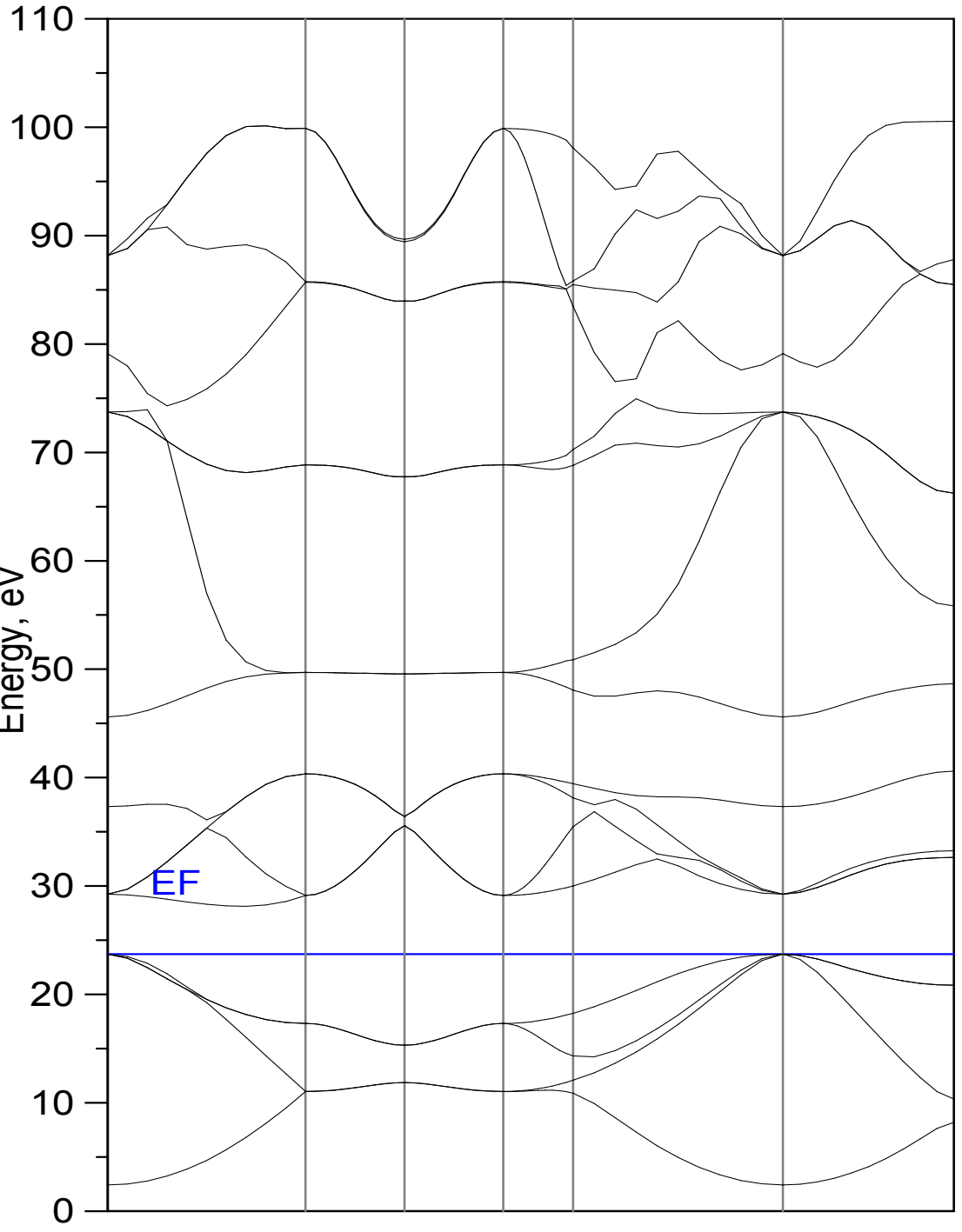
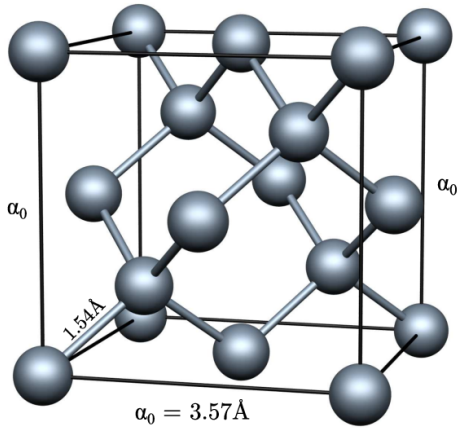
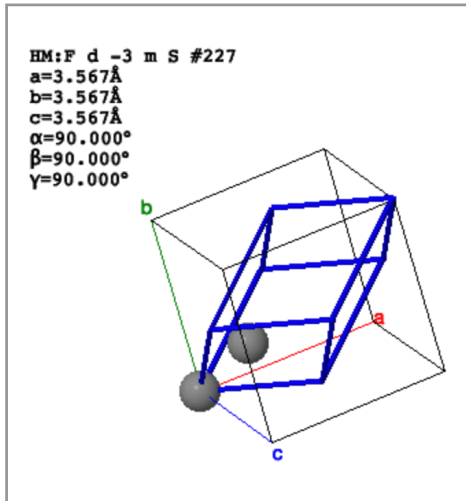


Diamond



Conventional unit cell



Primitive unit cell

2 atoms per unit cell
Electronic configuration $2s^2 2p^2$
1+3=4 bands per atom -> 8 bands
2x4=8 electrons per unit cell -> fill 4 bands (spin: /2)

8 bands
Fill 4

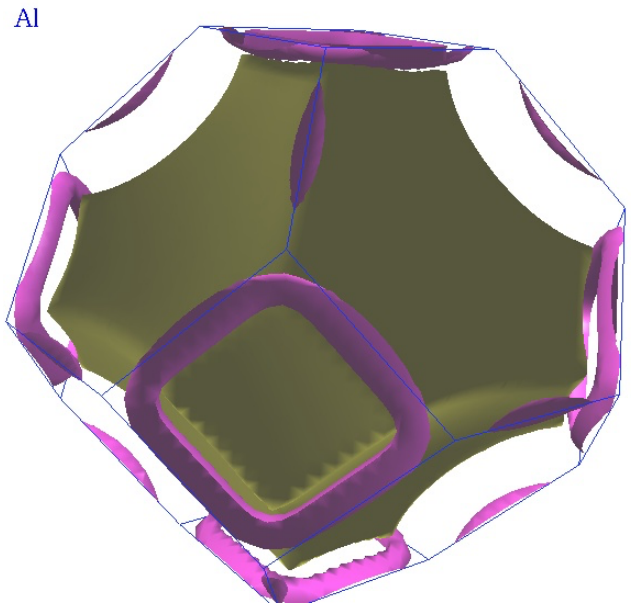
The conventional unit cell has redundant information and the extra bands that you calculate using that end up being degenerate with others because of symmetry considerations

In counting the orbitals, you have to count every state the electrons can fill, i.e. for the 2p level, 3 possible states.

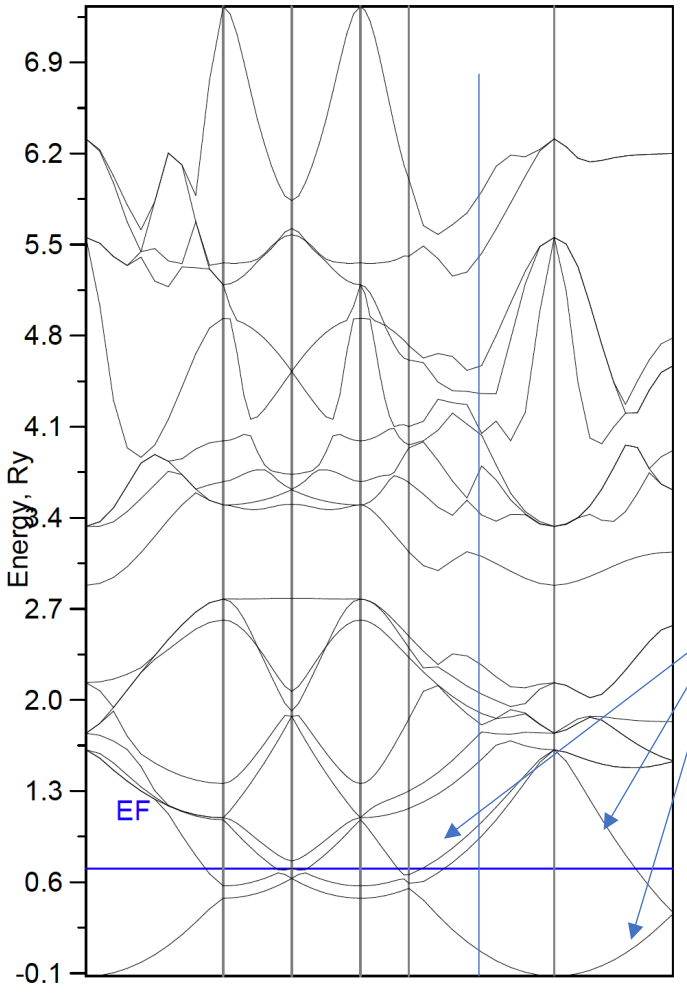
Other few examples:

Aluminum $3s^2\ 3p^6\ 3d^{10}$ x 1 atom total = 1+3+5 = 9 bands

Fermi surface



https://www.phys.ufl.edu/fermisurface/

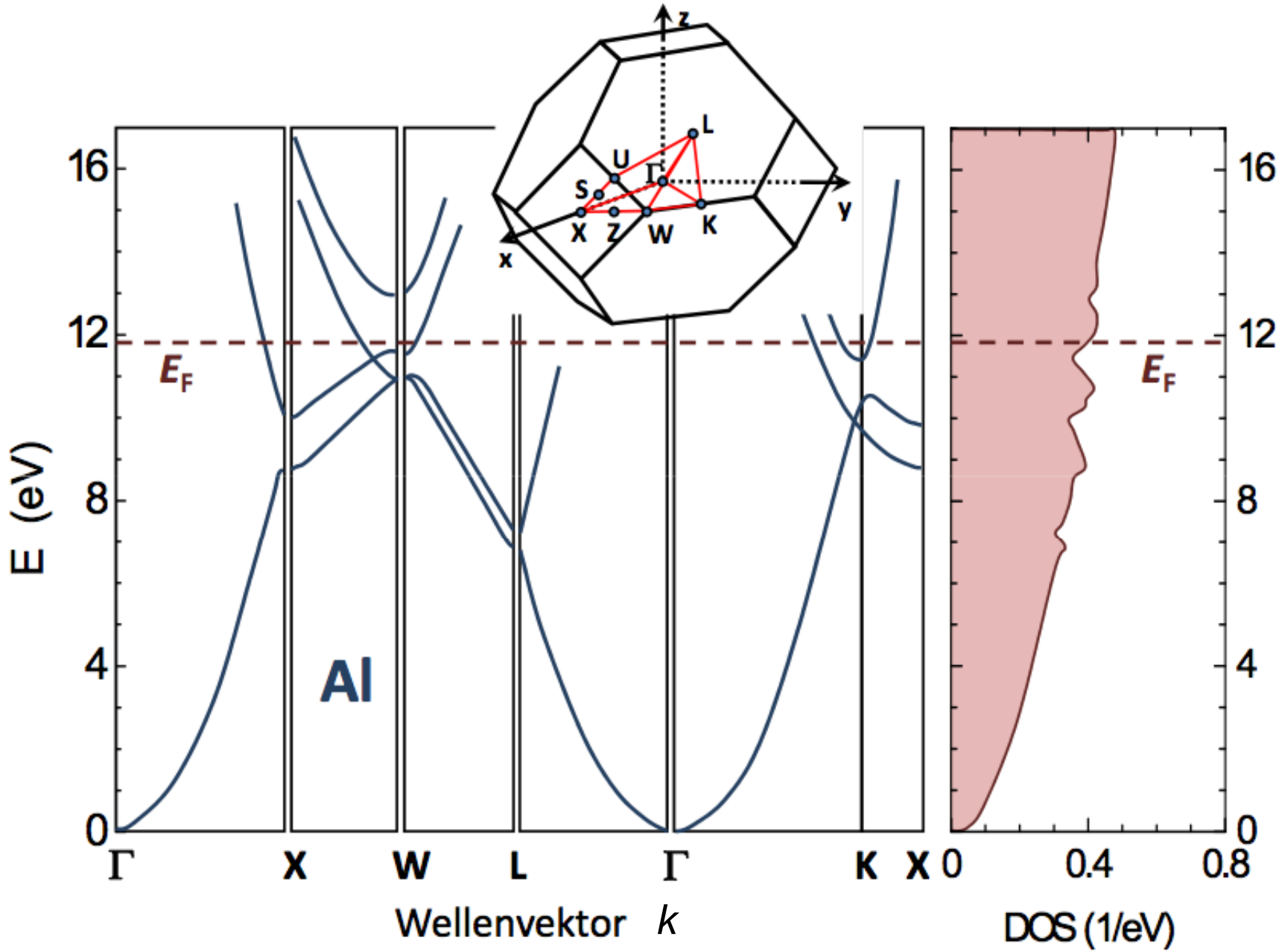


Notice how in Al you have $3s^2\ 3p^1$ electrons = 3 total
1 atom per primitive cell

You can fill 1.5 bands

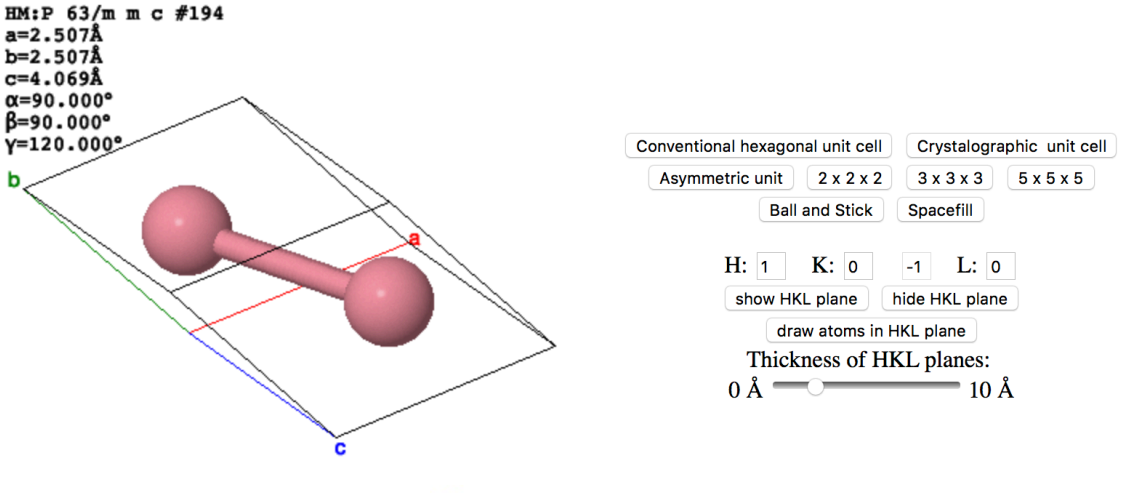
One is completely full, two are partially filled

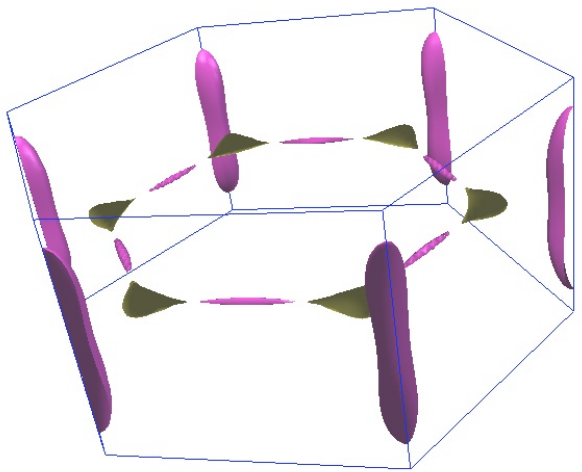
9 bands fill 1.5


z
y
x
L
U
Γ
S
X
Z
W
K
16
12
8
4
0
E (eV)
E_F
Al
Γ
X
W
L
Γ
K
X
Wellenvektor k
0
0.4
0.8
DOS (1/eV)

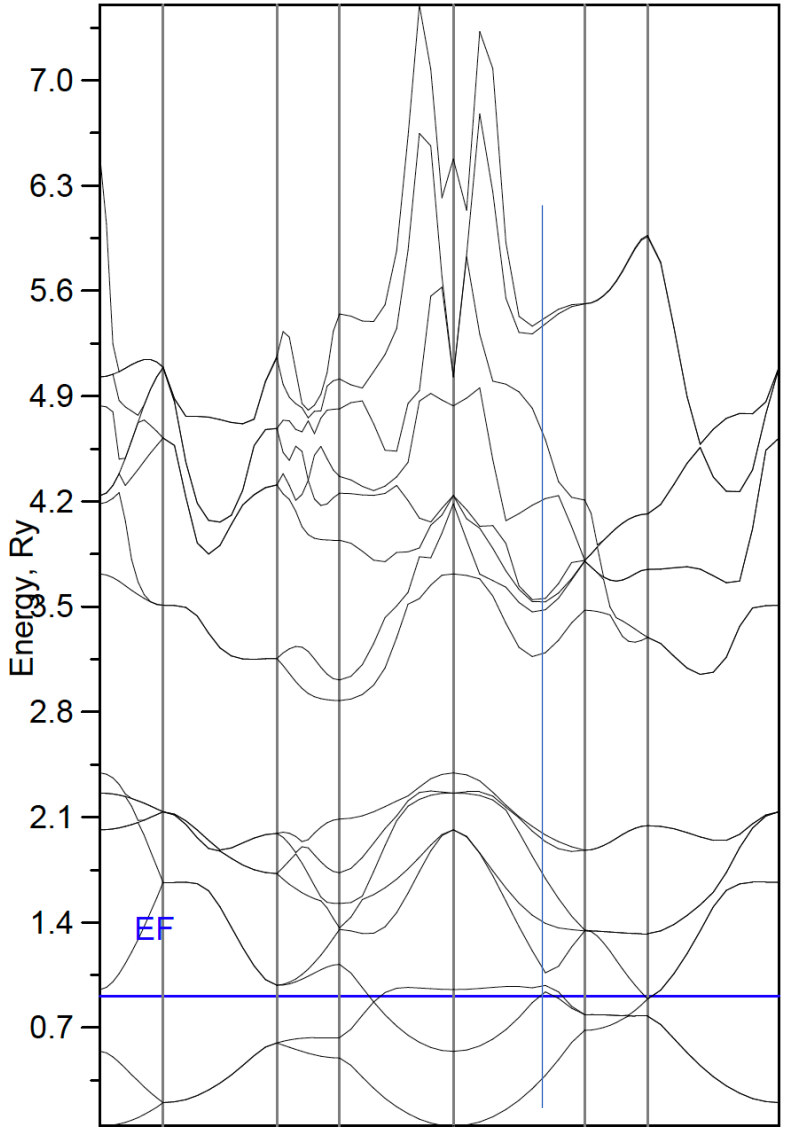
Beryllium

electronic configuration $2s^2$ primitive cell: 2 atoms. Total states: 1 (s orbitals) + 3(p orbitals) = 4 *2 = 8



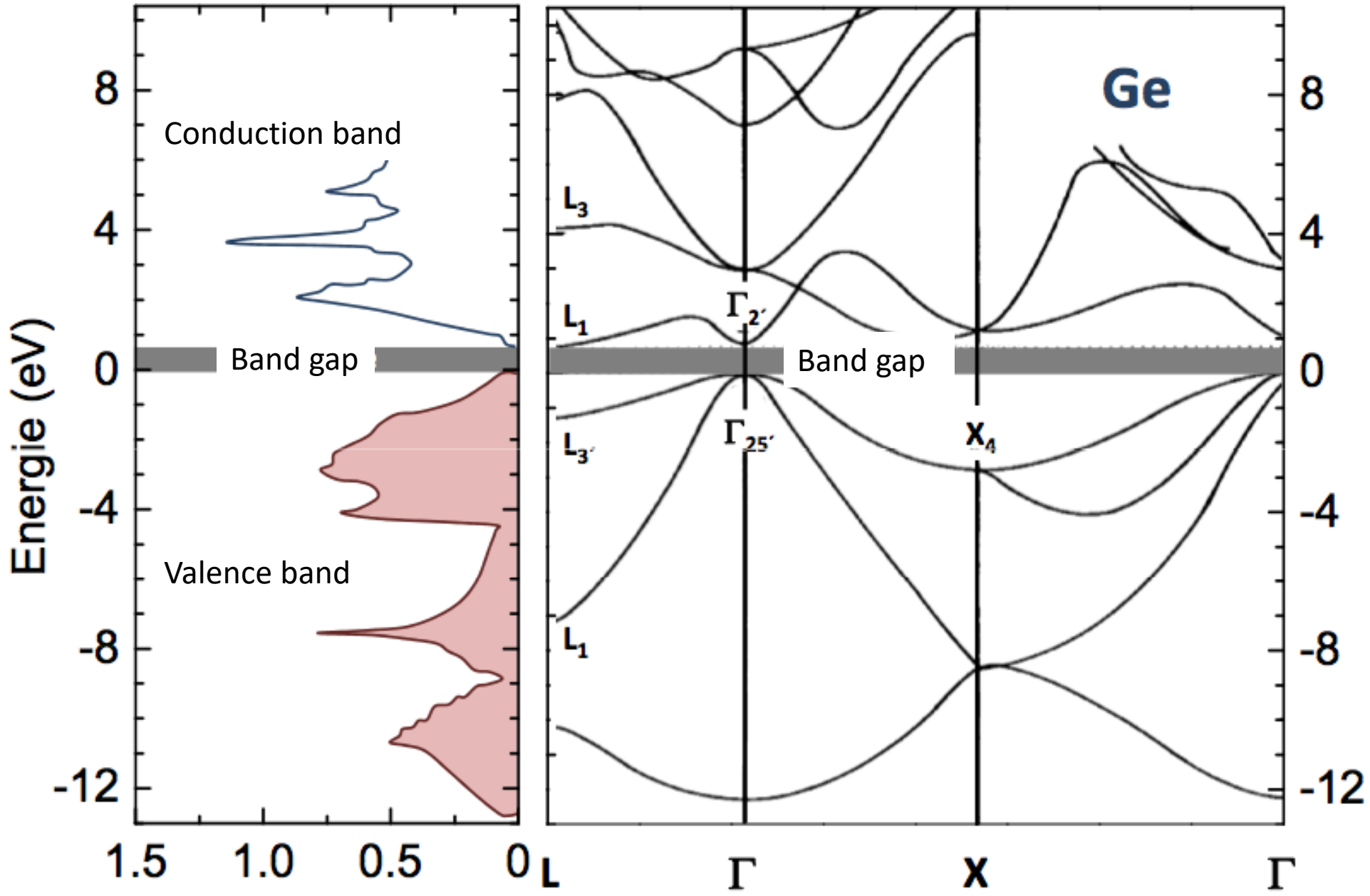


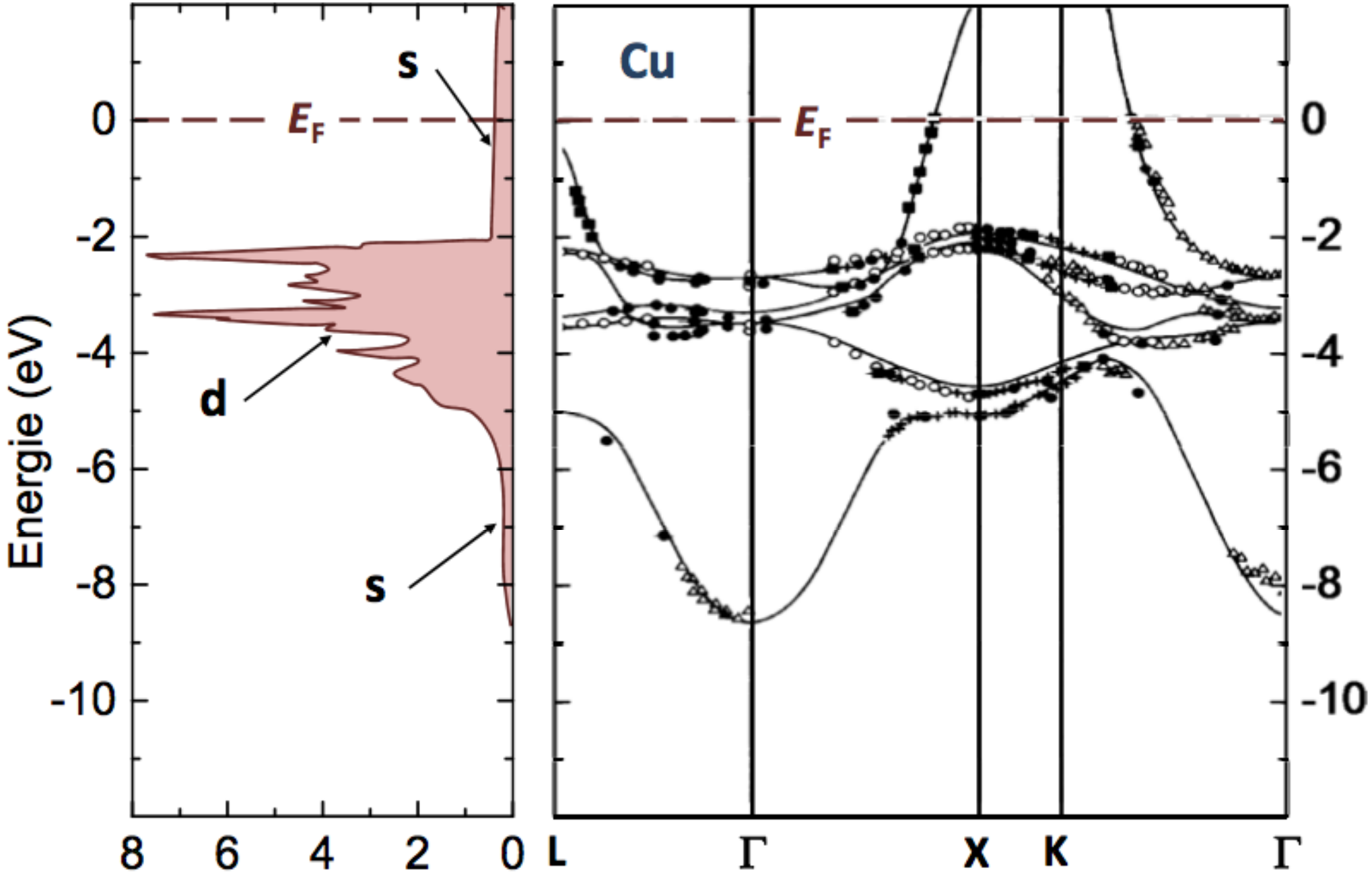
Fermi surface

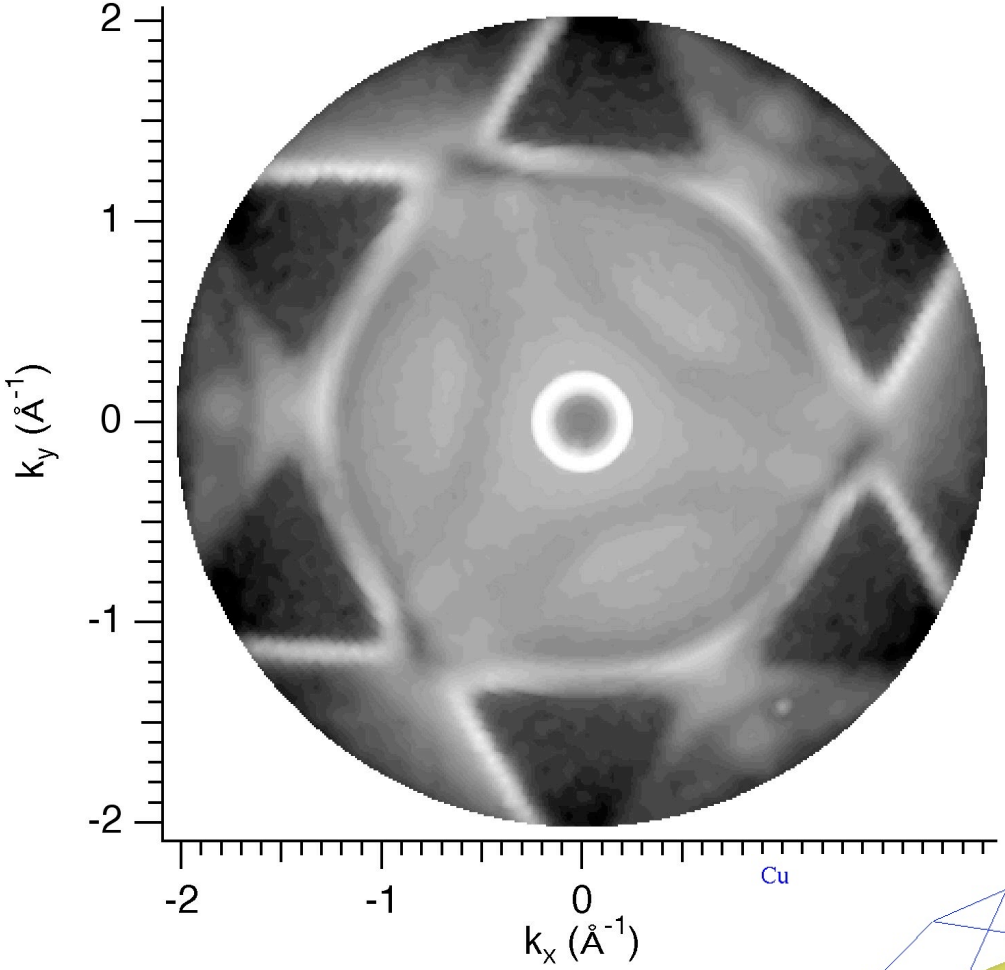


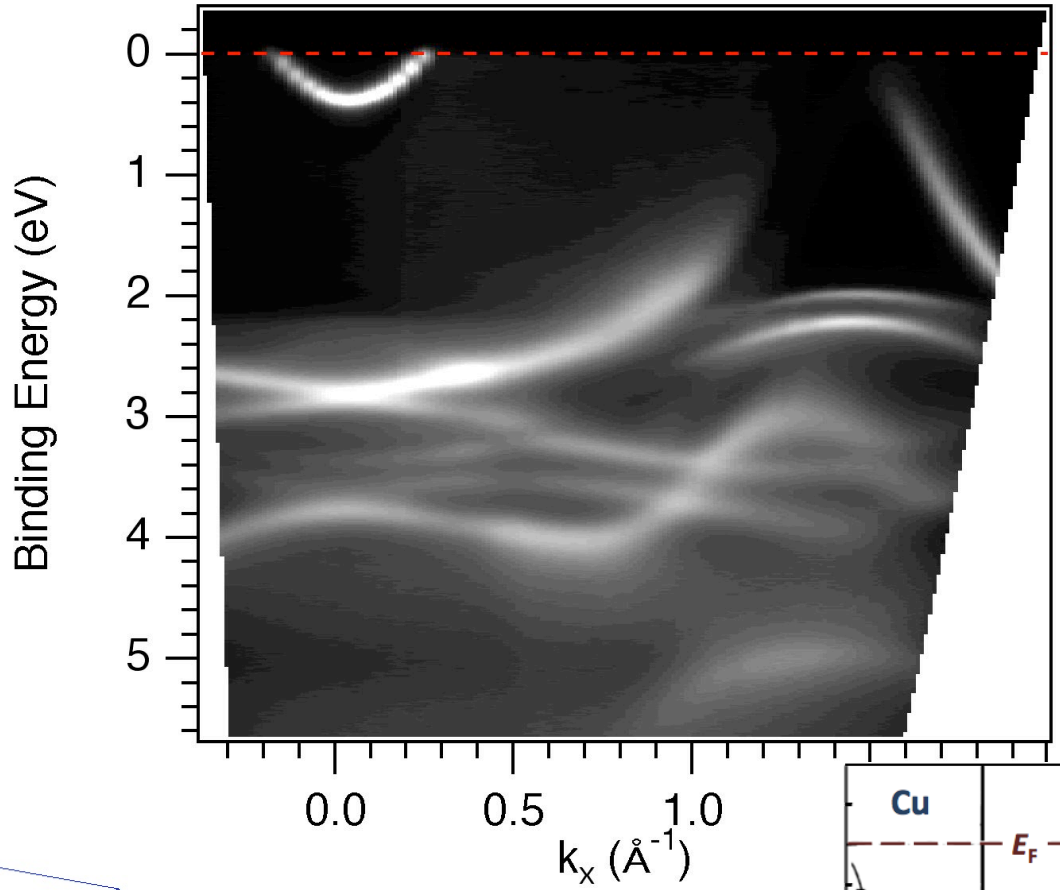
Adding 3s and 3 p another 8 bands

8 bands, fill 2

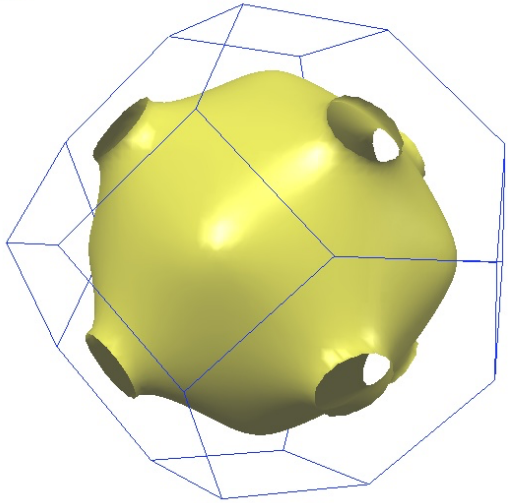

Ge
Conduction band
Valence band
Band gap
Band gap
Energie (eV)
8
4
0
-4
-8
-12
1.5
1.0
0.5
0
L
Γ
X
Γ
L3
L1
L3'
L1
Γ2'
Γ25'
X4

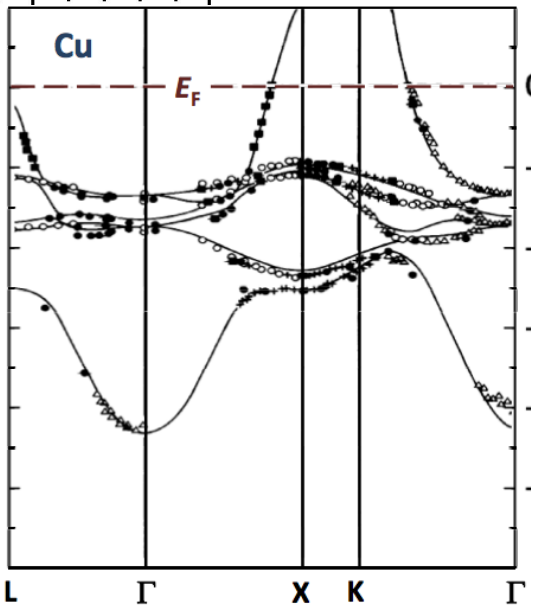

Cu
E_F
s
d
s
Energie (eV)
0
-2
-4
-6
-8
-10
8
6
4
2
0
L
Γ
X
K
Γ

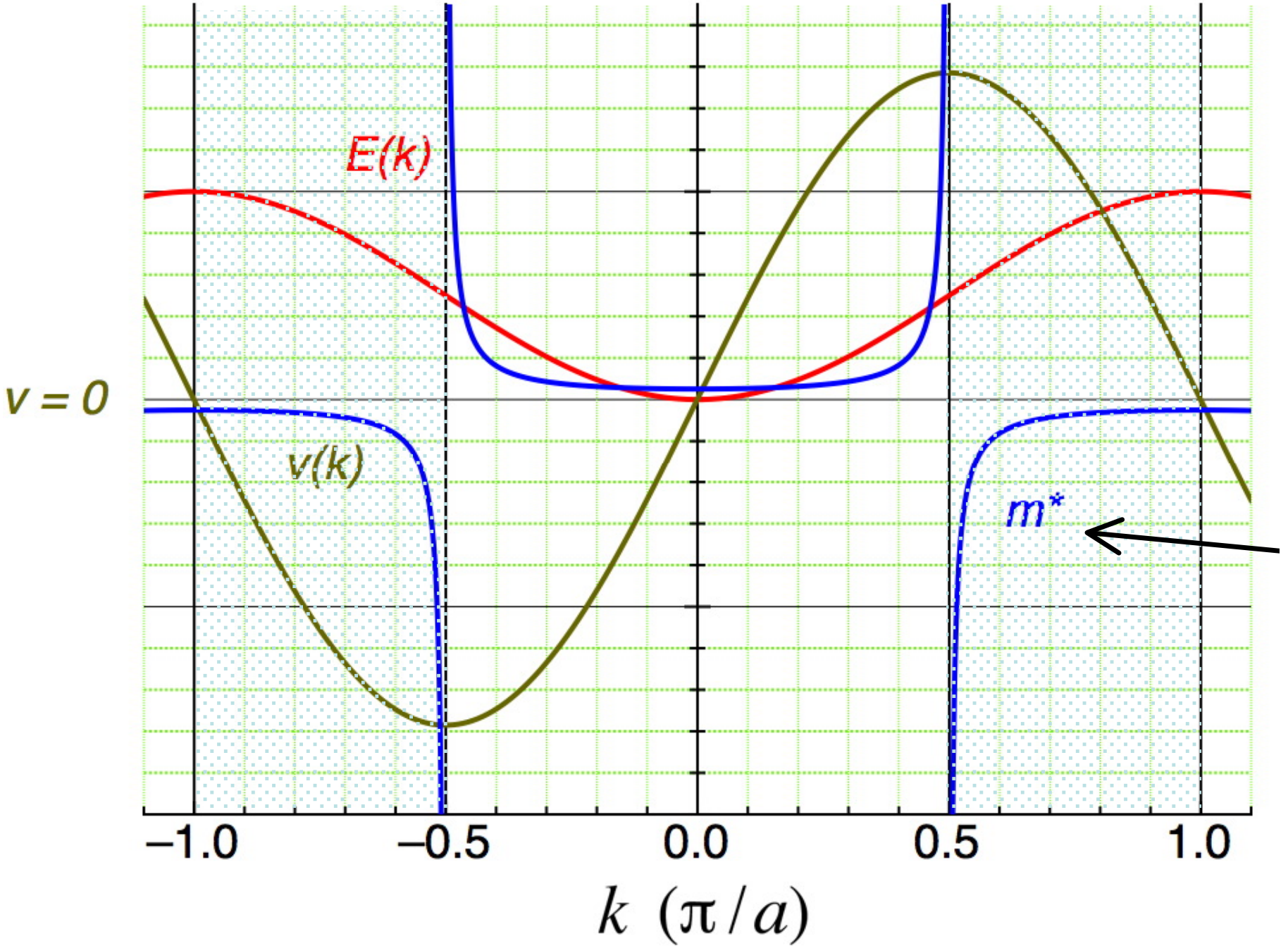




Angle-resolved photoemission spectroscopy (ARPES)






E(k)
v(k)
m*
v = 0
–1.0
–0.5
0.0
0.5
1.0
k (π/a)