



Computational Solid State Physics, part II

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Lab3: Electronic Structure Calculations

1. Electronic Structure: **General Concepts and definitions:**
2. Electronic Structure: **Effect of crystal symmetry (Group Theory).**
3. Electronic Structure Band Structure: **First Example, FCC Neon.**
4. 3d Band Structure: **Density of States and k-space integration methods**
5. Electronic Structure For **Metals: Fermi Surface.**
6. Exercises & **Home Assignments**



1. Electronic Structure: *General Concepts*

Bloch's Theorem

Bloch's theorem states that any excitation in a solid can be written as:

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$$

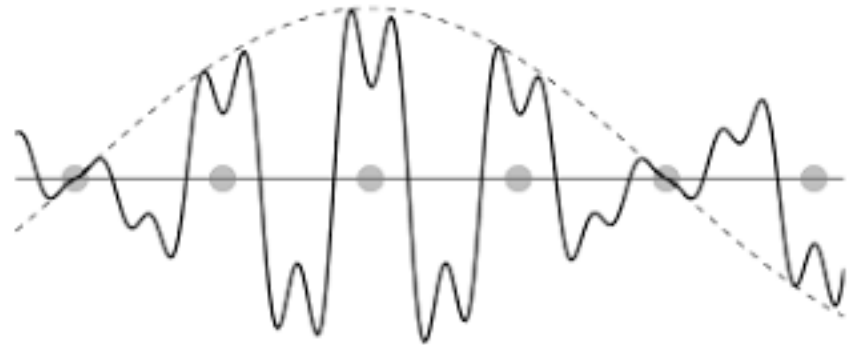
Where $u_{\mathbf{k}}(\mathbf{r})$ is a periodic function with the same periodicity as the crystal lattice:

$$u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})$$

And $e^{i\mathbf{k}\cdot\mathbf{r}}$ is a plane wave that modulates the periodic function.

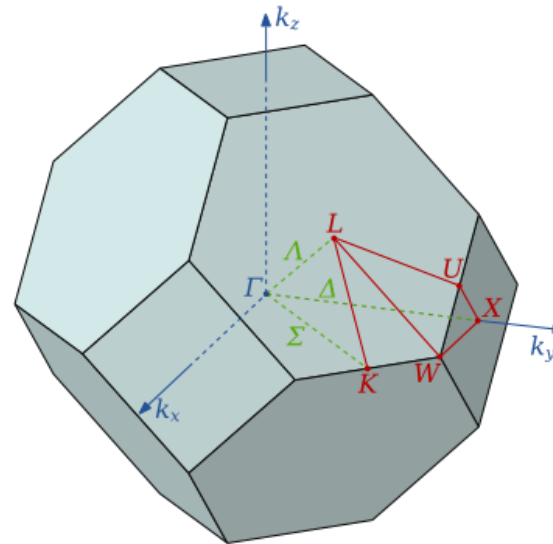
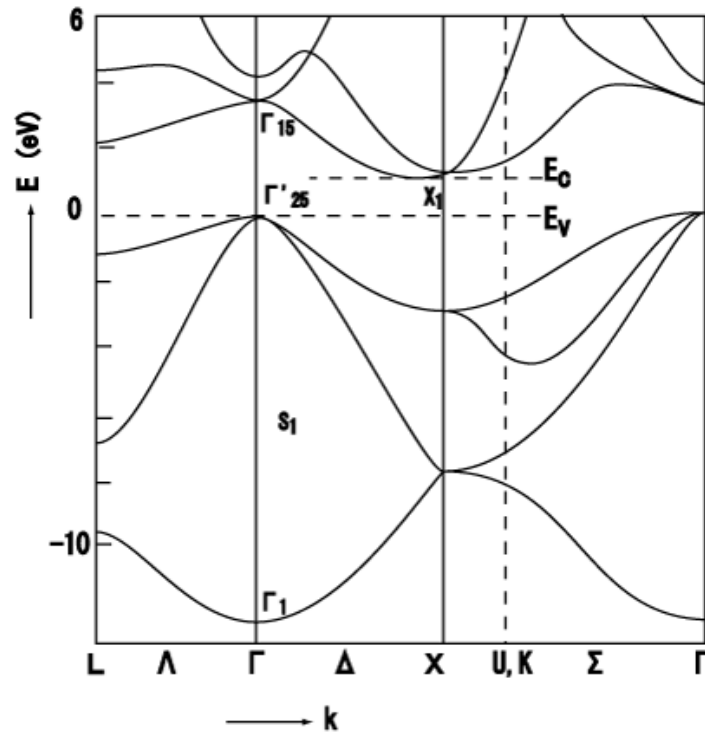
This also implies:

$$\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \psi_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{R}}$$



Band Structure:

A fundamental consequence of Bloch's theorem is that electronic energy levels in solids form **energy bands**; allowed energy levels can be separated by **gaps** of forbidden energies.



The number of \mathbf{k} points is equal to the number of unit cells in a crystal (practically infinite), hence bands are quasi-continuous variables.

The energy spectrum of a solid is a function of a 3-d variable $\mathbf{k}=(k_x, k_y, k_z)$; in order to **visualize** it one usually plots **band structure along high-symmetry lines** in \mathbf{k} space.

Density of States (DOS):

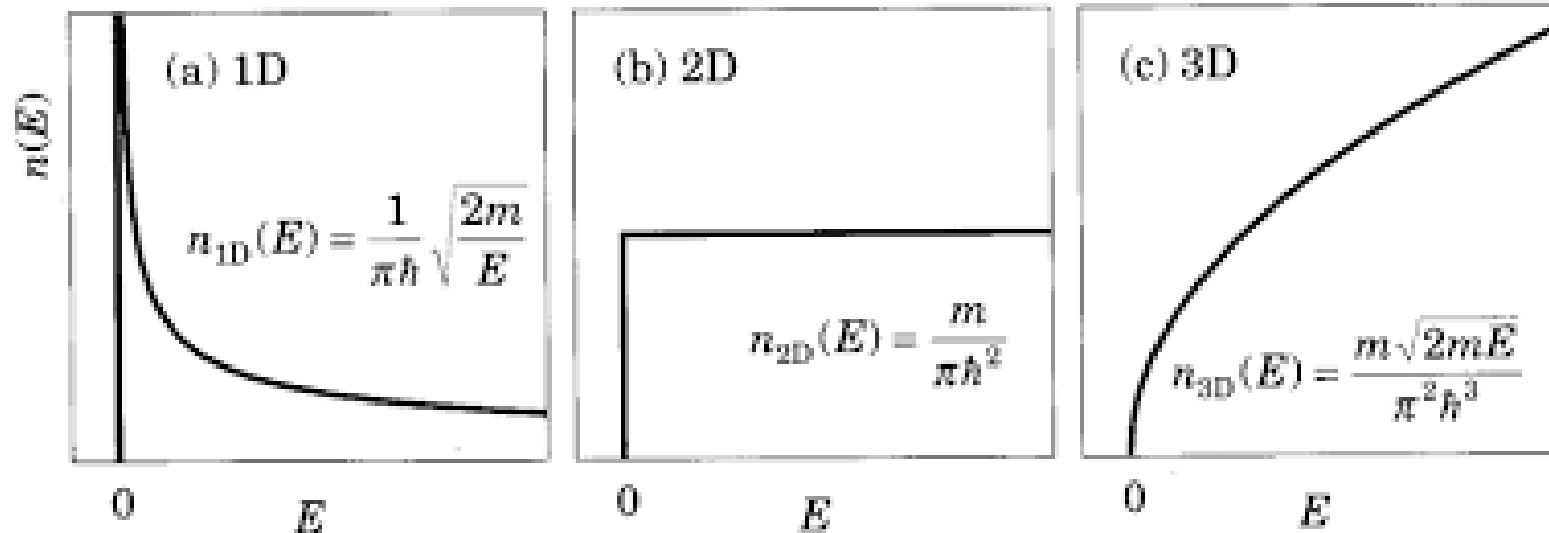
K-integrated quantities like the Density of States (DOS) give a more precise description.

$$D(\varepsilon) = \sum_{n,\mathbf{k}} \delta(\varepsilon - \varepsilon_{n,\mathbf{k}})$$

► **Free Electrons:**

$$\varepsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}$$

$$D(\varepsilon) \propto \varepsilon^{\frac{d-2}{2}}$$



Number of States (NOS):

The integral of the DOS gives the number of occupied states up to a certain energy:

$$N(\varepsilon) = \int_{-\infty}^{\varepsilon} D(\varepsilon') d\varepsilon'$$

This permits to define a **Fermi energy**, which separates occupied and unoccupied states.

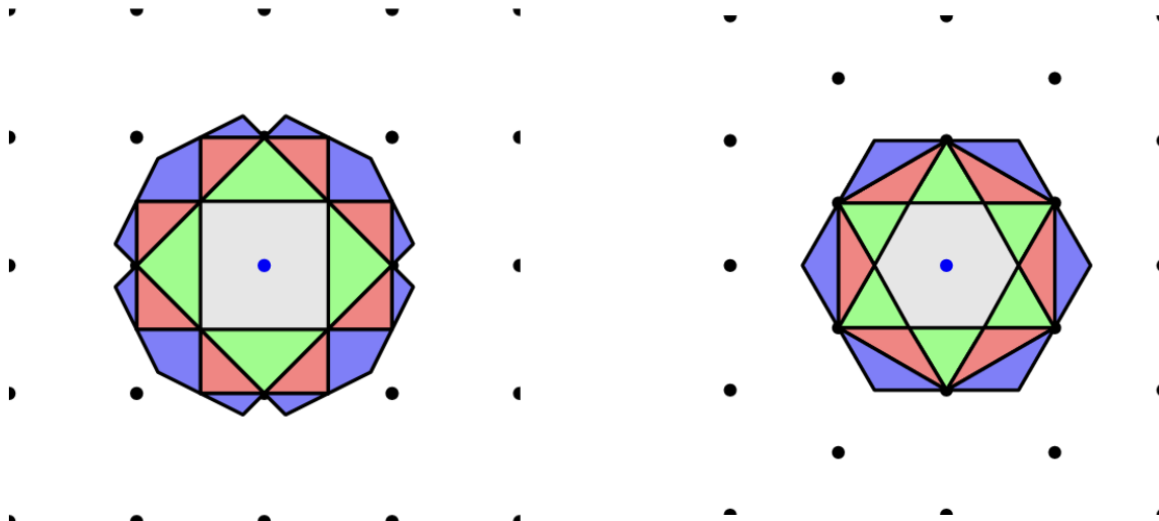
$$N_{el} = \int_{-\infty}^{E_F} D(\varepsilon) d\varepsilon$$

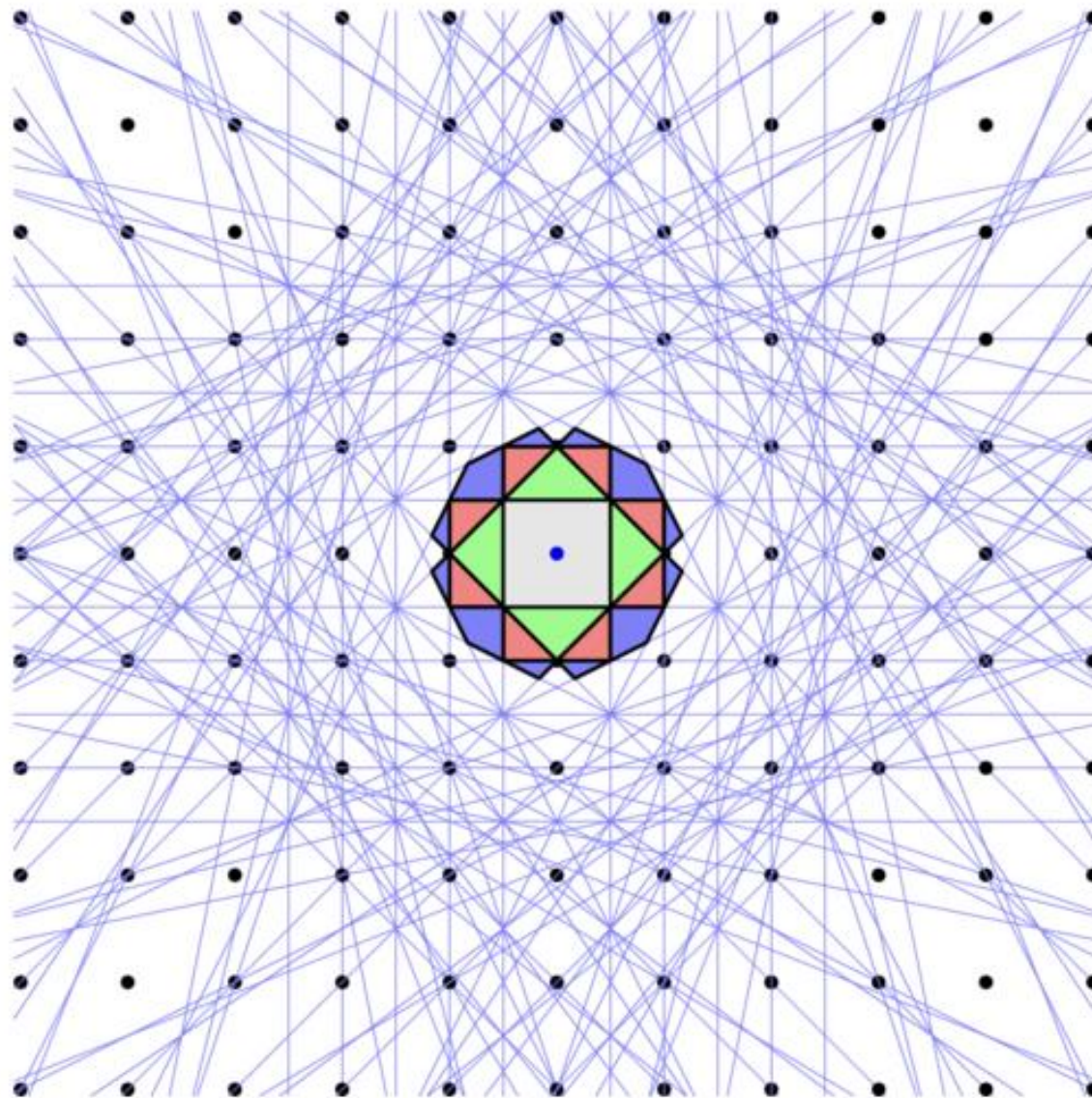
Brillouin Zone:

The **Brillouin zone** is the **Wigner-Seitz cell** of the **reciprocal lattice**.

$$\begin{aligned} \mathbf{G}_1 &= \frac{2\pi}{V} (\mathbf{R}_2 \times \mathbf{R}_3) \\ \mathbf{G}_2 &= \frac{2\pi}{V} (\mathbf{R}_3 \times \mathbf{R}_1) \\ \mathbf{G}_3 &= \frac{2\pi}{V} (\mathbf{R}_1 \times \mathbf{R}_2) \end{aligned}$$

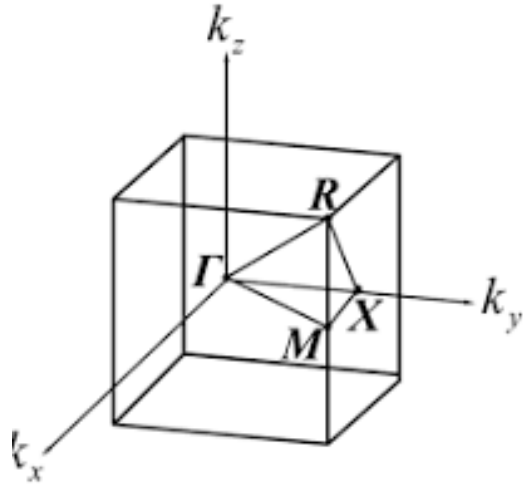
Wigner Seitz cell: Region of space closest to a given lattice point. It can be constructed finding the **perpendicular bisectors** to the lines connecting the point to other lattice points.



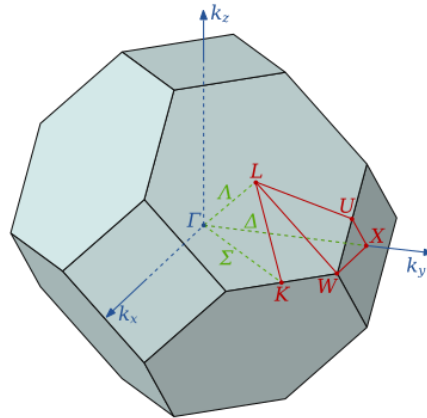


<https://eelvex.net/post/brillouin-zones-guide/>

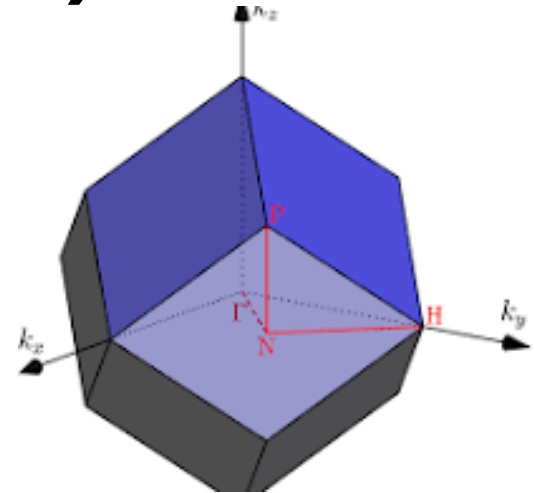
Brillouin Zone (3d):



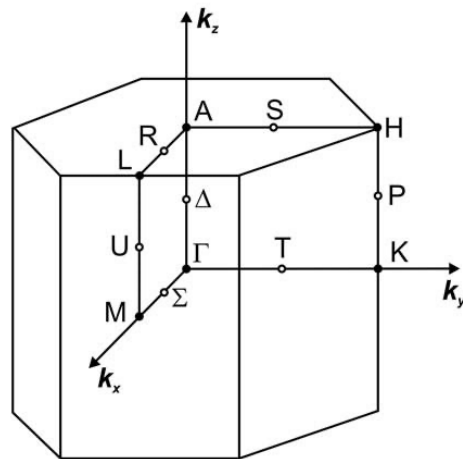
Simple Cubic



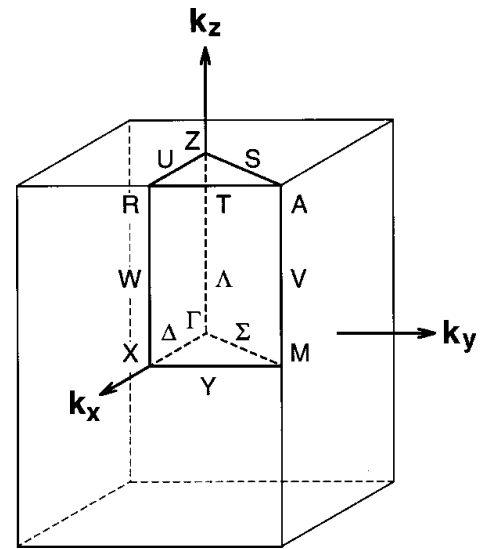
FCC



BCC



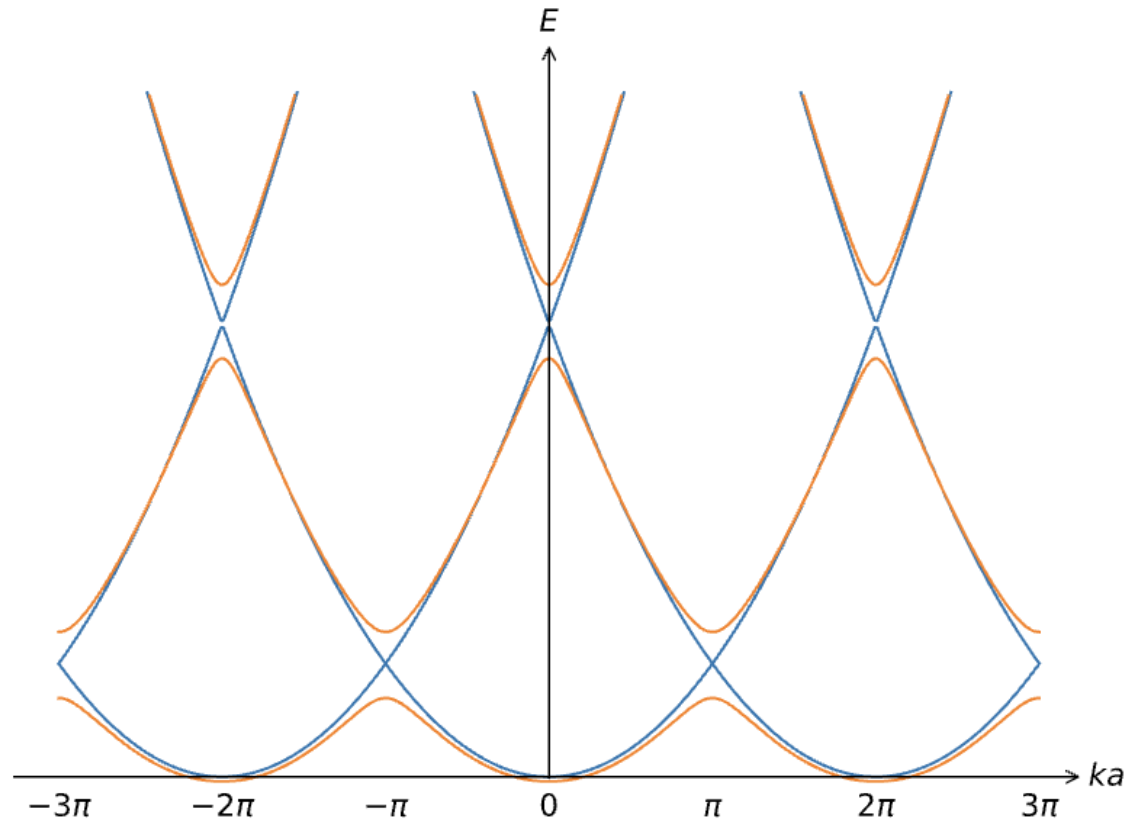
Hexagonal



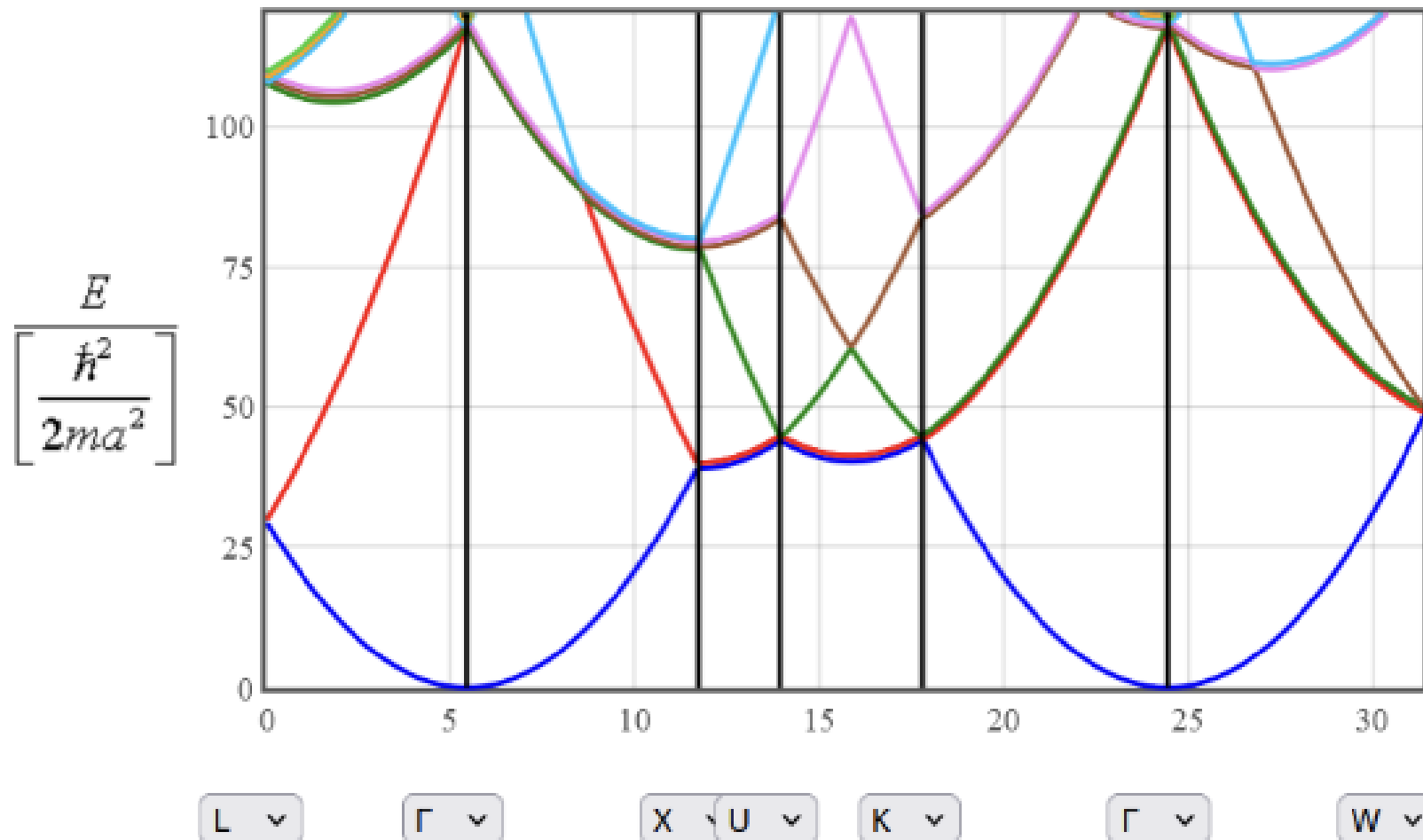
Tetragonal

Reduced Scheme:

Due to the presence of a periodic potential, bands are “folded in” to the first Brillouin zone:



Example: Free Electron bands - FCC lattice





2. Electronic Structure: *Group Theory*

Effect of symmetry in Reciprocal Space:

Example: IRREPS of Spg Group 221 (Simple Cubic)

k-Point	Location in BZ	Little Group	Symmetry Operations	Irreps
Γ (Gamma)	[0, 0, 0]	O _h	Full cubic symmetry: rotations (C ₄ , C ₃), inversion, mirror planes (m)	A ₁ , A ₂ , E, T ₁ , T ₂
X	$[\pi/a, 0, 0]$	D _{4h} (Tetragonal)	C ₂ rotations about x-axis, reflections through planes containing x-axis	A ₁ , A ₂ , B ₁ , B ₂ , E
M	$[\pi/a, \pi/a, 0]$	D _{2h} (Orthorhombic)	C ₂ rotations about principal axes, mirror planes containing k _x and k _y	A _g , B _g , B _{1g} , B _{2g}
Generic k-point	[k _x , k _y , k _z]	C ₁ (Trivial)	Identity only	A

Plotting bands along **high-Symmetry directions** gives an immediate way to visualize band behaviour in 3D. However, the behaviour of the solid is determined by the electronic structure **over the entire BZ**.

Effect of symmetry in Reciprocal Space:

Crystal symmetry in **real space** influences the behaviour of a solid in **reciprocal space** (band structure).

Little Group: Symmetry in reciprocal space is described by the **little group** of each k-point, which is the subgroup of the space group that leaves the k-point invariant.

High-Symmetry Points:

- High-Symmetry points (e.g., Γ , X, K, M) are invariant under many symmetry operations.
- These points often exhibit **degenerate bands**, constrained by the **irreducible representations** of their little group.

High-Symmetry Paths:

- Paths connecting k points – high-symmetry lines - (e.g., $\Gamma \rightarrow X$) are invariant under fewer symmetry operations than high-symmetry points.
- Bands along these paths may split or remain constrained depending on the path's symmetry.

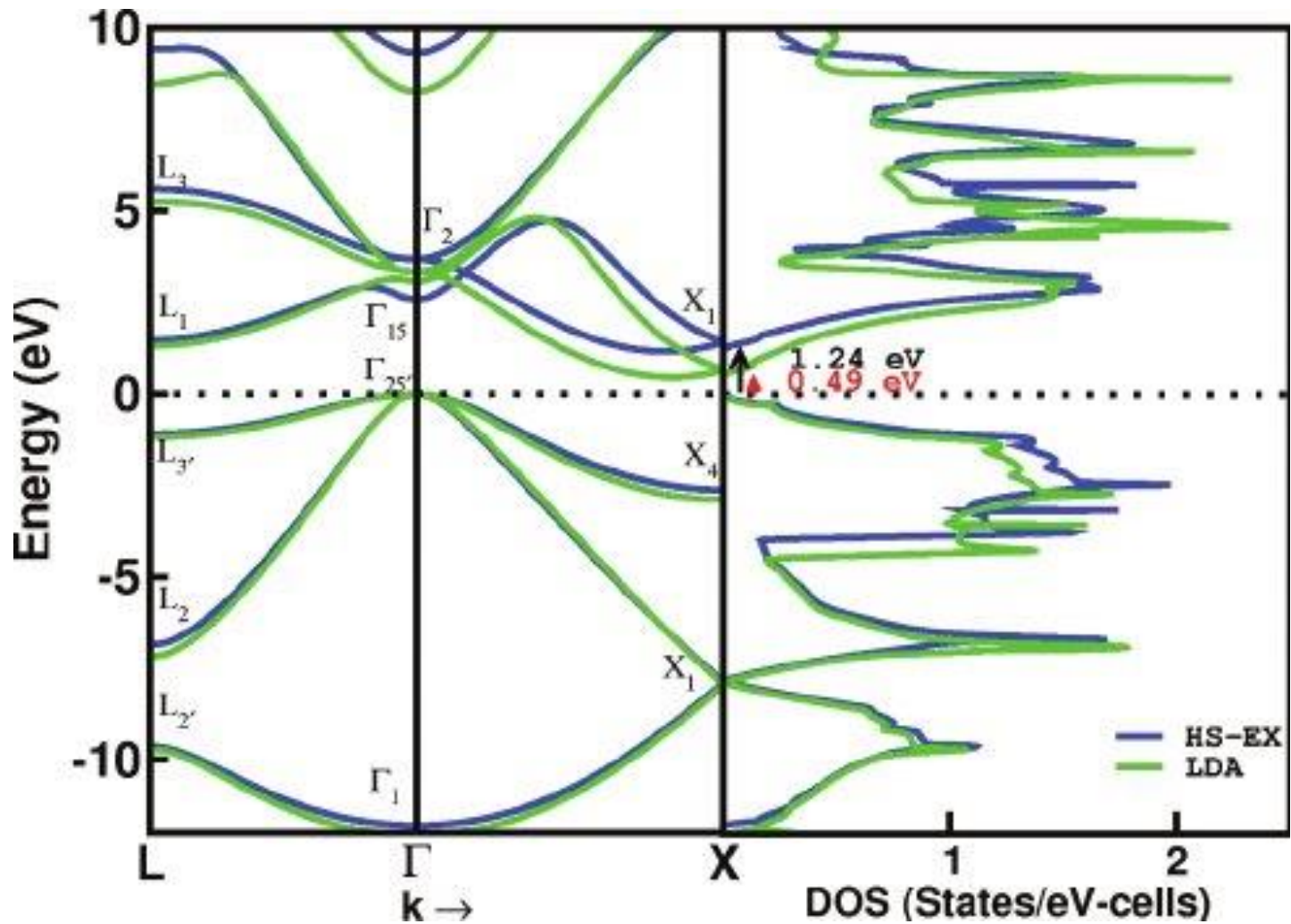
Generic k-Points:

- Generic points in the Brillouin zone (not on high-symmetry points or paths) have minimal symmetry; hence bands at these points are generally **non-degenerate**.

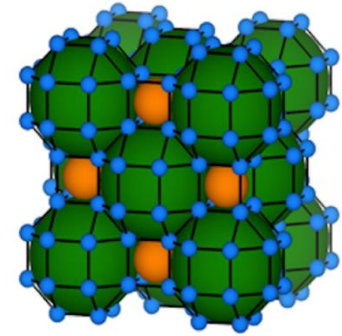
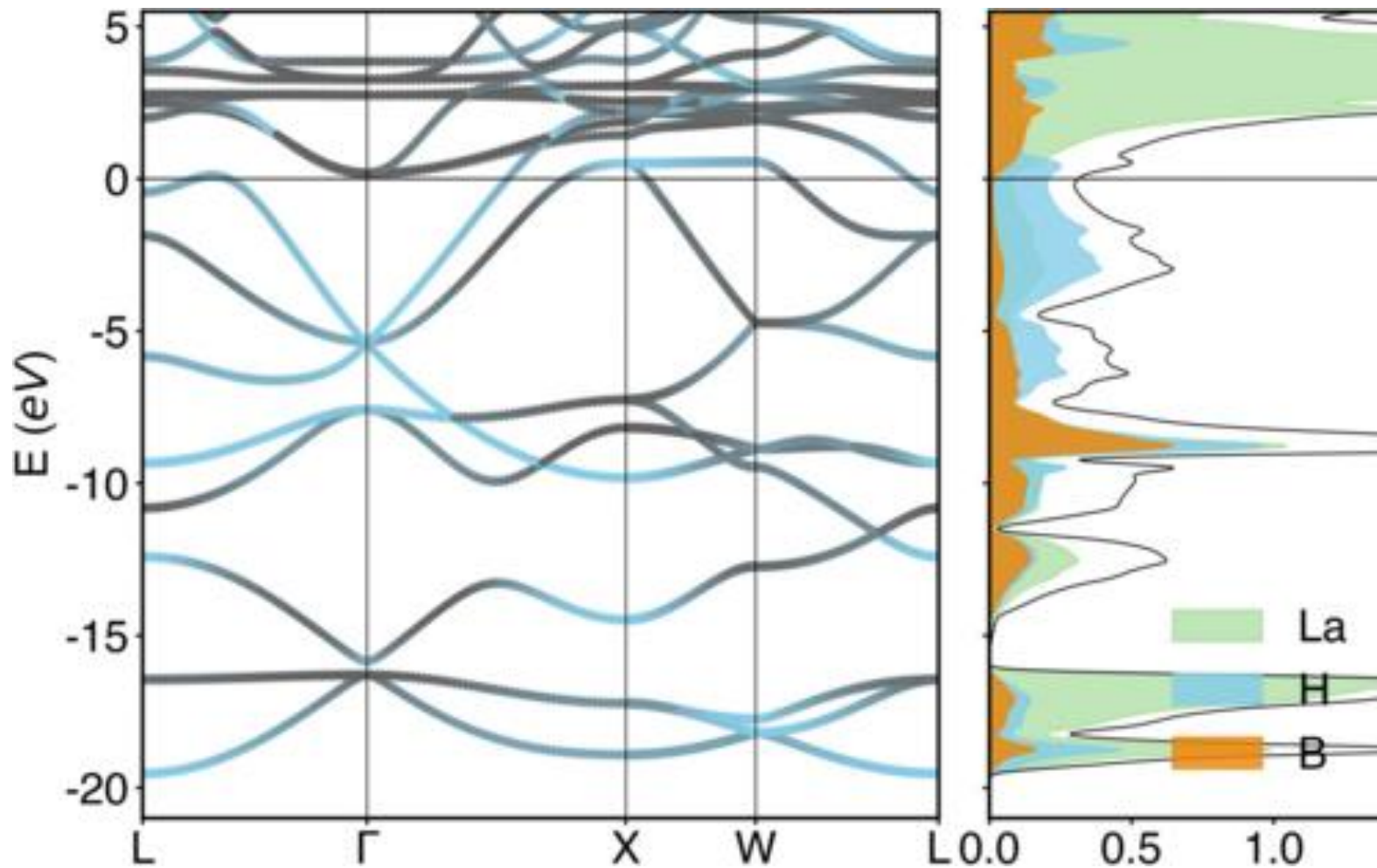
In Synthesis:

1. Real-space **periodicity** of the infinite crystal translates into **a quasi-continuous spectrum of electronic states** (bands) in reciprocal space (**Bloch Theorem**).
2. The **electronic band structure** is the main **signature** of a solid, and determines important properties such as electrical (and heat) transport, optical excitations, etc
3. **Symmetry operations** of the crystal in real space impose **constraints** and determine **degeneracies** of **bands** in reciprocal space.
4. Plotting the **bands** along **high-symmetry directions** is a useful way to understand the main features of the band structure of a crystal.
5. However, the actual behaviour of a crystal depends on what happens **in the entire Brillouin zone** (DOS, Fermi surface, k-space integrals).

Real World: Silicon



Real World: Metal



*Simone Di Cataldo, Christoph Heil, Wolfgang von der Linden, and Lilia Boeri, Phys. Rev. B **104**, L020511 (2021)*



2. Electronic Structure: *First Example with QE,* *Fcc Neon*

Band Structure Plots:

To create a **band structure plot** we need to compute the electronic energies (**Kohn-Sham eigenvalues**) along a **high-symmetry path** in k space.

How this is done in practice:

1. Run a **scf calculation** to generate a **converged charge density**:

(pw.x < neon.scf.in > neon.scf.out)

2. Run a non-scf calculation on a set of k points along high-symmetry lines in the Brillouin zone:

(pw.x < neon.bands.in > neon.bands.out)

Special k points for all Bravais lattices can be found for example in this paper:

<https://arxiv.org/abs/1004.2974>

3. Process the nscf output file to extract the eigenvalues in a convenient format:

(bands.x < bands.in > bands.out)

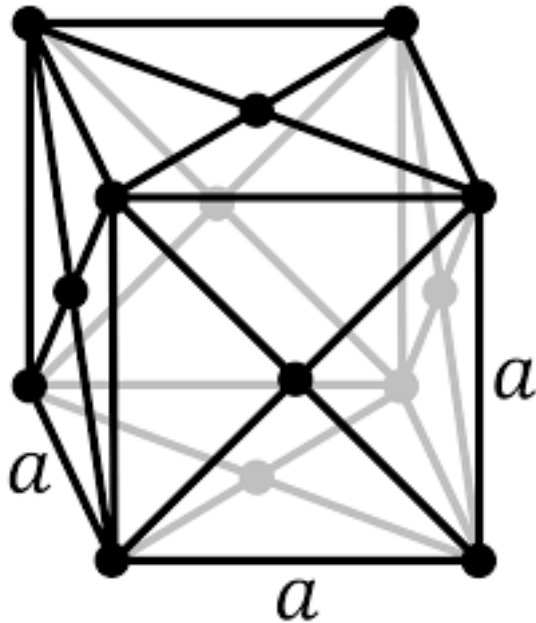
Remember to keep track of the special k points coordinates!

4. Use a 2d plotting program to visualize the band structure

(python3 bandstructure.py)

Example: fcc Neon

Real space:



- Neon, noble Gas (weak bonding)
- $Z=10$
- Electronic Configuration: $(1s^2)2s^2sp^6$

Length

4.46

Angstrom

=

8.428179

Bohr radius

Table 3.1 Lennard–Jones potential parameters for noble-gas crystals

	Neon	Argon	Krypton	Xenon
Crystal structure	fcc	fcc	fcc	fcc
Lattice constant (\AA)	4.46	5.31	5.64	6.13
ϵ (10^{-20} J)	0.050	0.167	0.225	0.320
ϵ (eV)	0.031	0.0104	0.014	0.0200
σ (\AA)	2.74	3.40	3.65	3.98

QE Input file (fcc neon):

&CONTROL

calculation = 'scf'

restart_mode = 'from_scratch'

outdir = './tmp'

pseudo_dir = './PSEUDO'

prefix = 'neon'

tstress = .true.

tpnfor = .true.

CONTROL SECTION: Calculation type, information on input/output info & files.

Pseudopotential files

/

&SYSTEM

ibrav = 2

celldm(1) = 8.43

nat = 1

ntyp = 1

ecutwfc = 80

occupations = 'fixed'

SYSTEM SECTION: Specifies the system (lattice type, lattice vectors, etc).

Plane waves (Basis set)

/

&ELECTRONS

conv_thr = 1.0e-6

ATOMIC SPECIES AND COORDINATES: Types and position of each atom.

/

ATOMIC_SPECIES

Ne 20.18 Ne.LDA.upf

ATOMIC_POSITIONS crystal

Ne 0.00 0.00 0.00

Crystal structure

K_POINTS automatic

4 4 4 0 0 0

https://www.quantum-espresso.org/Doc/INPUT_PW.html

First Test: fcc Neon

Reciprocal space:

$$\begin{cases} \mathbf{G}_1 = \frac{2\pi}{a} (-1, 1, 1) \\ \mathbf{G}_2 = \frac{2\pi}{a} (1, -1, 1) \\ \mathbf{G}_3 = \frac{2\pi}{a} (1, 1, -1) \end{cases}$$

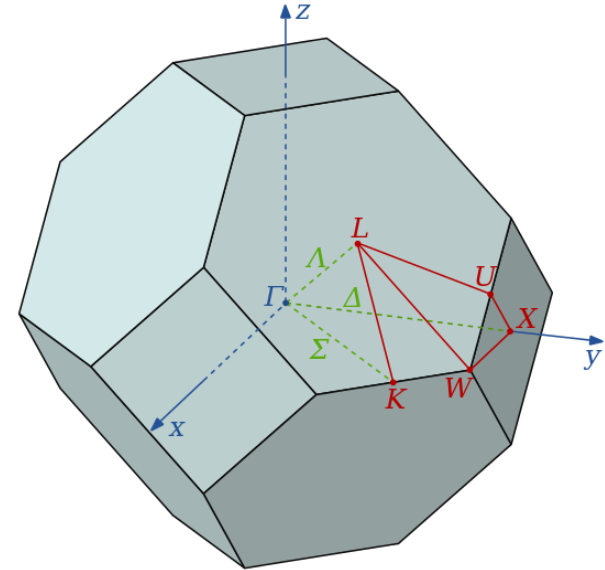
Special k points:

$$\Gamma = 0$$

$$\mathbf{X} = 1/2\mathbf{G}_1 + 1/2\mathbf{G}_2$$

$$\mathbf{W} = 3/4\mathbf{G}_1 + 1/2\mathbf{G}_2 + 1/4\mathbf{G}_3$$

$$\mathbf{L} = 1/2\mathbf{G}_1$$

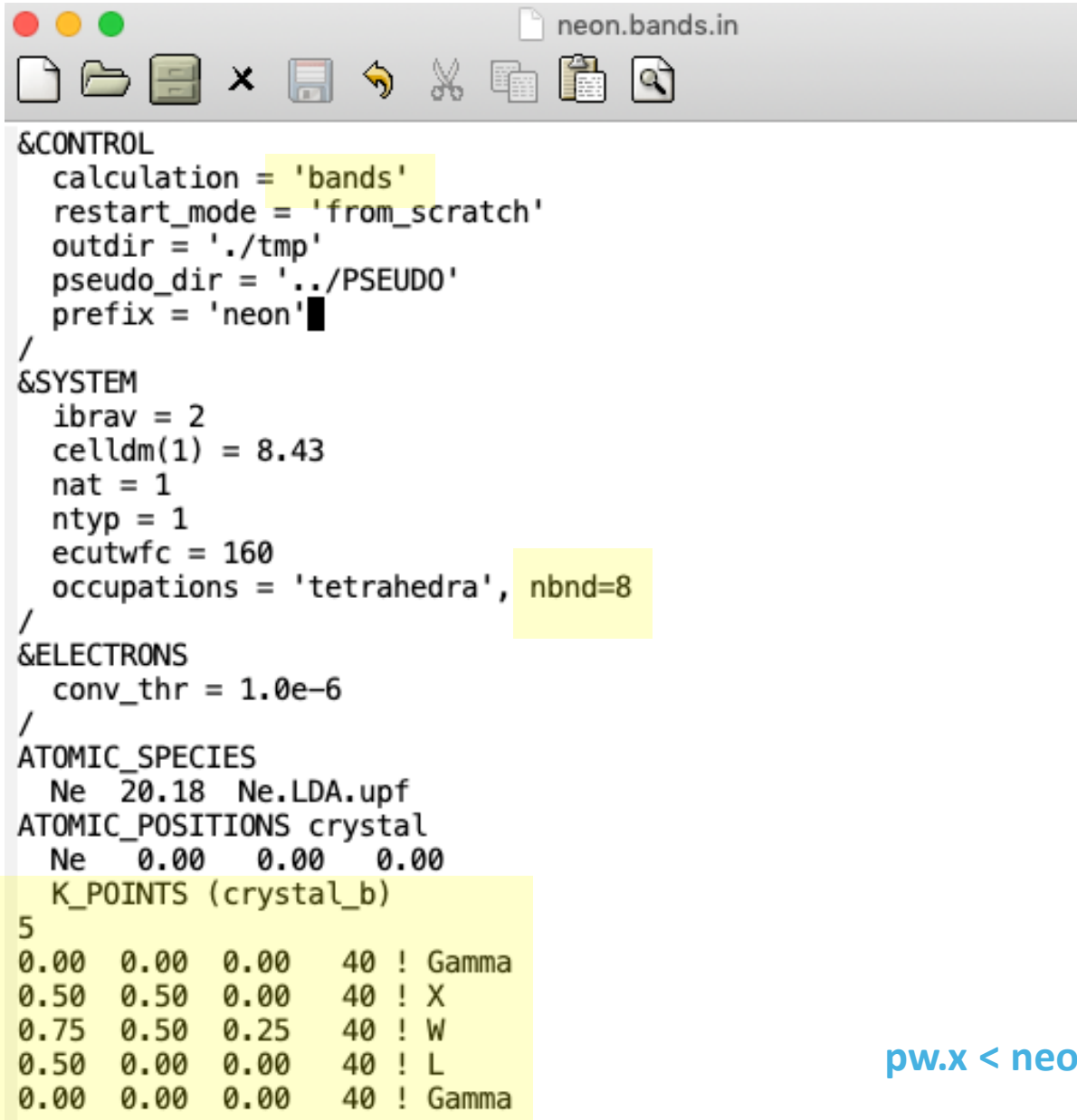


https://en.wikipedia.org/wiki/Brillouin_zone

For a list of special k points for all 3d Brillouin zones see for example:

<http://de.arxiv.org/abs/1004.2974>

Input file: fcc Neon (band structure)



```
&CONTROL
  calculation = 'bands'
  restart_mode = 'from_scratch'
  outdir = './tmp'
  pseudo_dir = '../PSEUDO'
  prefix = 'neon'
/
&SYSTEM
 ibrav = 2
  celldm(1) = 8.43
  nat = 1
  ntyp = 1
  ecutwfc = 160
  occupations = 'tetrahedra', nbnd=8
/
&ELECTRONS
  conv_thr = 1.0e-6
/
ATOMIC_SPECIES
  Ne 20.18 Ne.LDA.upf
ATOMIC_POSITIONS crystal
  Ne 0.00 0.00 0.00
K_POINTS (crystal_b)
5
0.00 0.00 0.00 40 ! Gamma
0.50 0.50 0.00 40 ! X
0.75 0.50 0.25 40 ! W
0.50 0.00 0.00 40 ! L
0.00 0.00 0.00 40 ! Gamma
```

`pw.x < neon.bands.in > neon.bands.out`

Input file: fcc Neon (bands.x)

```
&BANDS
prefix = 'neon',
outdir = './tmp/',
filband = 'neon.bands.dat',
lsym = .true.
&end
```

bands.x < bands.in > bands.out

The program **bands.x** will also produce two files containing the eigenvalues formatted in two different formats. We will use *neon.bands.dat.gnu*.

You can edit/modify the script *bandstructure.py*.

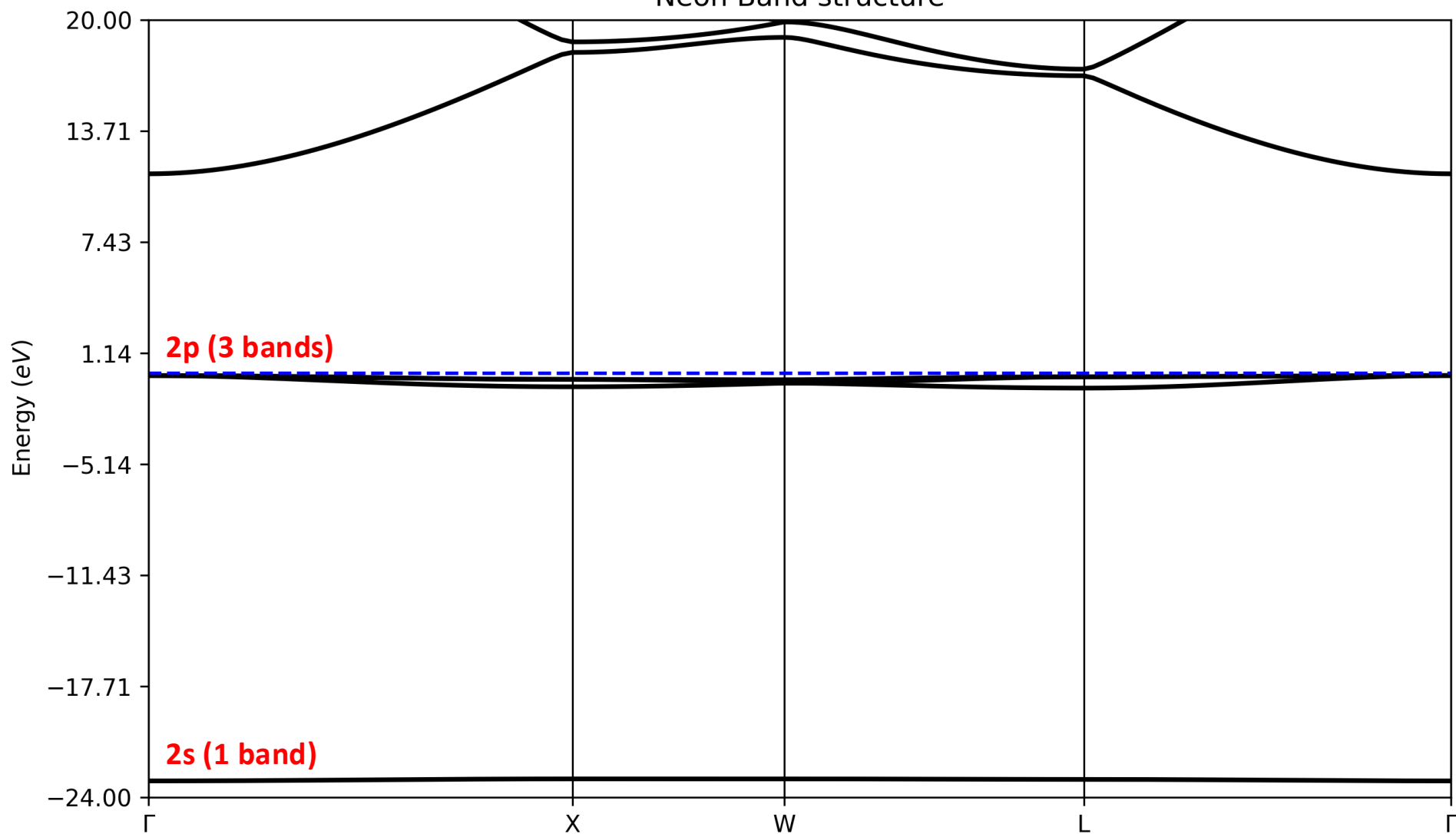
To set the special k points label you need the x coordinates in the bands.out file:

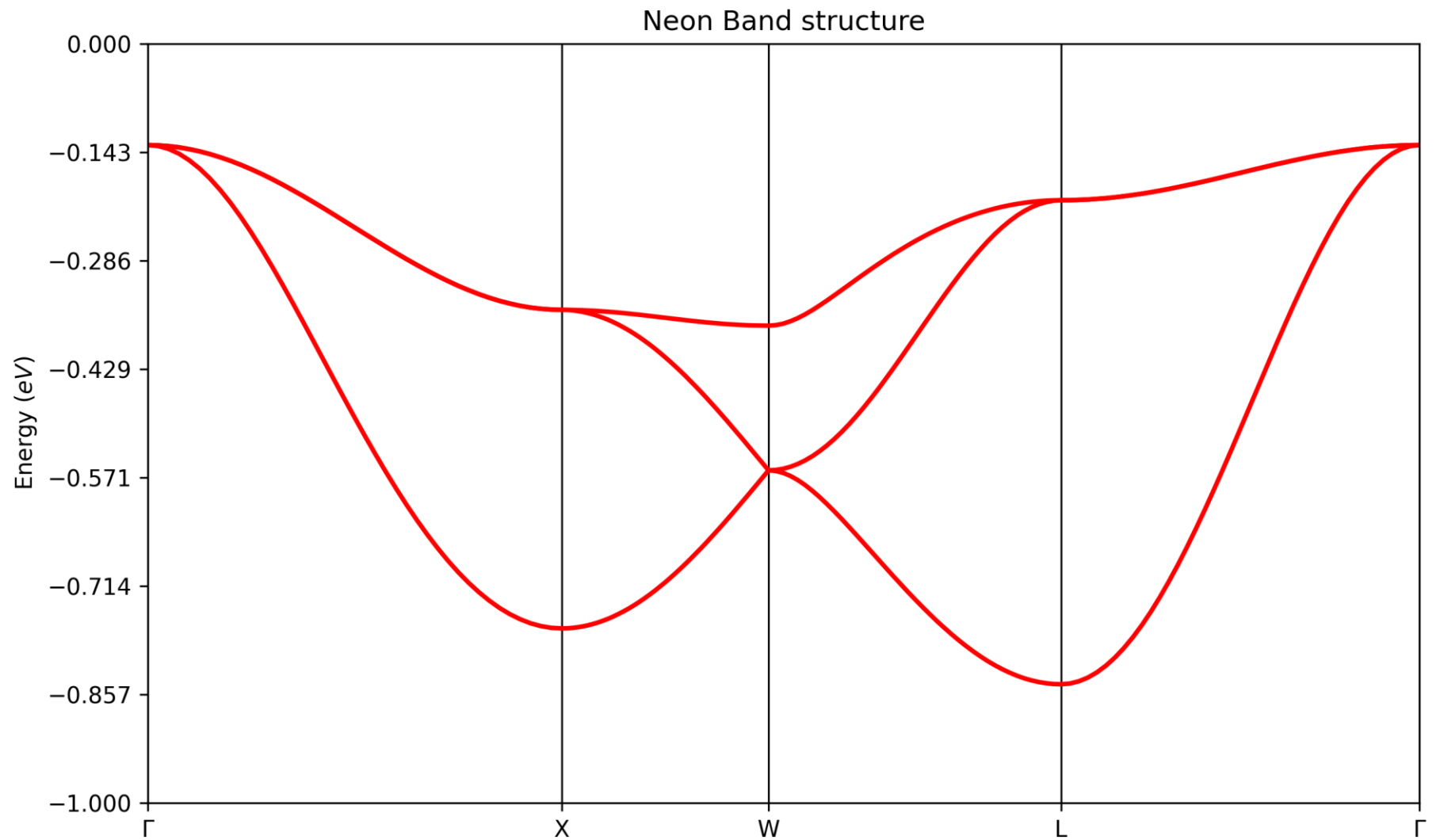
```
G-vector sticks info
-----
sticks:   dense  smooth    PW    G-vecs:   dense  smooth    PW
Sum       1561   1561     439           40857   40857    6183

high-symmetry point:  0.0000 0.0000 0.0000  x coordinate  0.0000
high-symmetry point:  0.0000 0.0000 1.0000  x coordinate  1.0000
high-symmetry point: -0.5000 0.0000 1.0000  x coordinate  1.5000
high-symmetry point: -0.5000-0.5000 0.5000  x coordinate  2.2071
high-symmetry point:  0.0000 0.0000 0.0000  x coordinate  3.0731

Plottable bands (eV) written to file neon.bands.dat.gnu
Bands written to file neon.bands.dat
```

Neon Band structure





Valence bands (2p): Modify y range



3. Density of States and k-space integration methods

Density of States (DOS):

The **density of states** counts how many electronic states exist with energies in $[e, e+de]$.

$$D(\varepsilon) = \sum_{n, \mathbf{k}} \delta(\varepsilon - \varepsilon_{n, \mathbf{k}})$$

The **number of states** counts how many electronic are occupied with energies up to e .

$$N(\varepsilon) = \int_{-\infty}^{\varepsilon} D(\varepsilon') d\varepsilon'$$

In order to calculate the Density of States, we need to perform an **accurate integral** over **reciprocal space** (Brillouin zone).

► What to do in practice:

1. Compute Kohn-Sham Eigenvalues on a **dense mesh of k points** in reciprocal space. (Integral -> discrete sum).
2. Exploit **Symmetry operations** to reduce the sum from the entire BZ to the **irreducible wedge**.
3. Approximate the integral using a **k -space integration method** (smearing, tetrahedron, etc).

Brillouin Zone integration Methods:

The **integral** over the Brillouin zone is replaced by a **discrete sum** over a finite number of \mathbf{k} points, with **weights**:

$$\int_{\text{BZ}} f(\mathbf{k}) d\mathbf{k} \approx \sum_i w_i f(\mathbf{k}_i)$$

► How to choose \mathbf{k}_i, w_i ? Generate a **discrete mesh** of points in reciprocal space.

1. **Uniform Mesh** - *H. J. Monkhorst and J. D. Pack, Phys. Rev. B 13, 5188 (1976).*
2. **Special K points** - *A. Baldereschi, Phys. Rev. B 7, 5212 (1973); D. J. Chadi and M. L. Cohen, Phys. Rev. B 8, 5747 (1973).*
3. **Adaptive Meshes** (importance sampling).

Brillouin Zone integration Methods:

1) Choose a grid: Uniform Grid

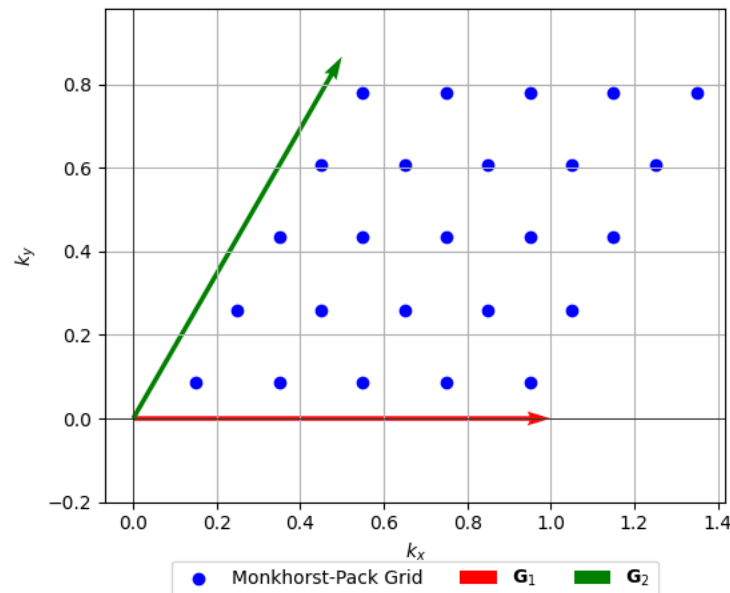
$$\mathbf{k}_n = \frac{n_1}{N_1} \mathbf{G}_1 + \frac{n_2}{N_2} \mathbf{G}_2 + \frac{n_3}{N_3} \mathbf{G}_3 + \mathbf{k}_{\text{shift}} \quad \text{with} \quad n_i = 0, 1, \dots, N_i - 1,$$

$\mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3$: Reciprocal lattice vectors of the crystal,

N_1, N_2, N_3 : Number of divisions along each reciprocal lattice direction,

$\mathbf{k}_{\text{shift}}$: Optional shift applied to the k-point grid to avoid high-symmetry points.

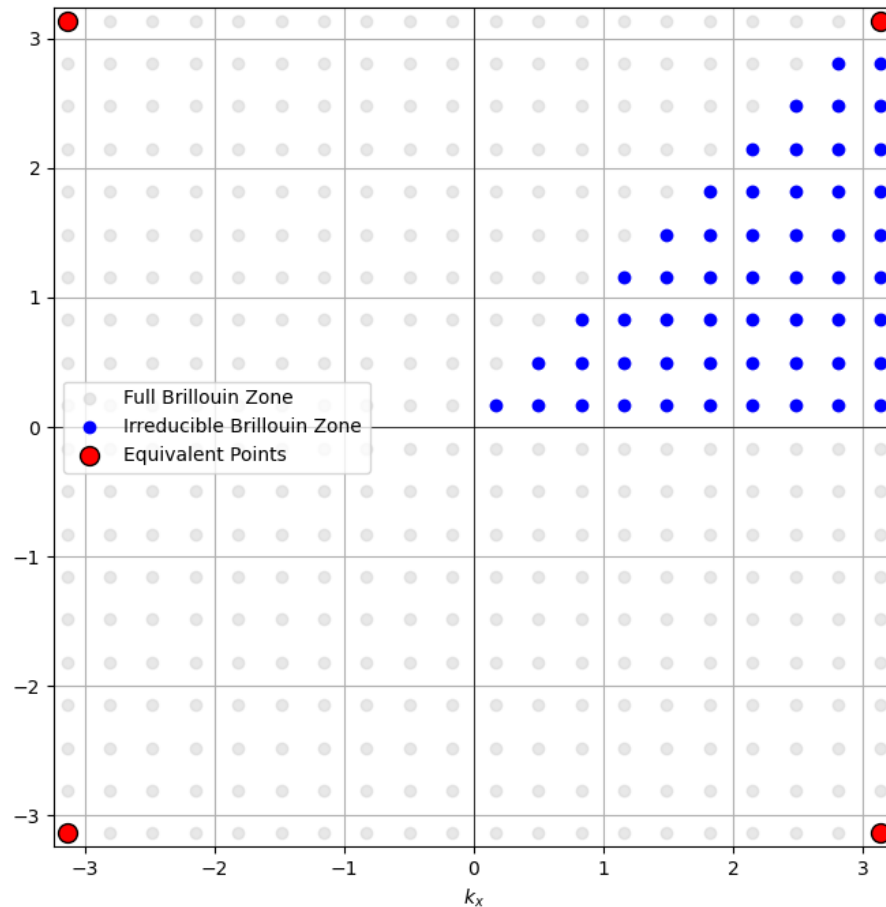
2d example:



Brillouin Zone integration Methods:

$$\int_{\text{BZ}} f(\mathbf{k}) d\mathbf{k} \approx \sum_i w_i f(\mathbf{k}_i)$$

2) Use **Symmetries** to reduce the Sum to the **Irreducible Wedge**:



Brillouin Zone integration Methods:

$$\int_{\text{BZ}} f(\mathbf{k}) d\mathbf{k} \approx \sum_i w_i f(\mathbf{k}_i)$$

3) Approximate the integral using a **k-space integration method**:

Even after reducing the summation to the Irreducible wedge, the number of k points to achieve convergence by brute-force summation is too large.

K-space integration methods permit to reduce the sum to a manageable number of k points:

- **Smearing Methods:** Delta functions are replaced by functions with a finite width (smearing).
Different flavours of smearing functions: gaussians, «cold smearing» functions, etc.
- **Tetrahedron Method:** The Brillouin zone is partitioned into (small) tetrahedra; bands are calculated at the corners of the tetrahedra, and linearly interpolated inside.

Brillouin Zone integration Methods:

► Smearing Method:

Delta functions are replaced by functions with a finite width (smearing).

Different flavours of smearing functions:

$$\delta(E - E_i) \approx \begin{cases} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(E - E_i)^2}{2\sigma^2}\right), & \text{(Gaussian smearing)} \\ \frac{1}{\pi} \frac{\sigma}{(E - E_i)^2 + \sigma^2}, & \text{(Lorentzian smearing)} \\ \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)}, & \text{(Fermi-Dirac smearing)} \end{cases}$$

More advanced methods: Methfessel-Paxton (Hermite Polynomials), cold smearing, etc...

Brillouin Zone integration Methods:

► Tetrahedron Method:

The Brillouin zone is partitioned into (small) tetrahedra; bands are calculated at the corners of the tetrahedra, and linearly interpolated inside.

$$\int_{\text{BZ}} f(\mathbf{k}) d\mathbf{k} \approx \sum_{\text{tetrahedra}} \int_{\text{tetrahedron}} f(\mathbf{k}) d\mathbf{k}.$$

$$f(\mathbf{k}) = \sum_{i=1}^4 w_i(\mathbf{k}) f_i,$$

where:

$w_i(\mathbf{k})$ are the barycentric weights, and
 f_i are the function values at the tetrahedron's four vertices.

Brillouin Zone integration Methods:

Tetrahedron Method:

The Brillouin zone is partitioned into (small) tetrahedra; bands are calculated at the corners of the tetrahedra, and linearly interpolated inside.

- **Original Method:** O. Jepsen and O. K. Andersen, Solid State Comm., **20**, 1763 (1971);
- **Improved Tetrahedron Method (Metals):** P. E. Blöchl, O. Jepsen, and O. K. Andersen, Physical Review B **49**, 16223 (1994);
- **Improved Tetrahedron Method (Forces & Phonons):** Mitsuaki Kawamura, Yoshihiro Gohda, and Shinji Tsuneyuki, Phys. Rev. B **89**, 094515 (2014).

HowTo: DOS plot

1. Run a **scf calculation** to generate a **converged charge density**:

`(pw.x < neon.scf.in > neon.scf.out)`

2. Run a **non-scf** calculation on a **fine grid in k space**:

`(pw.x < neon.nscf.in > neon.nscf.out)`

To perform a smooth integration you need a very fine k mesh and a «smart» integration method (tetrahedron or smearing)

3. Process the nscf output file to extract the eigenvalues in a convenient format:

`(dos.x < dos.in > dos.out)`

4. Use a **2d plotting program** to **visualize** the DOS:

`(python3 dos.py)`

Input file: fcc Neon (scf calculation)

```
&CONTROL
  calculation = 'scf'
  restart_mode = 'from_scratch'
  outdir = './tmp'
  pseudo_dir = './PSEUDO'
  prefix = 'neon'
  tstress = .true.
  tprnfor = .true.
/
&SYSTEM
  ibrav = 2
  celldm(1) = 8.43
  nat = 1
  ntyp = 1
  ecutwfc = 80
  occupations = 'fixed'
/
&ELECTRONS
  conv_thr = 1.0e-6
/
ATOMIC_SPECIES
  Ne 20.18 Ne.LDA.upf
ATOMIC_POSITIONS crystal
  Ne 0.00 0.00 0.00
K_POINTS automatic
  4 4 4 0 0 0
```

K-space integration

pw.x < neon.scf.in > neon.scf.out

neon.nscf.in

```
&CONTROL
  calculation = 'nscf'
  restart_mode = 'from_scratch'
  outdir = './tmp'
  pseudo_dir = '../PSEUDO'
  prefix = 'neon'
  tstress = .true.
  tprnfor = .true.
/
&SYSTEM
 ibrav = 2
  celldm(1) = 8.43
  nat = 1
  ntyp = 1
  ecutwfc = 160
  occupations = 'tetrahedra', nbnd=8
/
&ELECTRONS
  conv_thr = 1.0e-6
/
ATOMIC_SPECIES
  Ne 20.18 Ne.LDA.upf
ATOMIC_POSITIONS crystal
  Ne 0.00 0.00 0.00
K_POINTS automatic
  12 12 12 0 0 0
```

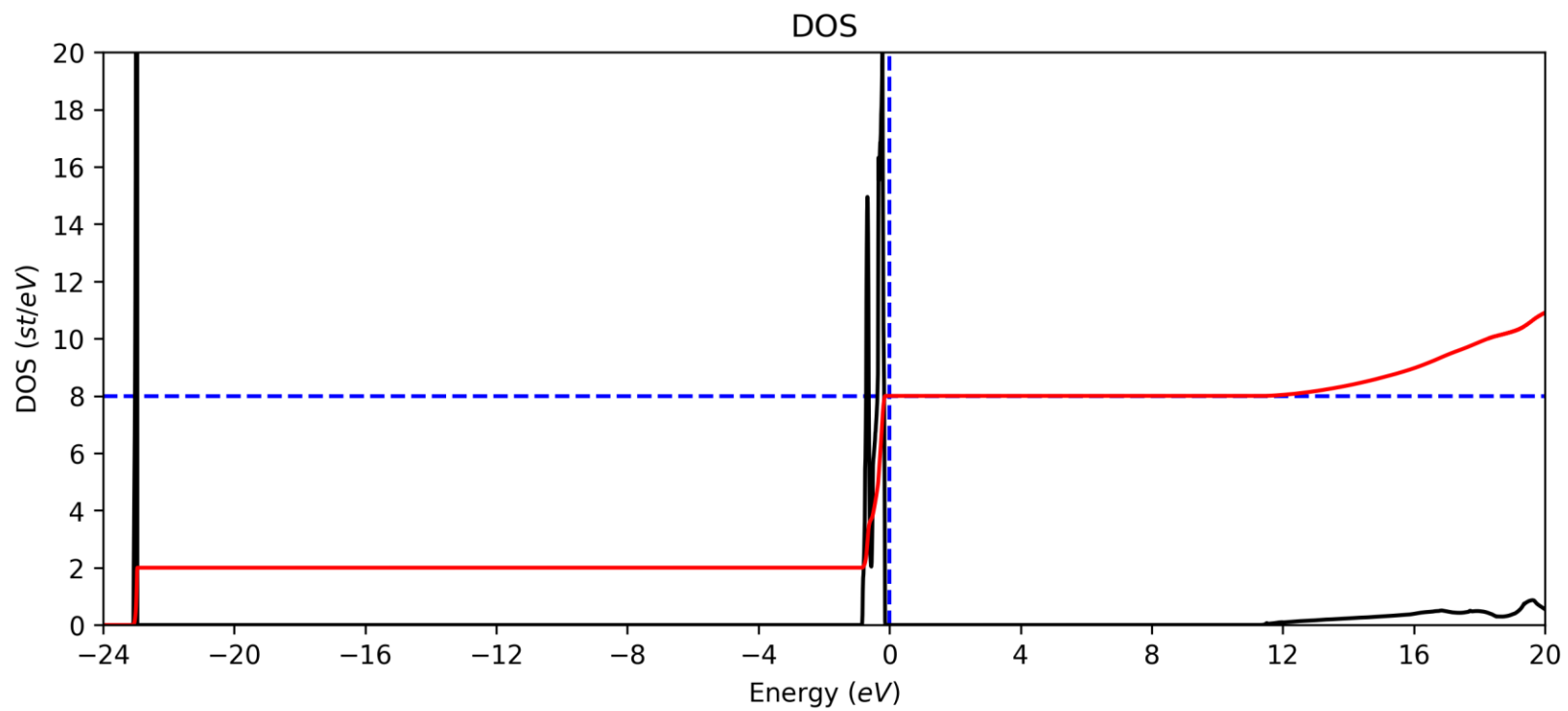
pw.x < neon.nscf.in > neon.nscf.out

Input file: fcc Neon (DOS)

```
&dos  
prefix = 'neon',  
outdir = './tmp',  
Emin = -40,  
Emax = 20,  
DeltaE = 0.01  
&end
```

dos.x < dos.in > dos.out

#	E (eV)	dos(E)	Int dos(E)	EFermi =
				-5.953 eV
	-40.000	0.0000E+00	0.0000E+00	
	-39.990	0.0000E+00	0.0000E+00	
	-39.980	0.0000E+00	0.0000E+00	
	-39.970	0.0000E+00	0.0000E+00	
	-39.960	0.0000E+00	0.0000E+00	
	-39.950	0.0000E+00	0.0000E+00	
	-39.940	0.0000E+00	0.0000E+00	
	-39.930	0.0000E+00	0.0000E+00	
	-39.920	0.0000E+00	0.0000E+00	
	-39.910	0.0000E+00	0.0000E+00	
	-39.900	0.0000E+00	0.0000E+00	
	-39.890	0.0000E+00	0.0000E+00	
	-39.880	0.0000E+00	0.0000E+00	
	-39.870	0.0000E+00	0.0000E+00	



2s (1 band)

2p (3 bands)

In summary (electronic Structure calculations **HOWTO**):

1. Run a **scf calculation** to generate a **converged charge density**:

`(pw.x < neon.scf.in > neon.scf.out)`

2. Run a **non-scf calculation** on **properly chosen k points** (*high-symmetry lines or dense grid*):

`(pw.x < neon.bands.in > neon.bands.out) / (pw.x < neon.nscf.in > neon.nscf.out)`

3. **Process** the nscf output file to extract the eigenvalues in a convenient format:

`(bands.x < bands.in > bands.out) / (dos.x < dos.in > dos.out)`

4. **Use a 2d plotting program** to **visualize** the band structure/Density of States:

`(python3 bandstructure.py)/(python3 dos.py)`



4. Electronic Structure *for Metals*

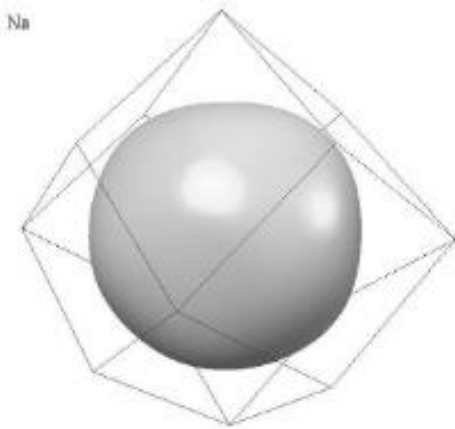
Fermi Energy and Fermi Surface:

The Fermi energy (E_F) is the highest energy state occupied by electrons in a solid, i.e.

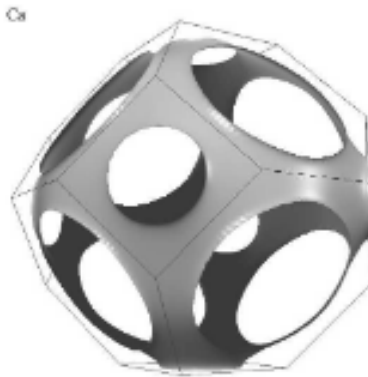
$$N_{el} = \int_{-\infty}^{E_F} D(\varepsilon) d\varepsilon$$

In metals, the Fermi energy (E_F) defines a surface in 3-dimensional space which separates full and empty space, known as the **Fermi surface**.

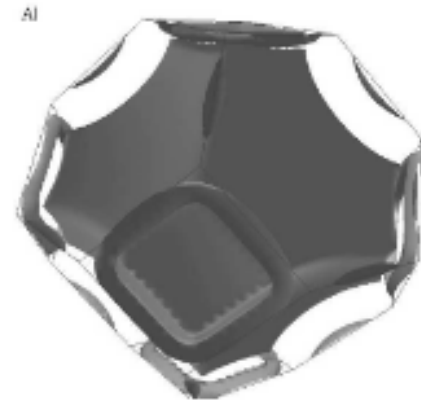
For **free electrons**, the Fermi surface is a **sphere**, folded into the first BZ (See *Ashcroft & Mermin*, chapter 9):



Na ($N_e=1$)



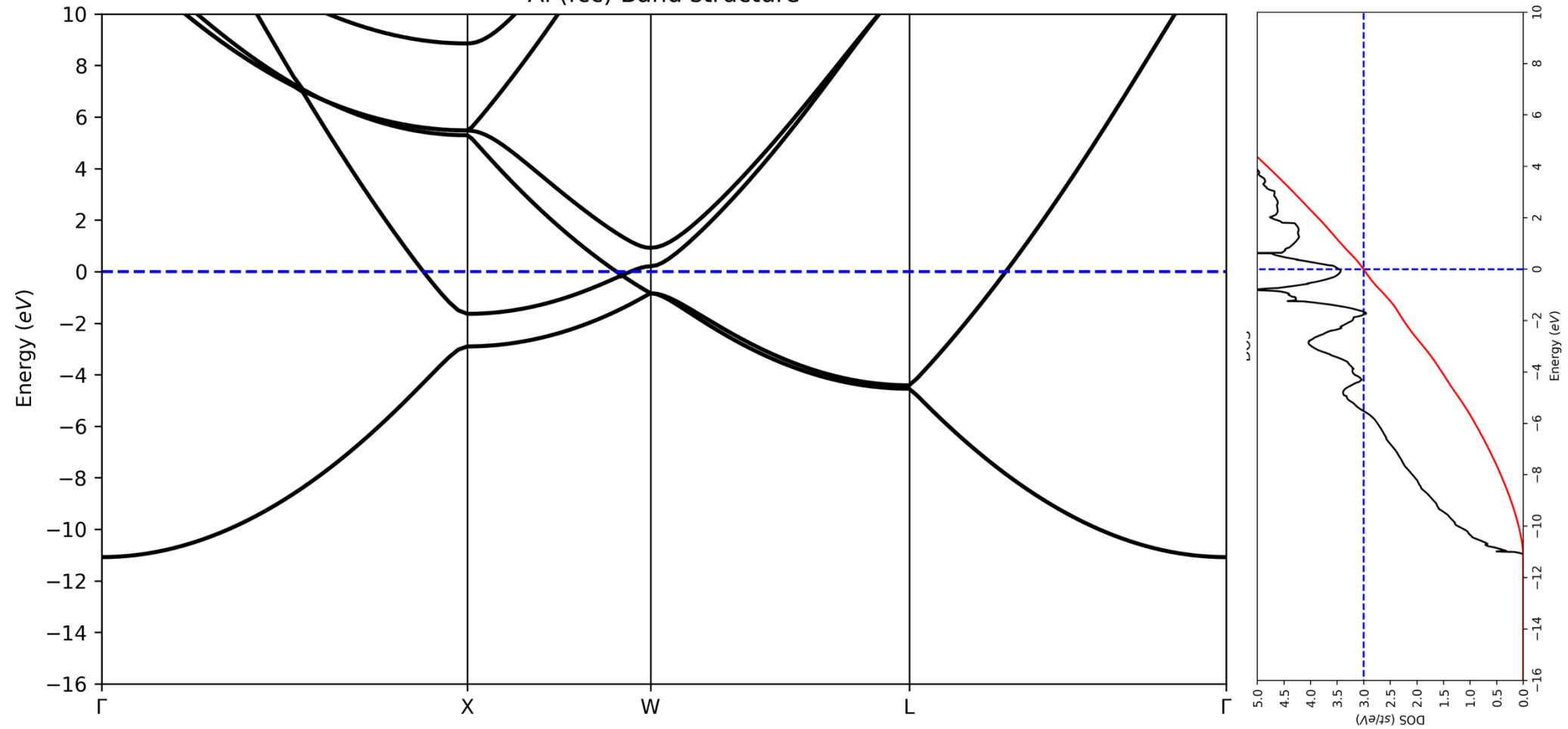
Ca ($N_e=2$)



Al ($N_e=3$)

Example: Aluminum

Al (fcc) Band structure



Input file: fcc Aluminum (scf)

```
&CONTROL
  calculation = 'scf'
  restart_mode = 'from_scratch'
  outdir = './tmp'
  pseudo_dir = '../PSEUDO'
  prefix = 'allu'
  tstress = .true.
  tprnfor = .true.
/
&SYSTEM
 ibrav = 2
  celldm(1) = 7.653391
  nat = 1
  ntyp = 1
  ecutwfc = 40
  occupations = 'tetrahedra'
/
&ELECTRONS
  conv_thr = 1.0e-6
/
ATOMIC_SPECIES
  Al 26.98 Al.LDA.upf
ATOMIC_POSITIONS crystal
  Al 0.00 0.00 0.00
K_POINTS automatic
  12 12 12 0 0 0
```

the Fermi energy is 7.6703 ev

```
! total energy = -4.72585935 Ry
  Harris-Foulkes estimate = -4.72585952 Ry
  estimated scf accuracy < 0.00000083 Ry
```

Input file: fcc Aluminum (bands)

```
&CONTROL
  calculation = 'bands'
  restart_mode = 'from_scratch'
  outdir = './tmp'
  pseudo_dir = '../PSEUDO'
  prefix = 'allu'
  tstress = .true.
  tprnfor = .true.
/
&SYSTEM
 ibrav = 2
  celldm(1) = 7.653391
  nat = 1
  ntyp = 1
  ecutwfc = 40, nbnd=10,
occupations='tetrahedra'
/
&ELECTRONS
  conv_thr = 1.0e-6
/
ATOMIC_SPECIES
  Al 26.98 Al.LDA.upf
ATOMIC_POSITIONS crystal
  Al 0.00 0.00 0.00
K_POINTS (crystal_b)
5
0.00 0.00 0.00 40
0.50 0.50 0.00 40
0.75 0.50 0.25 40
0.50 0.00 0.00 40
0.00 0.00 0.00 40
```

Input file: fcc Aluminum (DOS)

```
&CONTROL
  calculation = 'nscf'
  restart_mode = 'from_scratch'
  outdir = './tmp'
  pseudo_dir = '../PSEUDO'
  prefix = 'allu'
  tstress = .true.
  tprnfor = .true.
/
&SYSTEM
  ibrav = 2
  celldm(1) = 7.653391
  nat = 1
  ntyp = 1
  ecutwfc = 40, nbnd=10,
! occupations = 'smearing', smearing='gauss', degauss=0.02
occupations='tetrahedra'
/
&ELECTRONS
  conv_thr = 1.0e-6
/
ATOMIC_SPECIES
  Al 26.98 Al.LDA.upf
ATOMIC_POSITIONS crystal
  Al 0.00 0.00 0.00
K_POINTS automatic
  16 16 16 0 0 0
```



4. Exercises & Home Assignments

Electronic structure of **AlSi** in the **CsCl** structure

- Setup the scf calculation, converging the calculation with respect to all relevant parameters (ecut, k points, etc)
- Compute the band structure and DOS.
- Is the resulting structure a metal or an insulator/semiconductor?
- If it's an insulator/semiconductor, how large is the gap? Is it direct or indirect?

<https://materialsproject.org/materials/mp-1021666/>

Crystal Structure

Lattice (Conventional)

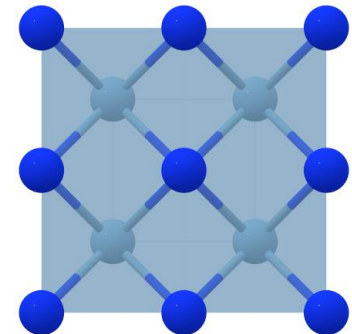
a	3.15 Å
b	3.15 Å
c	3.15 Å
α	90.00 °
β	90.00 °
γ	90.00 °
Volume	31.31 Å ³

Lattice is given in its ☒ conventional ☐ crystallographic setting.

Atomic Positions

Wyckoff	Element	x	y	z
1a	Al	0	0	0
1b	Si	1/2	1/2	1/2

Space group: 221 (simple cubic)



Electronic structure of **silicon** allotropes

- Plot the electronic structure and DOS of silicon in the diamond and lonsdaleite structure, i.e.
- Setup the scf calculation, converging the calculation with respect to all relevant parameters (ecut, k points, etc)
- Compute the band structure and DOS.
- Is the resulting structure a metal or an insulator/semiconductor?
- If it's an insulator/semiconductor, how large is the gap? Is it direct or indirect?
- If it's a metal, determine the Fermi level.

