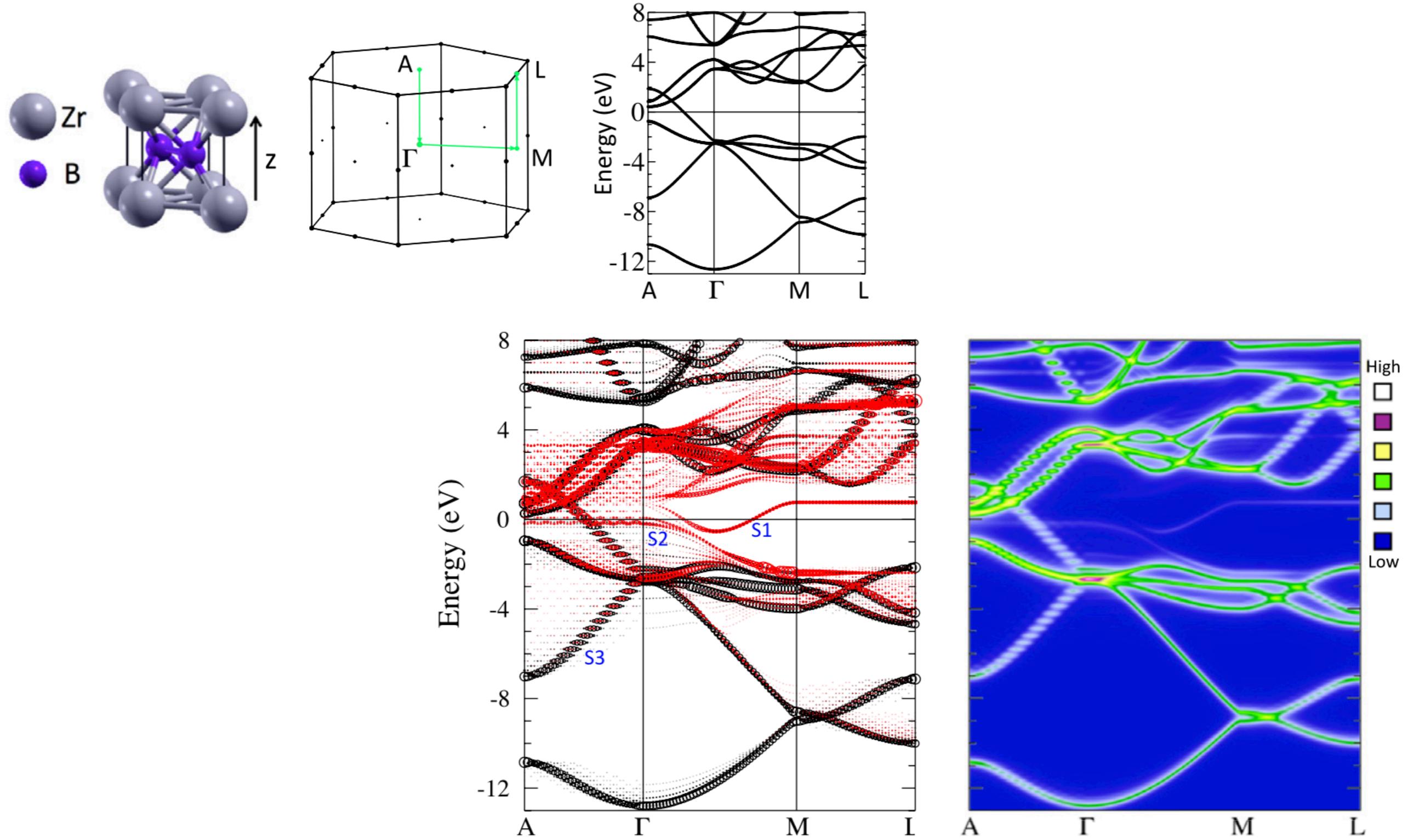
- The essential part is to relabel SC lattice vector by reference-cell lattice vector and relabel the SC orbital in terms of the reference-cell orbital:

$$R \rightarrow R + r_0(M) \text{ and } M \rightarrow m'(M)$$

- Example:



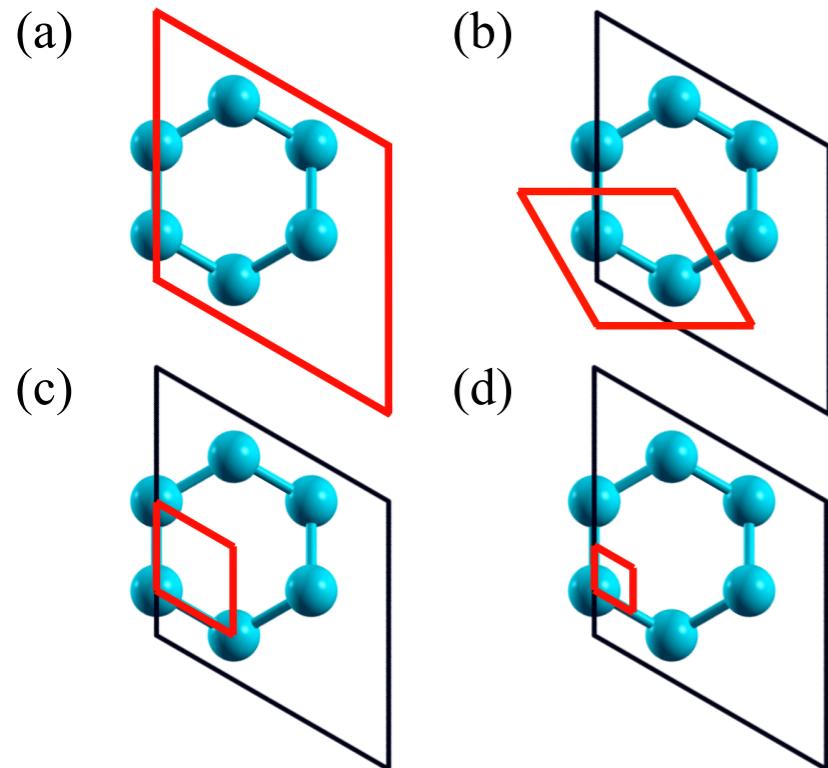
# ZrB<sub>2</sub> slab



# Example: Missing spectral weight

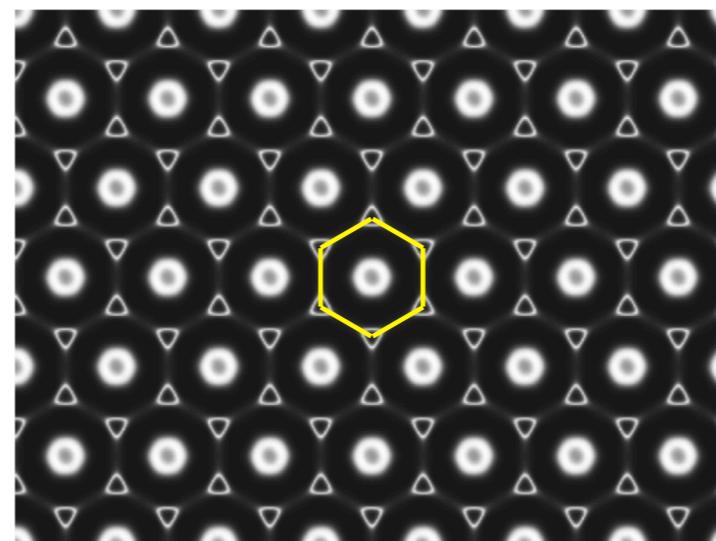
# Silicene: Missing spectral weight

## Free-standing planar-like silicene

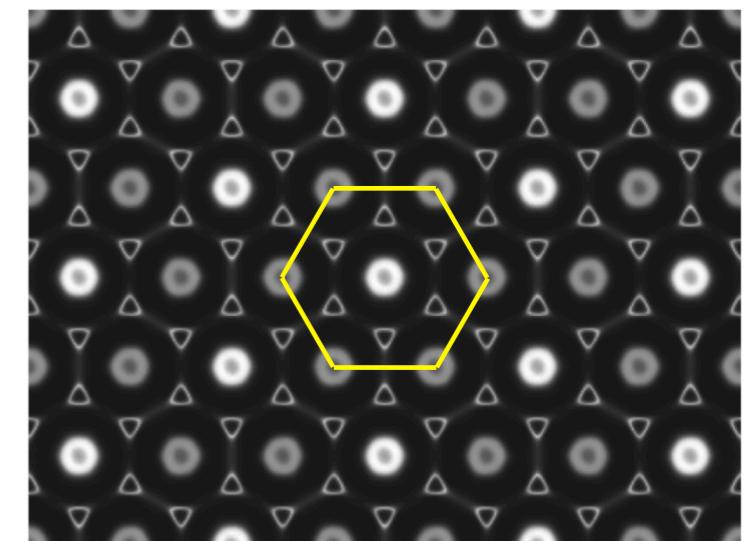


Energy = 1eV below the Fermi energy

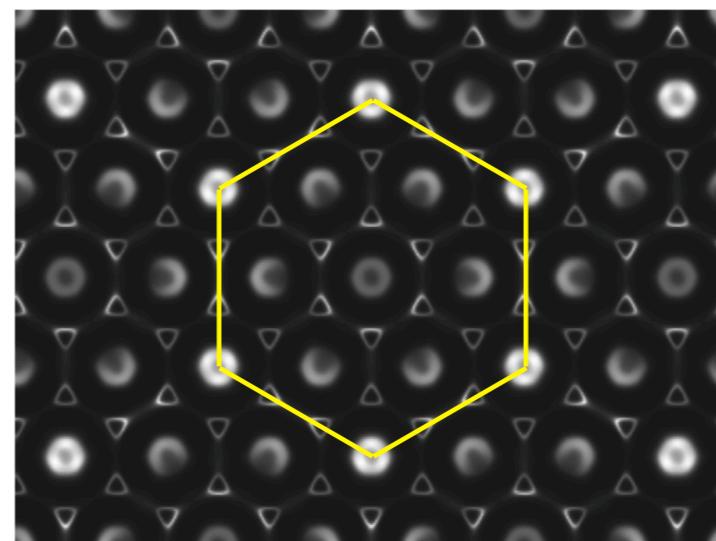
(i) Planar-like phase



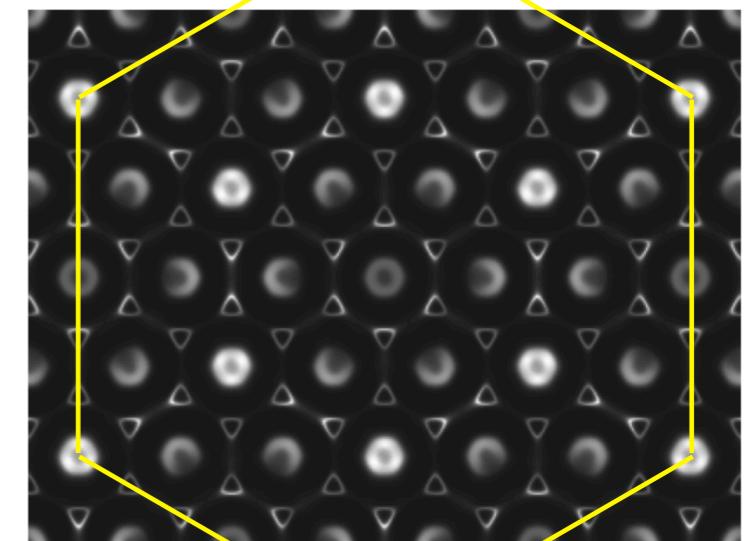
(j)



(k)



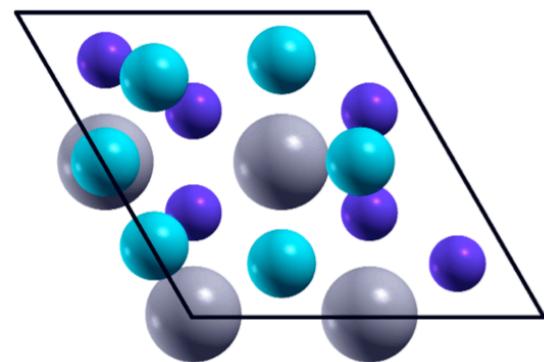
(l)



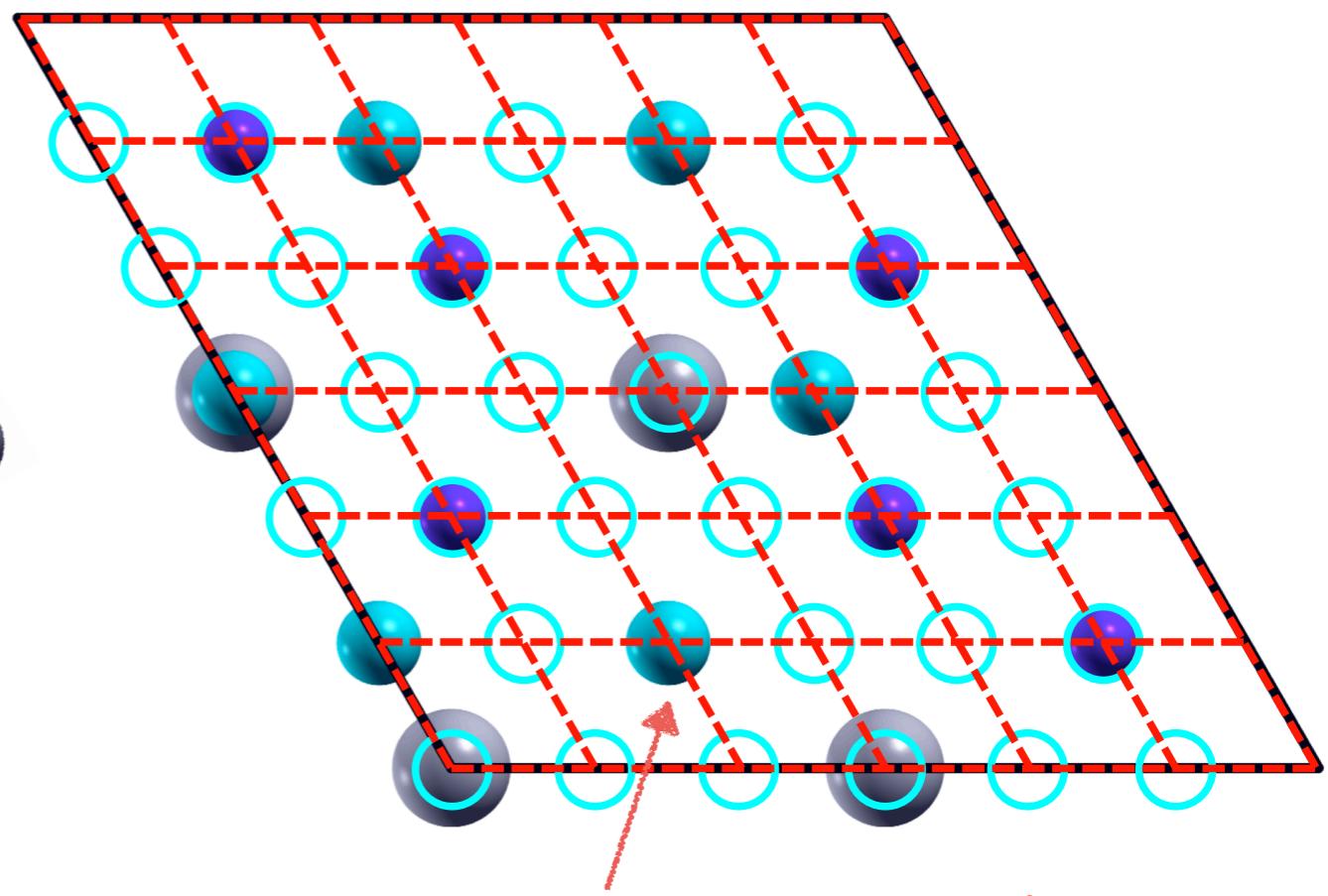
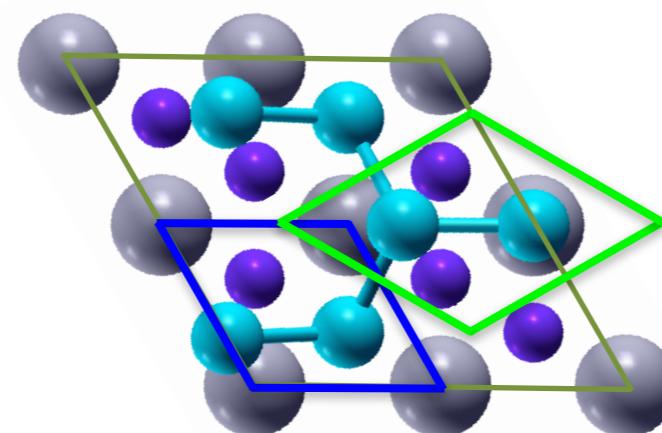
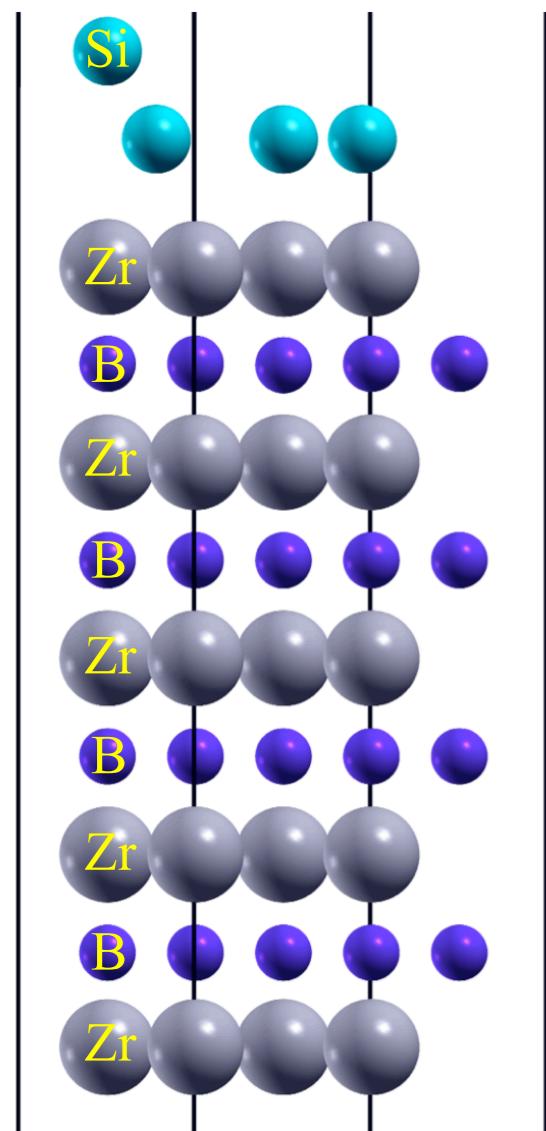
- Iso-energy surface, such as Fermi surface, could be disconnected!

# Silicene on ZrB<sub>2</sub>: Conceptual unit cell

## Planar-like silicene

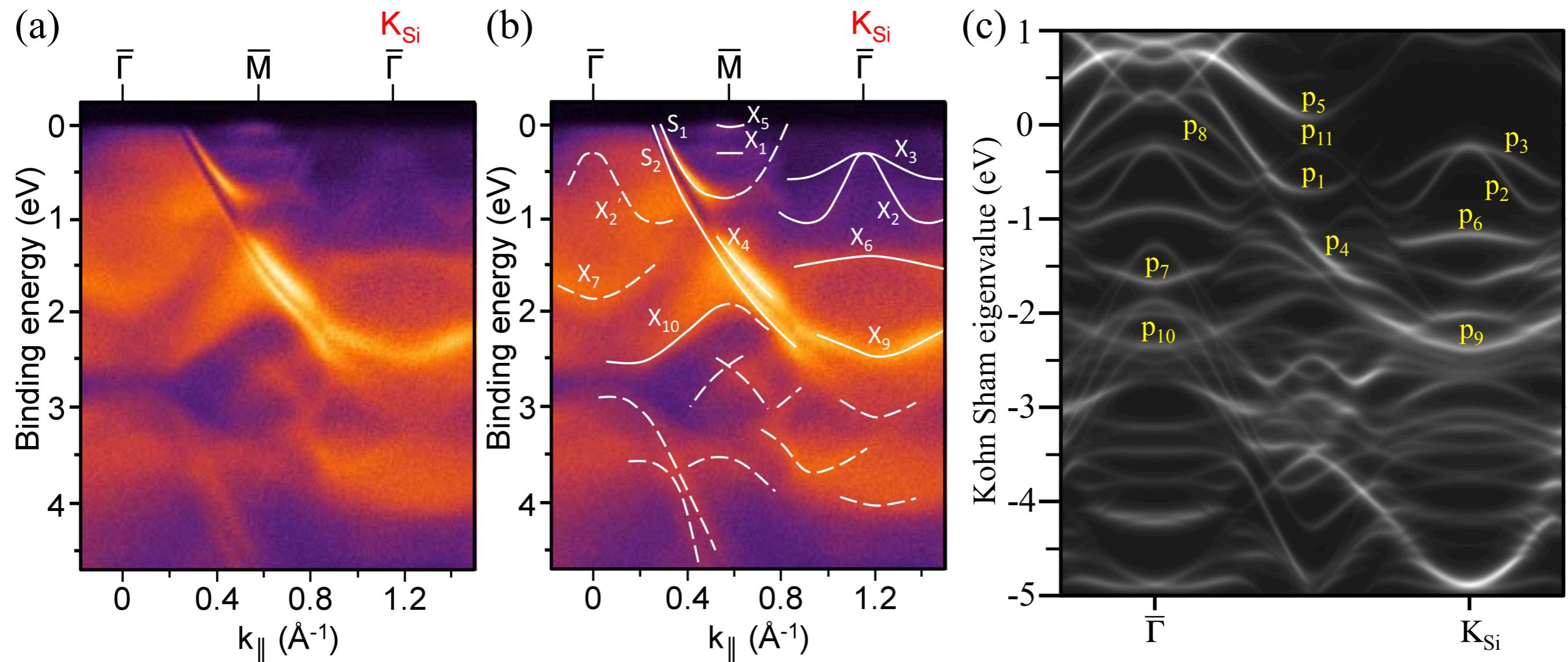


$\sqrt{3} \times \sqrt{3}$  - reconstructed silicene



**commensurate unit cell**

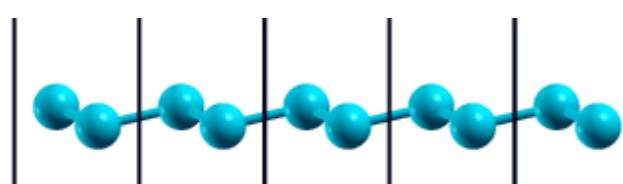
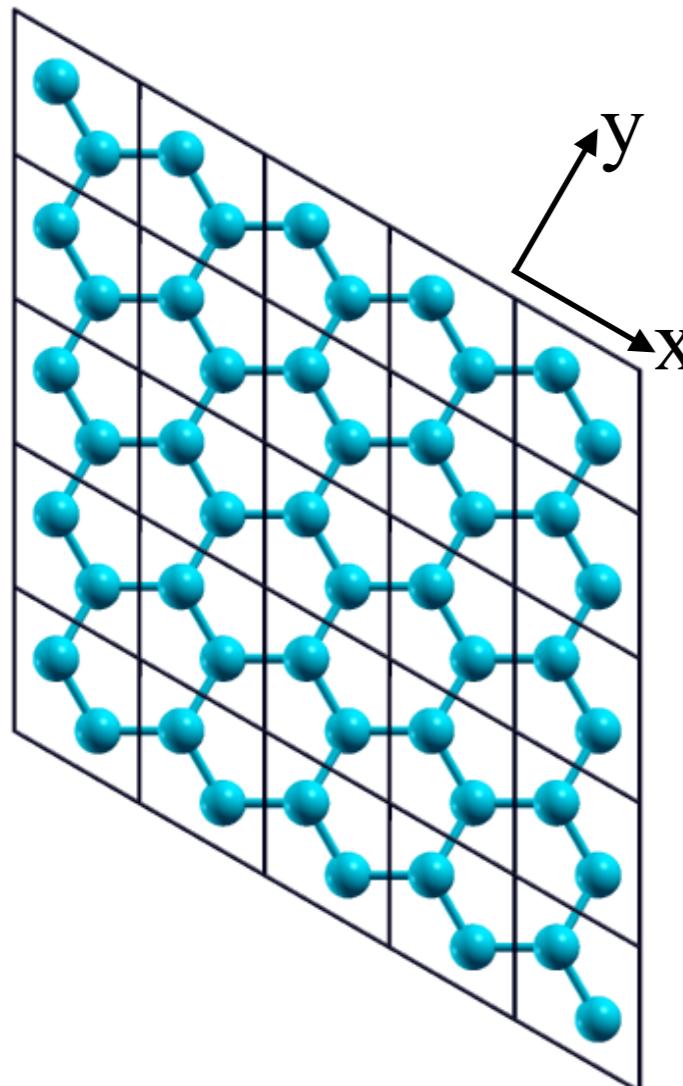
# Silicene on ZrB<sub>2</sub>: Concept unit cell



# How to run unfolding in OpenMX

# Free-standing silicene

## Step 1: Choose a system to study



```
System.CurrentDirectory          ./
System.Name                      Silicene
DATA.PATH                         /provide_your_path/DFT_DATA13

Species.Number           1
<Definition.of.Atomic.Species
  Si   Si7.0-s2p2d1  Si_PBE13
Definition.of.Atomic.Species>

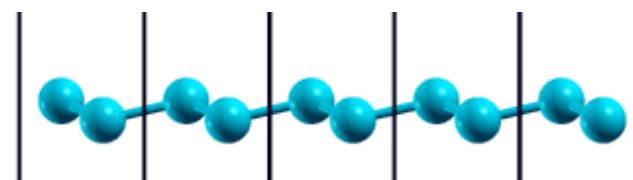
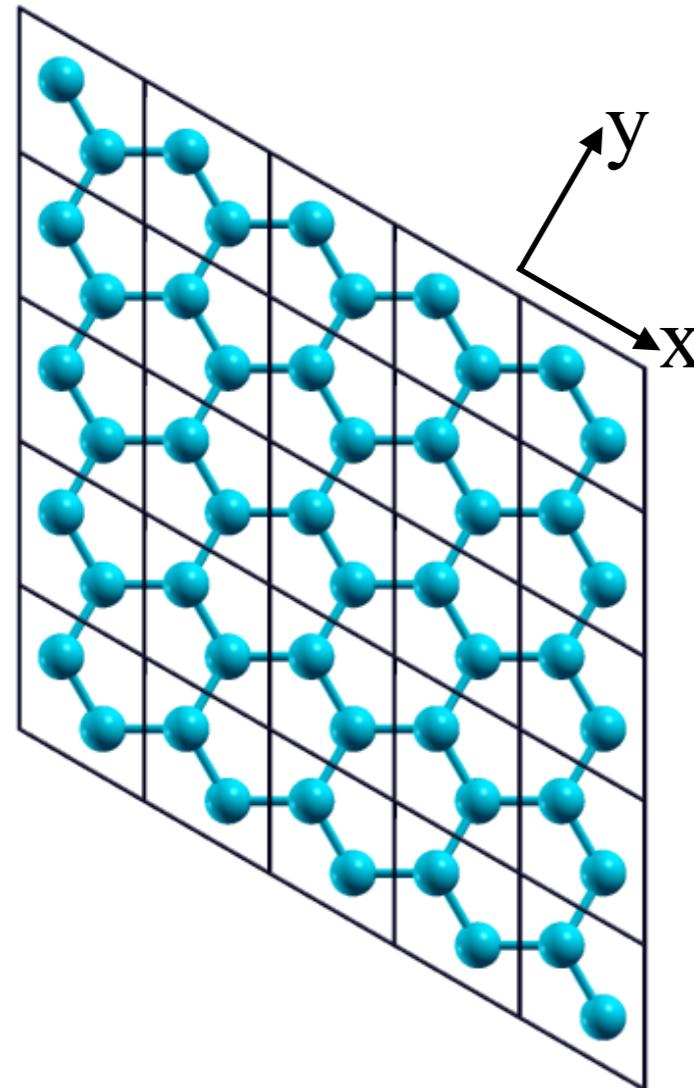
Atoms.Number           2
Atoms.SpeciesAndCoordinates.Unit    FRAC # Ang | AU
<Atoms.SpeciesAndCoordinates
  1      Si      0.33333  0.66666  0.4871  2. 2.
  2      Si      0.66666  0.33333  0.5128  2. 2.
Atoms.SpeciesAndCoordinates>

Atoms.UnitVectors.Unit    Ang
<Atoms.UnitVectors
  3.8577926 0 0
  -1.9288963 3.3409463939 0
  0 0 20
Atoms.UnitVectors>

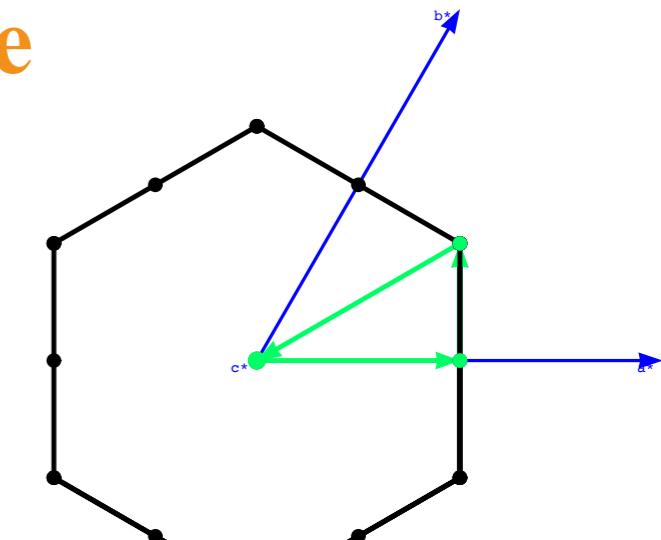
scf.XcType            GGA-PBE      # LDA|LSDA-CA|LSDA-PW|GGA-PBE
scf.SpinPolarization Off         # On|Off
scf.energy cutoff     250.0       # default=150 (Ry)
scf.maxIter           100         # default=40
scf.EigenvalueSolver band        # Recursion|Cluster|Band
scf.Kgrid              8 8 1      # means n1 x n2 x n3
scf.Mixing.Type        rmm-diisk # Simple|Rmm-Diis|Gr-Pulay
scf.criterion          1.0e-8     # default=1.0e-6 (Hartree)
```

# Free-standing silicene

## Step 2: Choose $k$ paths for your band structure



We can plot band structure using unfolding keyword



```
Unfolding.Electronic.Band      on
Unfolding.LowerBound           -12.0
Unfolding.UpperBound           8.0
# on|off, default=off
# default=-10 eV
# default= 10 eV

Unfolding.Nkpoint              4

<Unfolding.kpoint
G 0 0 0
M 0.5 0 0
K 0.3333333 0.3333333 0
G 0 0 0
Unfolding.kpoint>

Unfolding.desired_totalnkpt    50
```

- Although the keyword is “unfolding”, the unfolding is not performed! More precisely, the band is unfolded to itself (the same zone).

# Free-standing silicene

**Step 3: Looking for the output files: Silicene.unfold\_totup**

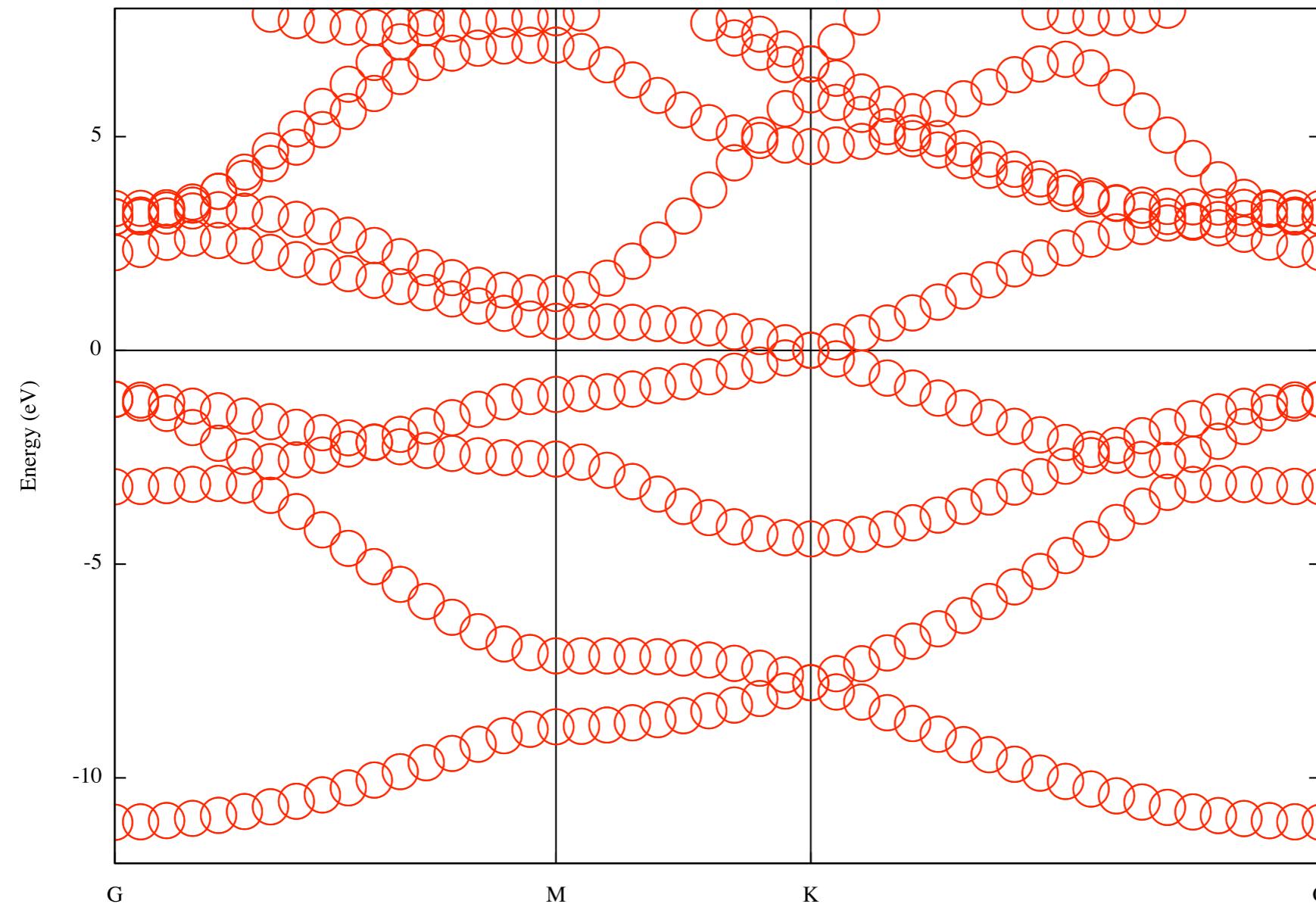
**Silicene.unfold\_orbup**

**Silicene.unfold\_plotexample**

gnuplot

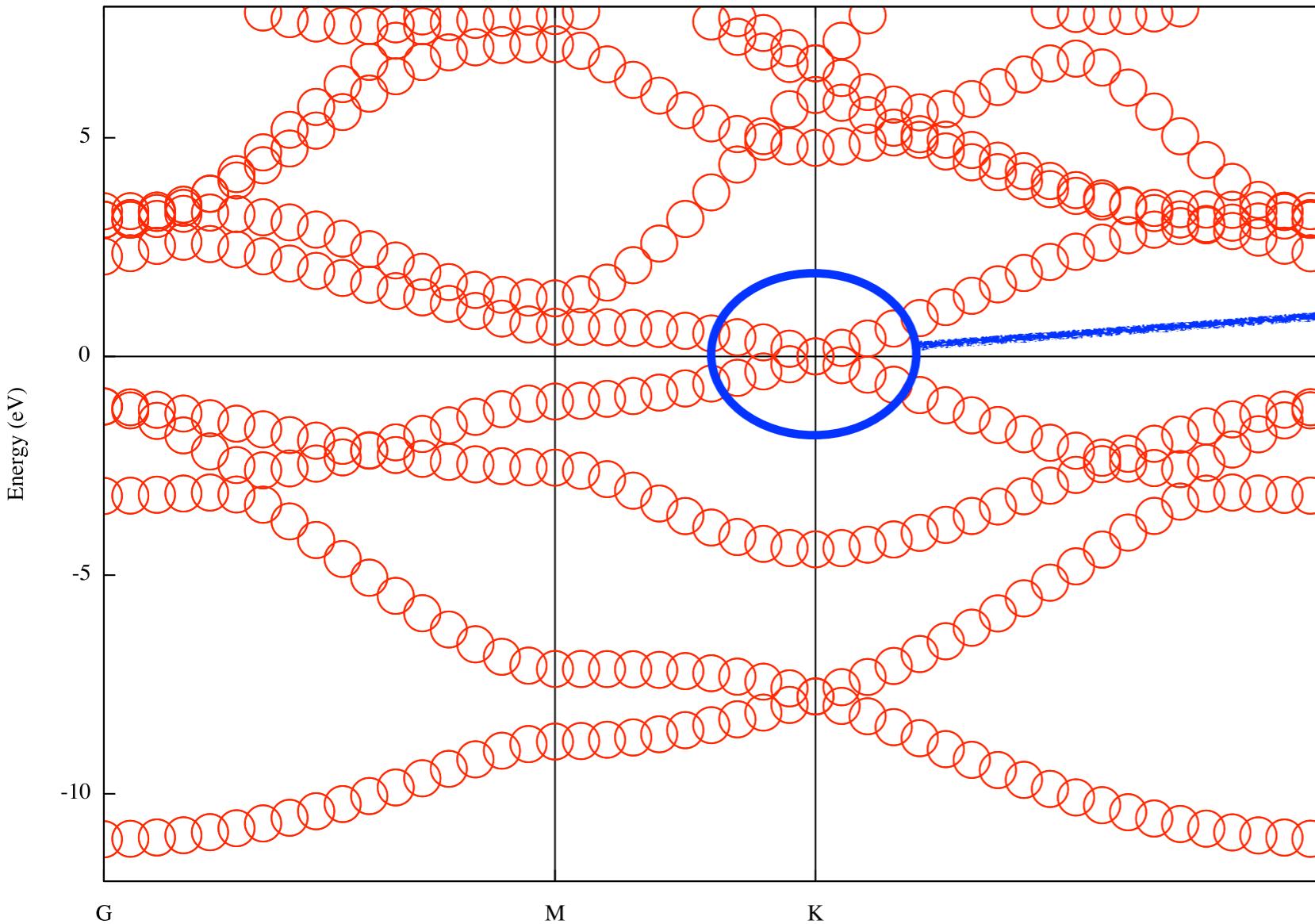
gnuplot> load 'Silicene.unfold\_plotexample'

plot 'Silicene.unfold\_totup' using 1:2:(\$3)\*0.02 notitle with circles lc rgb 'red'



# Free-standing silicene

## Step 4: Try to find something interesting



We have a Dirac cone.  
What is the orbital  
contribution?

- The orbital contribution can be found in `Silicene.unfold_orbup` and the format is `k_dis` ( $\text{Bohr}^{-1}$ ), `energy(eV)`, and `weight`. The sequence of the orbital weights can be found in `Silicene.out`.

# Free-standing silicene

## Step 5: Read output file for picking up the investigated orbitals

In Silicene.out, we can find

The sequence for the orbital weights in System.Name.unfold\_orbup(dn) is given below.

|    |   |    |   |             |   |  |
|----|---|----|---|-------------|---|--|
| 1  | 1 | Si | 0 | s           | 3 |  |
| 2  |   |    | 1 | s           | 4 |  |
| 3  |   |    | 0 | px          | 5 |  |
| 4  |   |    | 0 | py          | 6 | $k_{\text{dis}}$ (Bohr $^{-1}$ ), energy(eV) |
| 5  |   |    | 0 | pz          | 7 | 1  |
| 6  |   |    | 1 | px          |   | 2  |
| 7  |   |    | 1 | py          |   |  |
| 8  |   |    | 1 | pz          |   |  |
| 9  |   |    | 0 | $d3z^2-r^2$ |   |  |
| 10 |   |    | 0 | $dx^2-y^2$  |   |  |
| 11 |   |    | 0 | dxy         | . |  |
| 12 |   |    | 0 | dxz         | . |  |
| 13 |   |    | 0 | dyz         | . |  |
| 14 | 2 | Si | 0 | s           |   |  |
| 15 |   |    | 1 | s           |   | $p_z: \$7+\$10+\$20+\$23$                    |
| 16 |   |    | 0 | px          |   |  |
| 17 |   |    | 0 | py          |   |  |
| 18 |   |    | 0 | pz          |   |  |
| 19 |   |    | 1 | px          |   |  |
| 20 |   |    | 1 | py          |   |  |
| 21 |   |    | 1 | pz          |   |  |
| 22 |   |    | 0 | $d3z^2-r^2$ |   |  |
| 23 |   |    | 0 | $dx^2-y^2$  |   |  |
| 24 |   |    | 0 | dxy         |   |  |
| 25 |   |    | 0 | dxz         |   |  |
| 26 |   |    | 0 | dyz         |   |  |

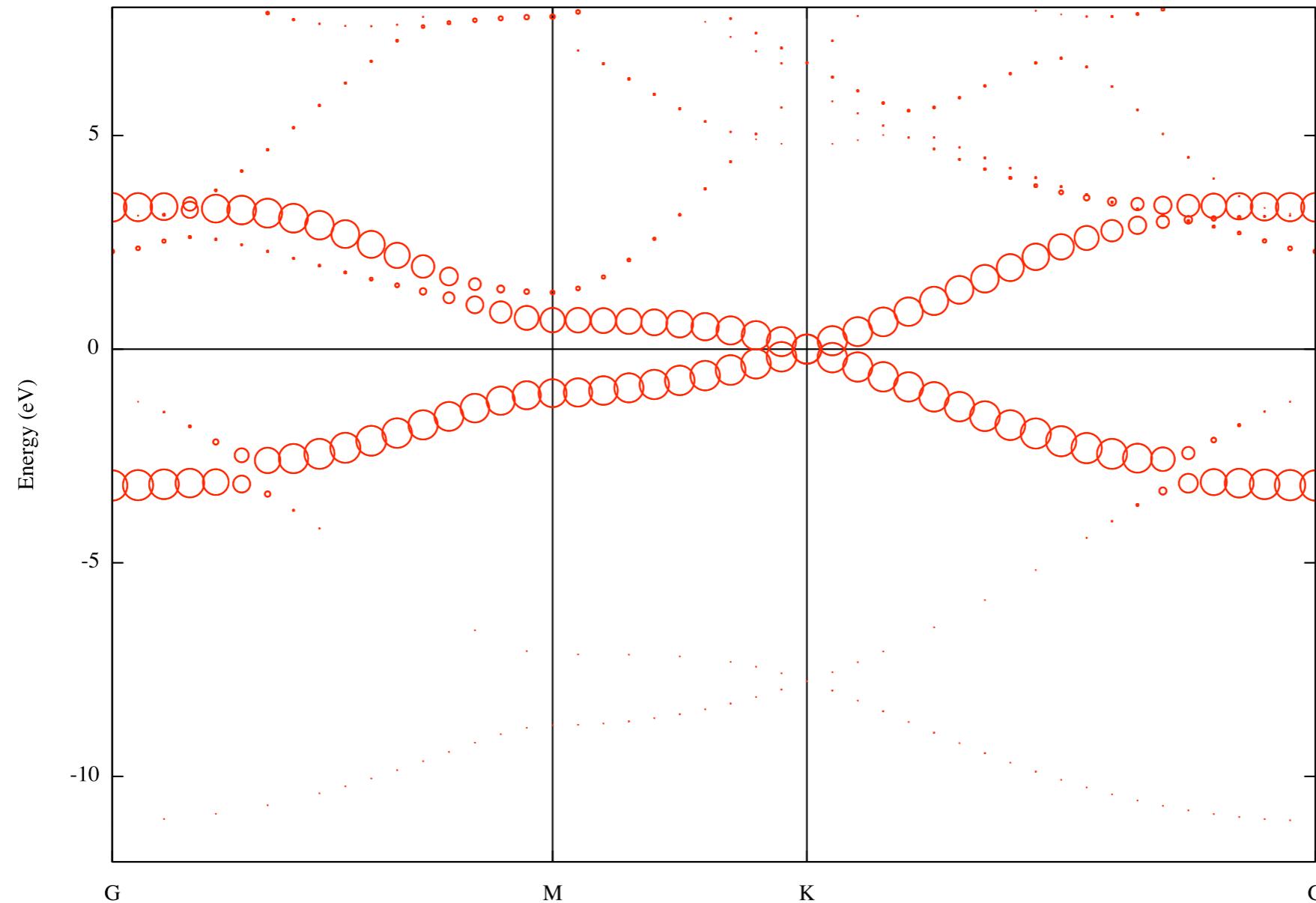
# Free-standing silicene

## Step 6: Examine orbital contribution

gnuplot

```
gnuplot> load 'Silicene.unfold_plotexample'
```

```
plot 'Silicene.unfold_orbup' using 1:2:(\$7+\$10+\$20+\$23)*0.02 notitle with circles lc rgb 'red'
```

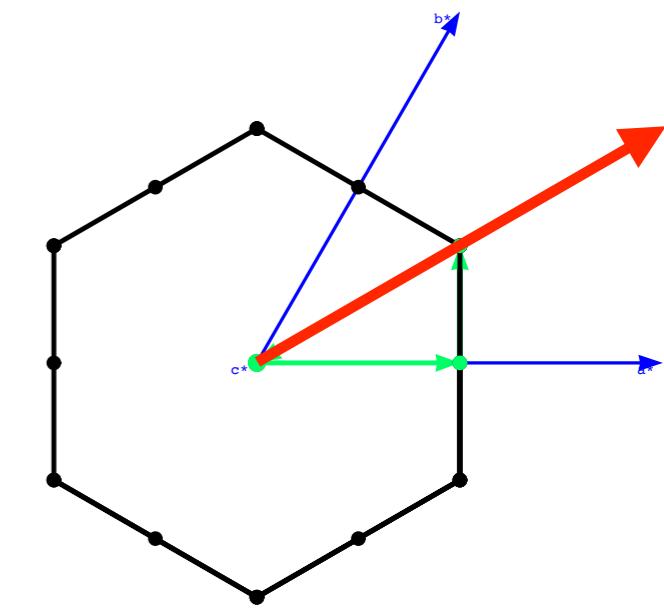
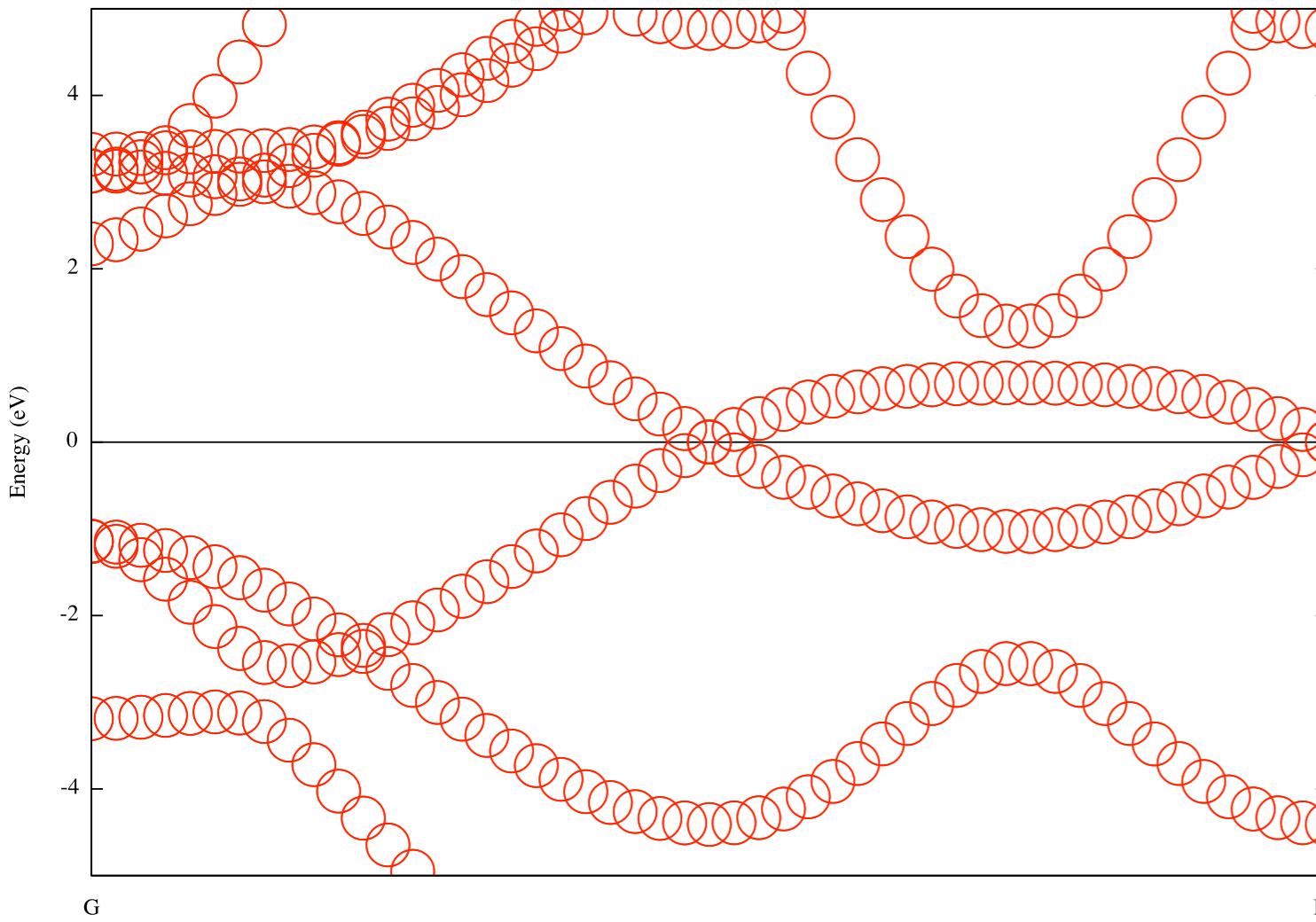


- The Dirac cone is composed of  $p_z$  orbitals

# Free-standing silicene

## Step 7: Find something even more interesting Prepare for performing unfolding

```
Unfolding.Electronic.Band      on      # on|off, default=off
Unfolding.LowerBound           -5.0   # default=-10 eV
Unfolding.UpperBound           5.0    # default= 10 eV
Unfolding.Nkpoint              2
<Unfolding.kpoint>
G 0 0 0
K2 0.6666666 0.6666666 0
Unfolding.kpoint>
Unfolding.desired_totalnkpt  51
```

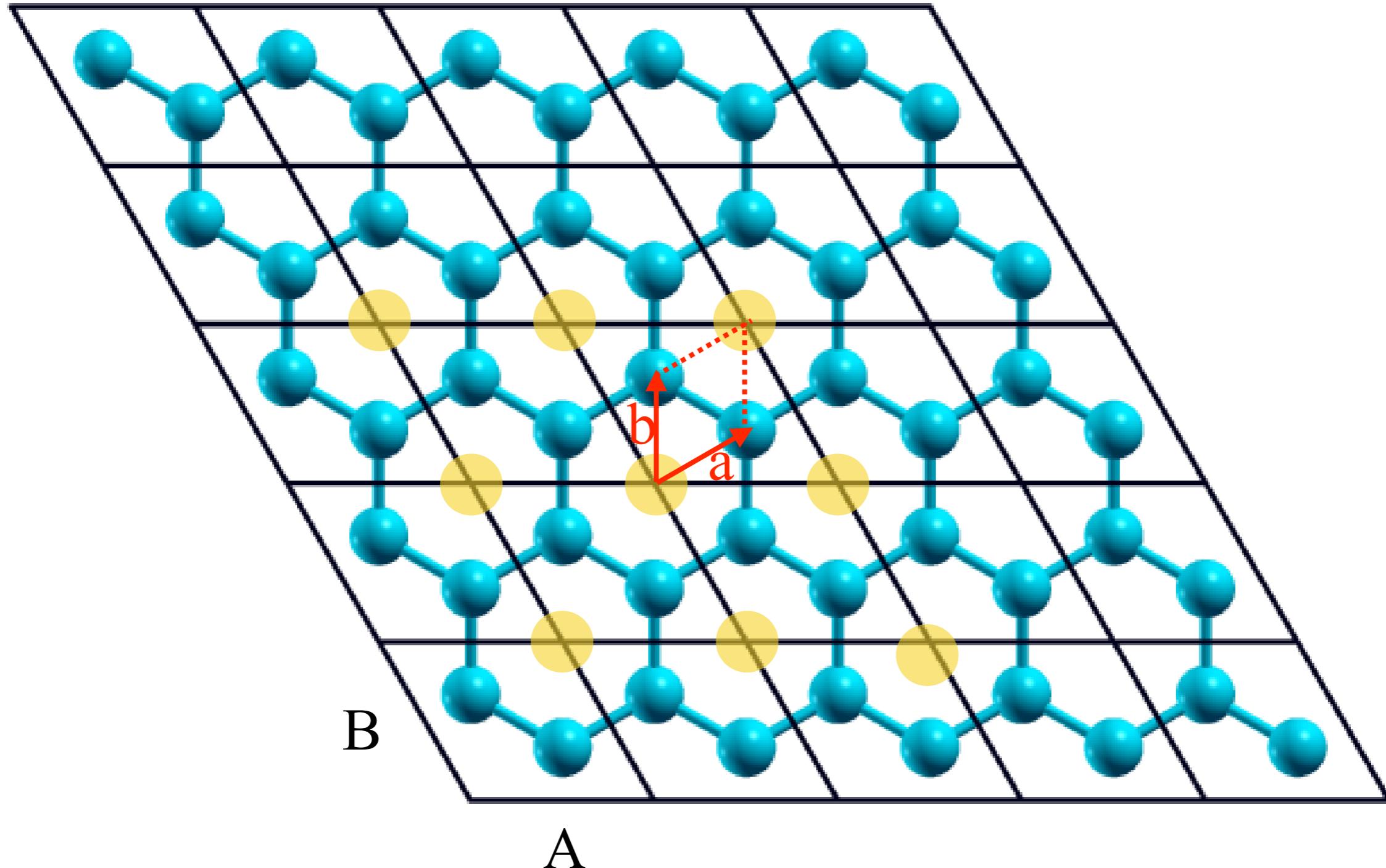


Will the result be different if we choose a larger BZ and unfold the bands to that zone?

The choice of a new conceptual unit cell seems to be important.

# Free-standing silicene

Step 8: Find a conceptual unit cell for your purpose



- The conceptual unit cell is still commensurate with the primitive unit cell

# Free-standing silicene

## Step 9: Unfolding: Provide conceptual cell information

### Calculated unit cell (supercell)

```
Atoms.UnitVectors.Unit Ang  
<Atoms.UnitVectors  
  3.8577926 0 0  
  -1.9288963 3.3409463939 0  
  0 0 20  
Atoms.UnitVectors>
```

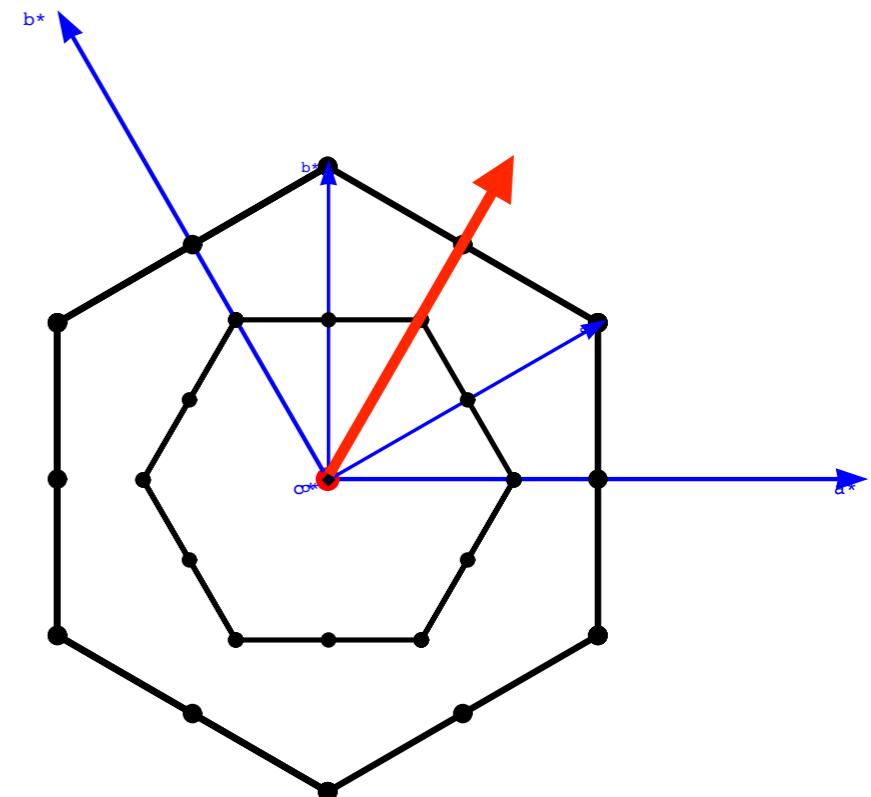
### Conceptual unit cell for defining the new Brillouin zone

```
<Unfolding.ReferenceVectors  
  1.9288963033 1.1136488 0  
  0 2.2272976 0  
  0 0 20  
Unfolding.ReferenceVectors>
```

```
Unfolding.Electronic.Band      on  
Unfolding.LowerBound          -5.0  
Unfolding.UpperBound          5.0  
Unfolding.Nkpoint              2  
Unfolding.desired_totalnkpt   51
```

```
<Unfolding.kpoint → using the reciprocal lattice  
G 0 0 0  
K2 0.6666666 0.6666666 0  
Unfolding.kpoint>  
  
<Unfolding.Map  
1 1  
2 1  
Unfolding.Map>
```

using the reciprocal lattice vectors of the conceptual unit cell as the units



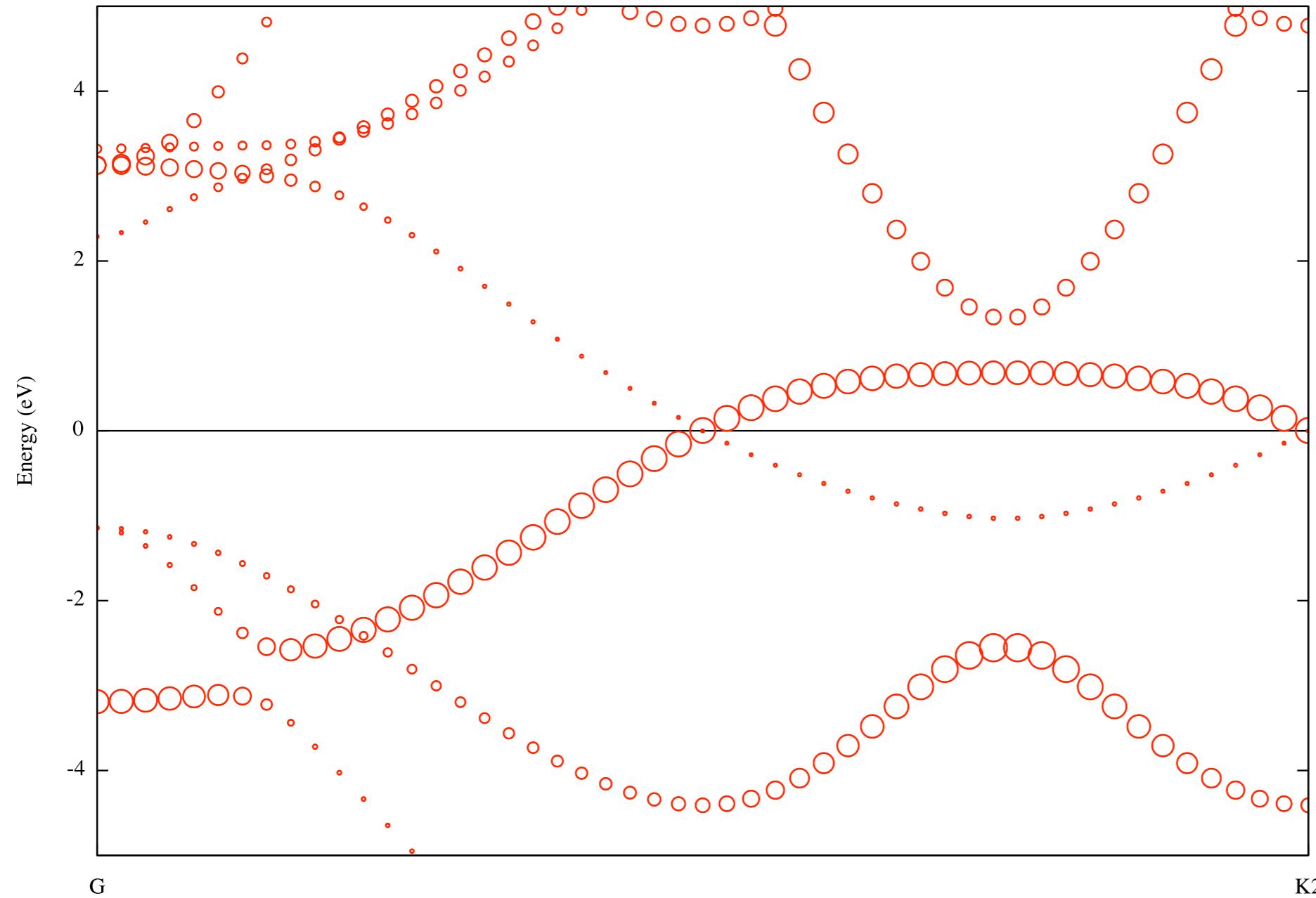
# Free-standing silicene

## Step 10: Plot unfolded spectral weight

gnuplot

```
gnuplot> load 'Silicene.unfold_plotexample'
```

```
plot 'Silicene.unfold_totup' using 1:2:($3)*0.02 notitle with circles lc rgb 'red'
```



# Free-standing silicene

## Step 10: Or using intensity map

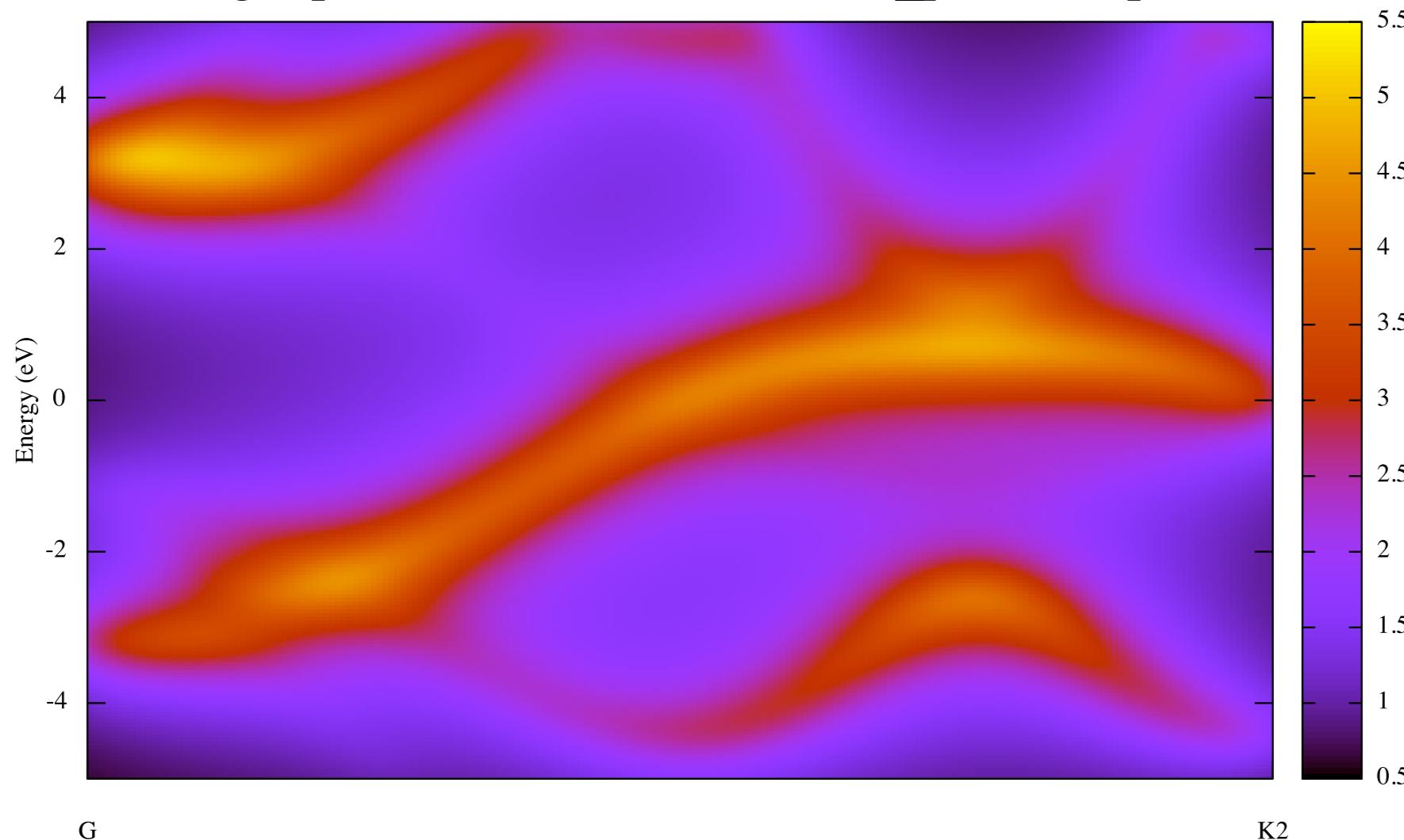
```
gcc intensity_map.c -lm -o intensity_map (do this in the “source” directory)
```

```
./intensity_map Silicene.unfold_totup -c 3 -k 0.5 -e 0.05 -l -5 -u 5 > map.txt
```

modify the Silicene.unfold\_plotexample as the following:

```
set yrang [-5.000000:5.000000]
set ylabel 'Energy (eV)'
set xtics('G' 0.000000,'K2' 1.149161)
set xrange [0:1.149161]
set arrow nohead from 0,0 to 1.149161,0
set pm3d map
sp 'map.txt'
```

gnuplot> load 'Silicene.unfold\_plotexample'



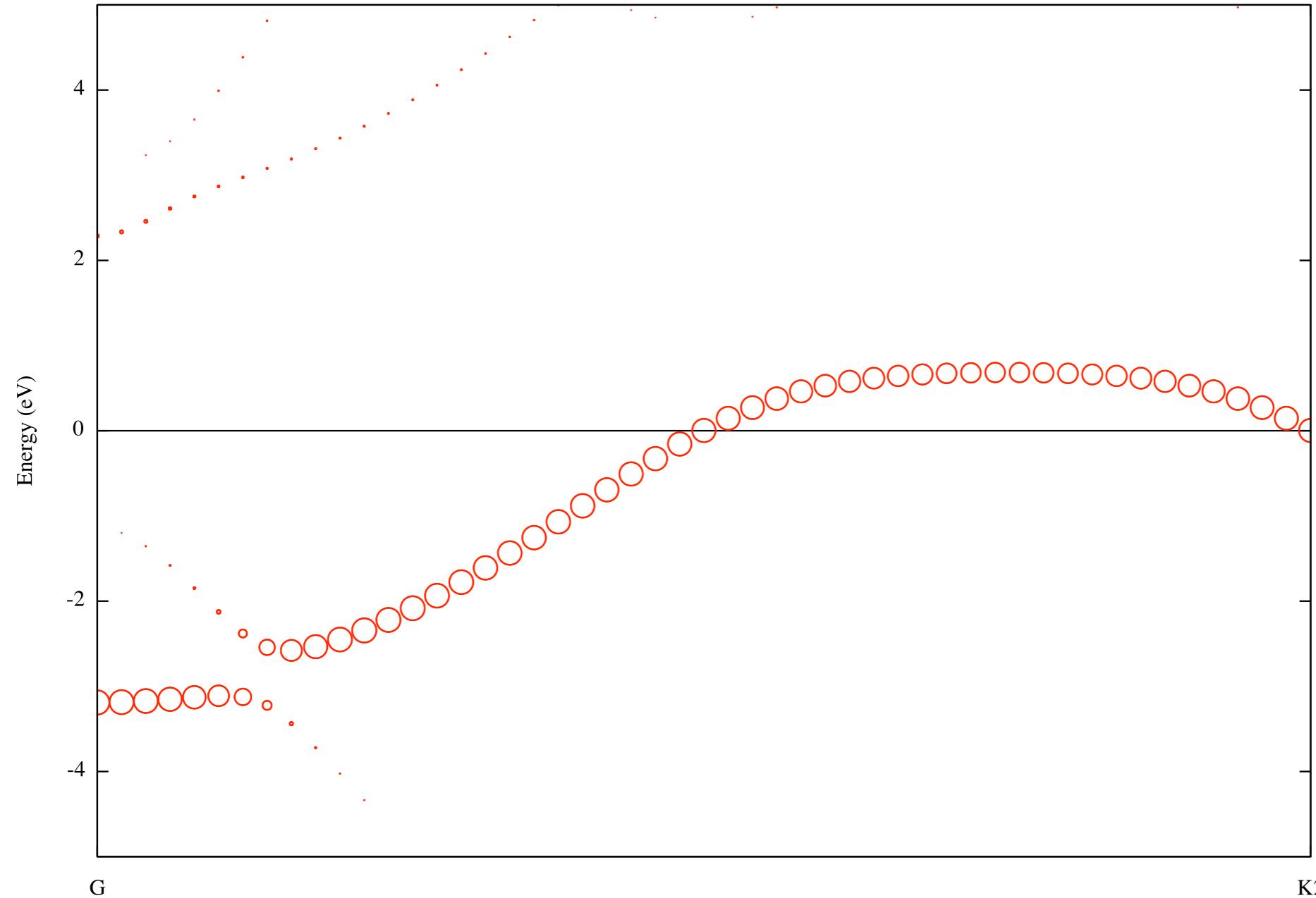
# Free-standing silicene

## Step 10: Or plot unfolded spectral weight of certain orbitals

gnuplot

gnuplot> load 'Silicene.unfold\_plotexample'

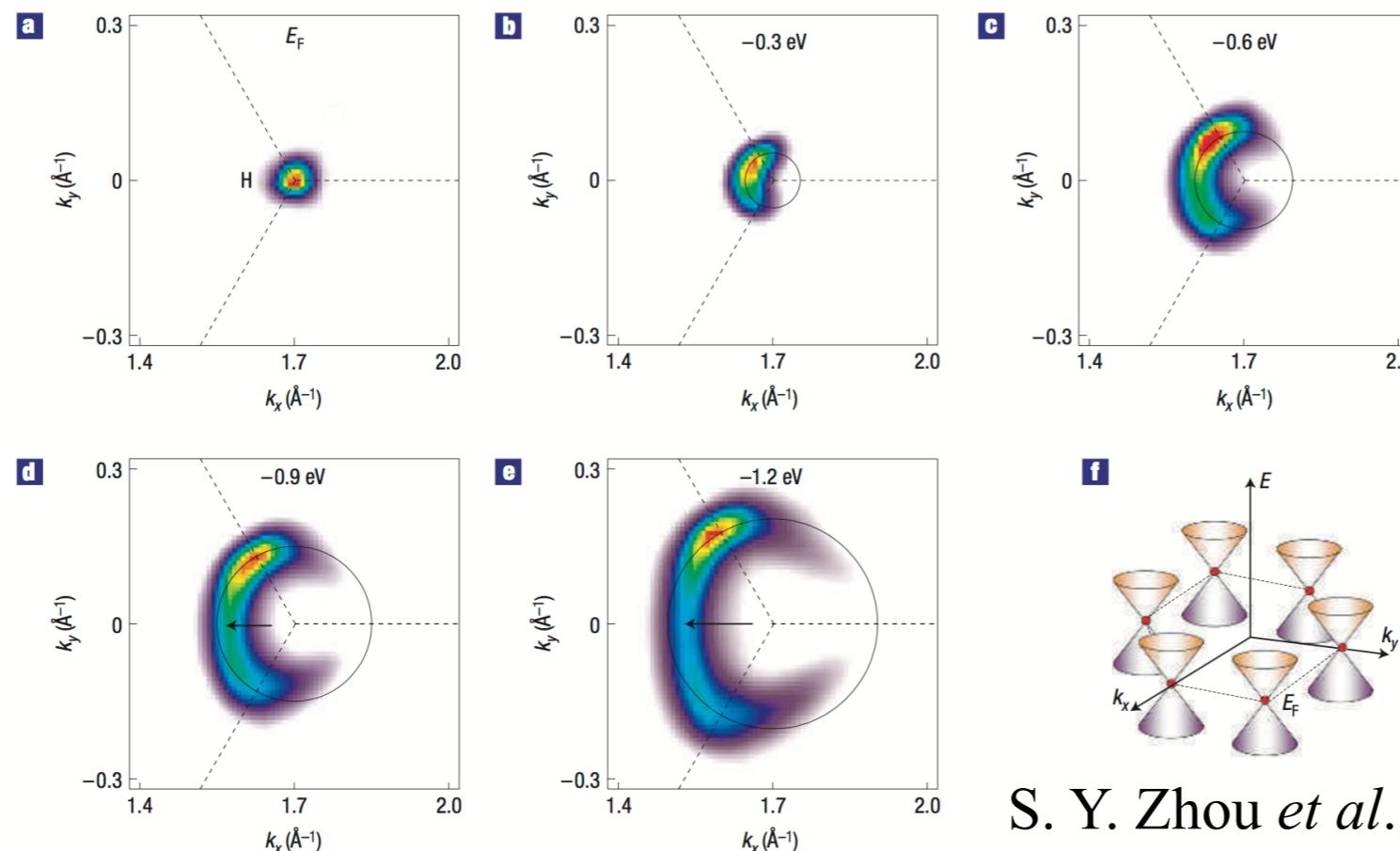
plot 'Silicene.unfold\_orbup' using 1:2:(\\$7+\\$10+\\$20+\\$23)\*0.02 notitle with circles lc rgb 'red'



# Free-standing silicene

## Step 11: Think about what is going on

- The translational symmetry breaking seen by the conceptual unit cell is two-fold. One is the periodic Si vacancies and the other is the dislocation due to the buckling. We can see the  $\text{Si}_\text{A}$ - $\text{Si}_\text{B}$  interference because we label them as the same atom. In the map, we define 1 and 1 (not 2).
- The missing spectral weight indicates an incomplete loop of Dirac cone at constant Energy.
- An example of incomplete loop of Dirac cone in graphene:



S. Y. Zhou *et al.*, Nature Physics 2, 595 (2006)

hands-on workshop

# Another case for running unfolding

# Free-standing silicene

## Step 1: Build a perfect supercell but unfold to primitive zone

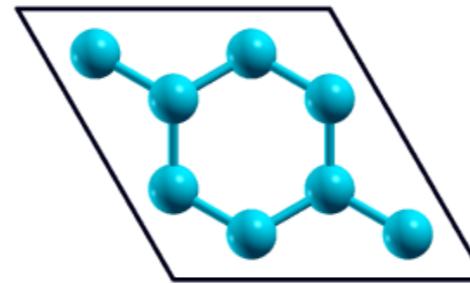
```
System.CurrentDirectory      ./  
System.Name                  Silicene  
DATA.PATH                    /provide_your_path/DFT_DATA13
```

```
Species.Number    1  
<Definition.of.Atomic.Species  
  Si  Si7.0-s2p2d1  Si_PBE13  
Definition.of.Atomic.Species>
```

```
Atoms.Number     8  
Atoms.SpeciesAndCoordinates.Unit   FRAC # Ang|AU  
<Atoms.SpeciesAndCoordinates  
  1  Si  0.166667  0.333333  0.4871  2. 2.  
  2  Si  0.333333  0.166667  0.5128  2. 2.  
  3  Si  0.666667  0.333333  0.4871  2. 2.  
  4  Si  0.833333  0.166667  0.5128  2. 2.  
  5  Si  0.166667  0.833333  0.4871  2. 2.  
  6  Si  0.333333  0.666667  0.5128  2. 2.  
  7  Si  0.666667  0.833333  0.4871  2. 2.  
  8  Si  0.833333  0.666667  0.5128  2. 2.  
Atoms.SpeciesAndCoordinates>
```

```
Atoms.UnitVectors.Unit  Ang  
<Atoms.UnitVectors  
  7.7155852 0 0  
  -3.8577926 6.6818927878 0  
  0 0 20  
Atoms.UnitVectors>
```

```
scf.XcType          GGA-PBE      # LDA|LSDA-CA|LSDA-PW|GGA-PBE  
scf.SpinPolarization Off         # On|Off  
scf.energycutoff   250.0       # default=150 (Ry)  
scf.maxIter        100          # default=40  
scf.EigenvalueSolver band         # Recursion|Cluster|Band  
scf.Kgrid           4 4 1       # means n1 x n2 x n3  
scf.Mixing.Type    rmm-diisk  # Simple|Rmm-Diis|Gr-Pulay  
scf.criterion      1.0e-8      # default=1.0e-6 (Hartree)
```



```
Unfolding.Electronic.Band      on  
Unfolding.LowerBound          -12.0  
Unfolding.UpperBound          8.0
```

```
Unfolding.Nkpoint              4  
Unfolding.desired_totalnkpt  50
```

```
<Unfolding.ReferenceVectors  
  3.8577926 0 0  
  -1.9288963 3.3409463939 0  
  0 0 20  
Unfolding.ReferenceVectors>
```

```
<Unfolding.kpoint  
  G 0 0 0  
  M 0.5 0 0  
  K 0.3333333 0.3333333 0  
  G 0 0 0  
Unfolding.kpoint>
```

```
<Unfolding.Map  
  1 1  
  2 2  
  3 1  
  4 2  
  5 1  
  6 2  
  7 1  
  8 2  
Unfolding.Map>
```

# Free-standing silicene

## Step 2: Plot unfolded band structure with SC bands

To do that, we need to turn on band dispersion

```
Band.dispersion          on
<Band.KPath.UnitCell
 3.8577926 0 0
 -1.9288963 3.3409463939 0
 0 0 20
 Band.KPath.UnitCell>
Band.Nkpath              3
<Band.kpath
17 0 0 0 0.5 0 0 G M
10 0.5 0 0 0.333333 0.333333 0 M K
20 0.333333 0.333333 0 0 0 0 K G
Band.kpath>
```

We also need to compile

```
gcc bandgnu13.c -lm -o bandgnu13
```

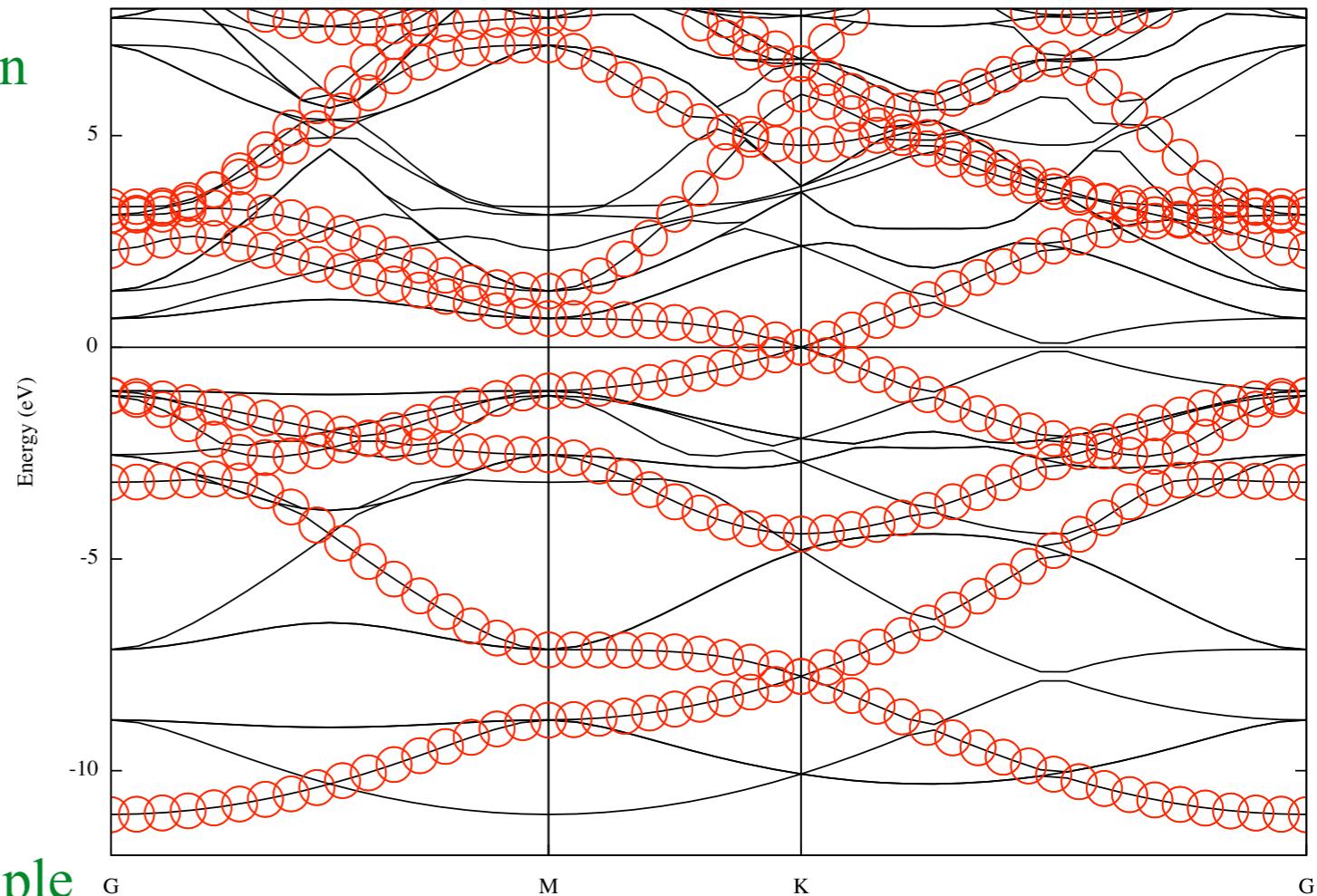
and perform (to get Silicene.BANDDAT1)

```
./bandgnu13 Silicene.Band
```

We can modify the Silicene.unfold\_plotexample

```
set xrange [-12.00000:8.00000]
set ylabel 'Energy (eV)'
set xtics('G' 0.00000,'M' 0.497601,'K' 0.784892,'G' 1.359472)
set xrange [0:1.359472]
set arrow nohead from 0,0 to 1.359472,0
set arrow nohead from 0.497601,-12.00000 to 0.497601,8.000000
set arrow nohead from 0.784892,-12.00000 to 0.784892,8.000000
set style circle radius 0
set style data lines
p "Silicene.BANDDAT1" notitle lc rgb 'black',"Silicene.unfold_totup" u 1:2:(\$3)*0.02 notitle w circles lc rgb 'red'
We have 1 and 0 in the weight
0.000000 -11.038611 1.0000000
0.000000 -8.808899 0.0000000
0.000000 -8.804652 0.0000000
0.000000 -8.804652 0.0000000
...
(Silicene.unfold_totup)
```

We can run gnuplot and load 'Silicene.unfold\_plotexample'



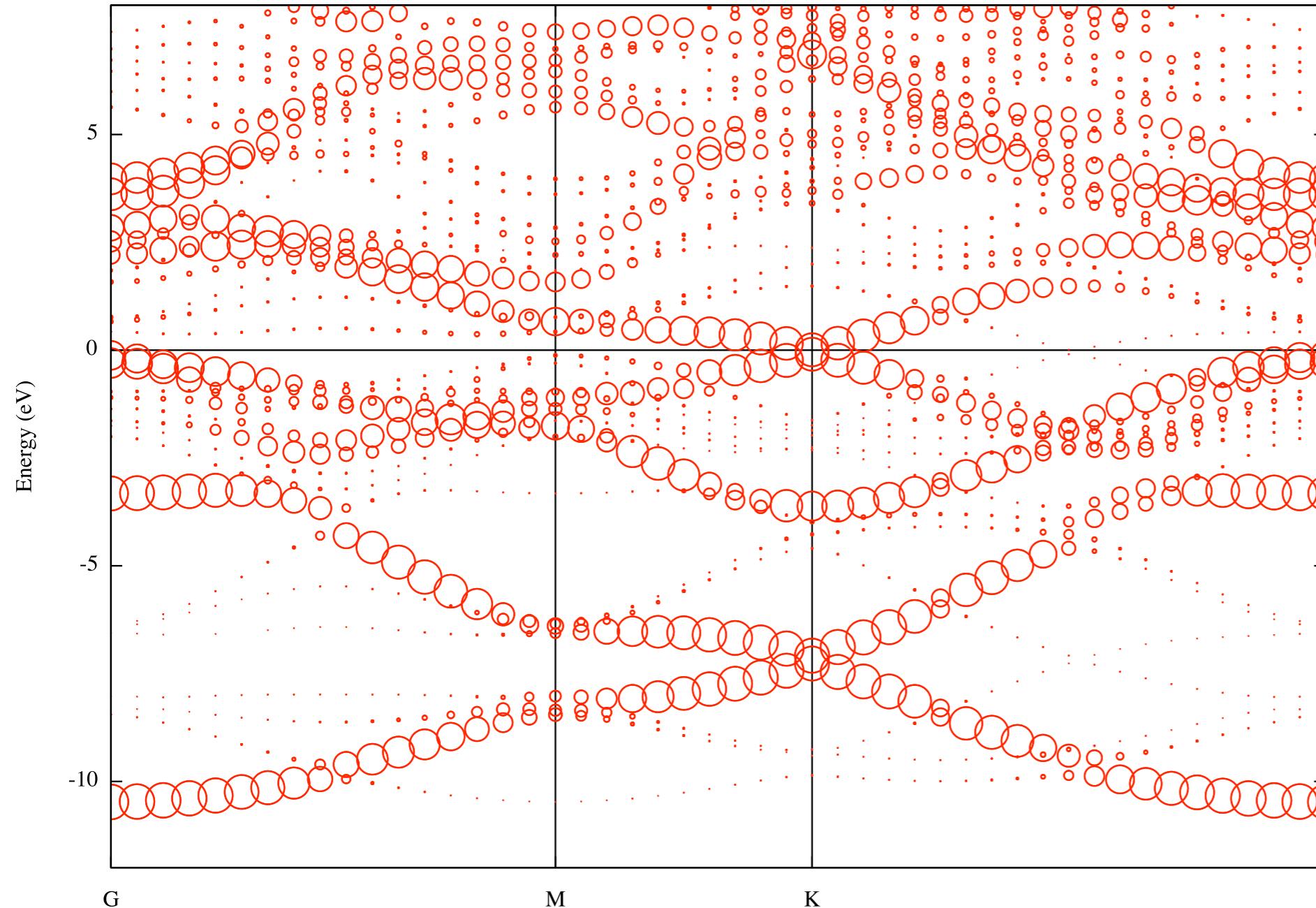
# Free-standing silicene

## Step 3: Perturb the atomic positions

```
System.CurrentDirectory          ./  
System.Name                      Silicene  
DATA.PATH                         /provide_your_path/DFT_DATA13  
  
Species.Number                   1  
<Definition.of.Atomic.Species  
  Si  Si7.0-s2p2d1  Si_PBE13  
>  
Atoms.Number                     8  
Atoms.SpeciesAndCoordinates.Unit FRAC # Ang|AU  
<Atoms.SpeciesAndCoordinates  
  1  Si  0.186667  0.353333  0.4971  2. 2.  
  2  Si  0.313333  0.146667  0.5228  2. 2.  
  3  Si  0.656667  0.313333  0.4871  2. 2.  
  4  Si  0.823333  0.156667  0.5128  2. 2.  
  5  Si  0.156667  0.853333  0.4771  2. 2.  
  6  Si  0.343333  0.686667  0.5328  2. 2.  
  7  Si  0.656667  0.813333  0.4671  2. 2.  
  8  Si  0.843333  0.686667  0.5128  2. 2.  
>  
Atoms.SpeciesAndCoordinates>  
  
Atoms.UnitVectors.Unit   Ang  
<Atoms.UnitVectors  
  7.7155852 0 0  
 -3.8577926 6.6818927878 0  
  0 0 20  
>  
Atoms.UnitVectors>  
  
scf.XcType                  GGA-PBE      # LDA|LSDA-CA|LSDA-PW|GGA-PBE  
scf.SpinPolarization        Off         # On|Off  
scf.energycutoff            250.0       # default=150 (Ry)  
scf.maxIter                 100         # default=40  
scf.EigenvalueSolver        band        # Recursion|Cluster|Band  
scf.Kgrid                   4 4 1       # means n1 x n2 x n3  
scf.Mixing.Type              rmm-diisk  # Simple|Rmm-Diis|Gr-Pulay  
scf.criterion               1.0e-8     # default=1.0e-6 (Hartree)
```

# Free-standing silicene

## Step 4: Plot the unfolded band structure



We have 0 ~ 1 in the weight

```
0.000000 -10.475841  0.9734492  
0.000000 -8.449300  0.0185308  
0.000000 -8.348240  0.0048797  
0.000000 -8.022265  0.0074129  
...
```

(Silicene.unfold\_totup)

# Free-standing silicene

## Step 5: How about change one Si atom to C atom as an impurity

```

System.CurrentDirectory      ./
System.Name                  Silicene
DATA.PATH                    /provide_your_path/DFT_DATA13
Unfolding.Electronic.Band   on
Unfolding.LowerBound        -12.0
Unfolding.UpperBound         8.0

Species.Number               2
<Definition.of.Atomic.Species
  Si  Si7.0-s2p2d1  Si_PBE13
  C   C7.0-s2p2d1  C_PBE13
Definition.of.Atomic.Species>

Atoms.Number                 8
Atoms.SpeciesAndCoordinates.Unit  FRAC # Ang|AU
<Atoms.SpeciesAndCoordinates
  1  Si  0.166667  0.333333  0.4871  2. 2.
  2  Si  0.333333  0.166667  0.5128  2. 2.
  3  C   0.666667  0.333333  0.4871  2. 2.
  4  Si  0.833333  0.166667  0.5128  2. 2.
  5  Si  0.166667  0.833333  0.4871  2. 2.
  6  Si  0.333333  0.666667  0.5128  2. 2.
  7  Si  0.666667  0.833333  0.4871  2. 2.
  8  Si  0.833333  0.666667  0.5128  2. 2.
<Atoms.SpeciesAndCoordinates>
Atoms.SpeciesAndCoordinates>

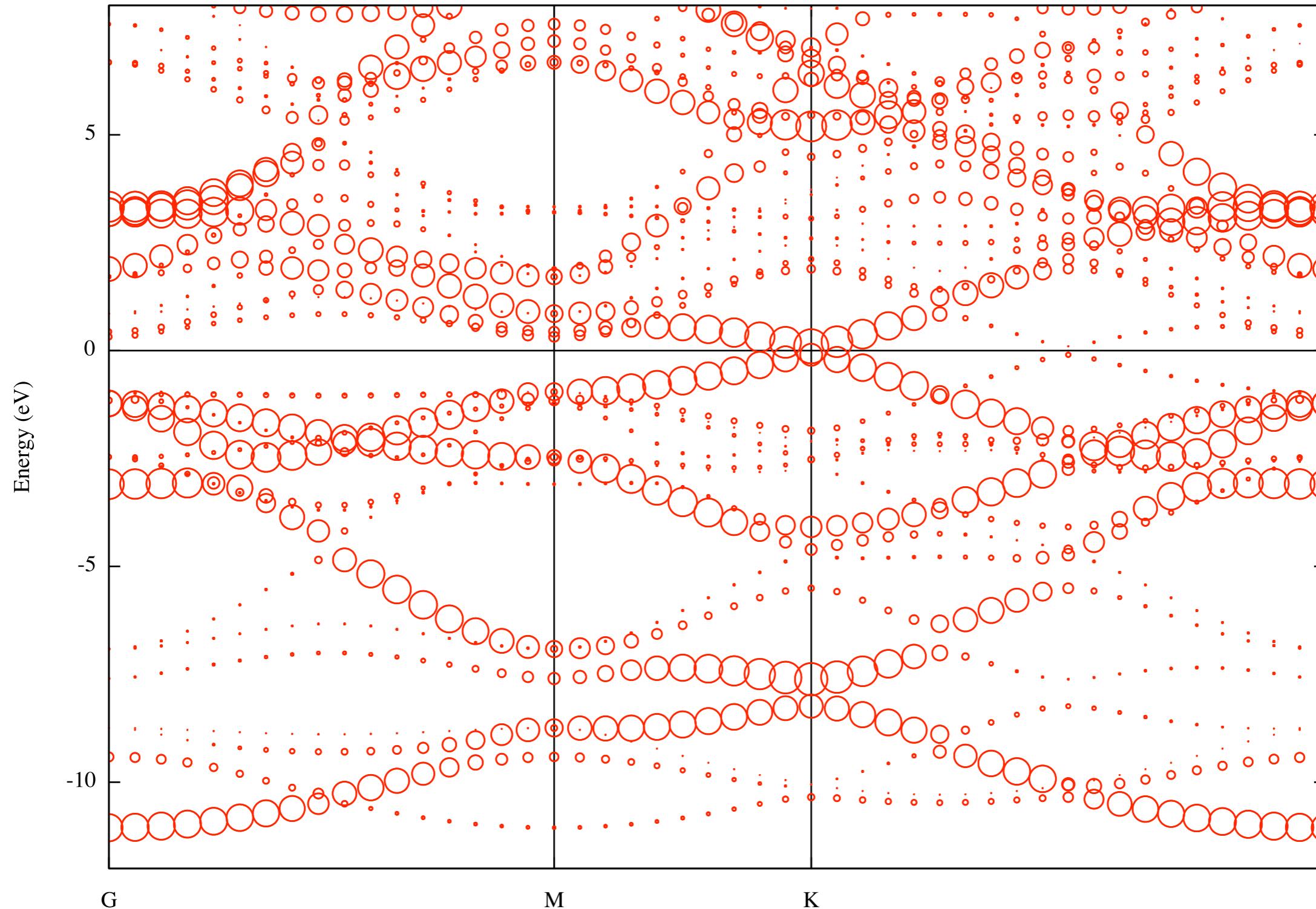
Atoms.UnitVectors.Unit     Ang
<Atoms.UnitVectors
  7.7155852 0 0
  -3.8577926 6.6818927878 0
  0 0 20
Atoms.UnitVectors>

scf.XcType                  GGA-PBE      # LDA|LSDA-CA|LSDA-PW|GGA-PBE
scf.SpinPolarization        Off          # On|Off
scf.energycutoff            250.0       # default=150 (Ry)
scf.maxIter                 100          # default=40
scf.EigenvalueSolver        band         # Recursion|Cluster|Band
scf.Kgrid                   4 4 1       # means n1 x n2 x n3
scf.Mixing.Type              rmm-diisk  # Simple|Rmm-Diis|Gr-Pulay
scf.criterion               1.0e-8     # default=1.0e-6 (Hartree)
Unfolding.Map>
  1 1
  2 2
  3 3
  4 2
  5 1
  6 2
  7 1
  8 2
Unfolding.Map>

```

# Free-standing silicene

## Step 6: Plot the unfolded band structure



# Reference

- The theory part can be found in  
Chi-Cheng Lee *et al.*, J. Phys.: Condens. Matter **25**, 345501 (2013).
- All other details can be found in  
[http://www.openmx-square.org/openmx\\_man3.8/openmx.html](http://www.openmx-square.org/openmx_man3.8/openmx.html)
  - Unfolding method for band structures
    - Analysis of band structures
    - Unfolding of band structures
    - The origin of the reference unit cell
    - Intensity map of unfolded spectral weight
    - In case of non-collinear DFT calculations
    - Examples

For example, you can also define the origin of the conceptual unit cell by yourself via “<Unfolding.ReferenceOrigin”.