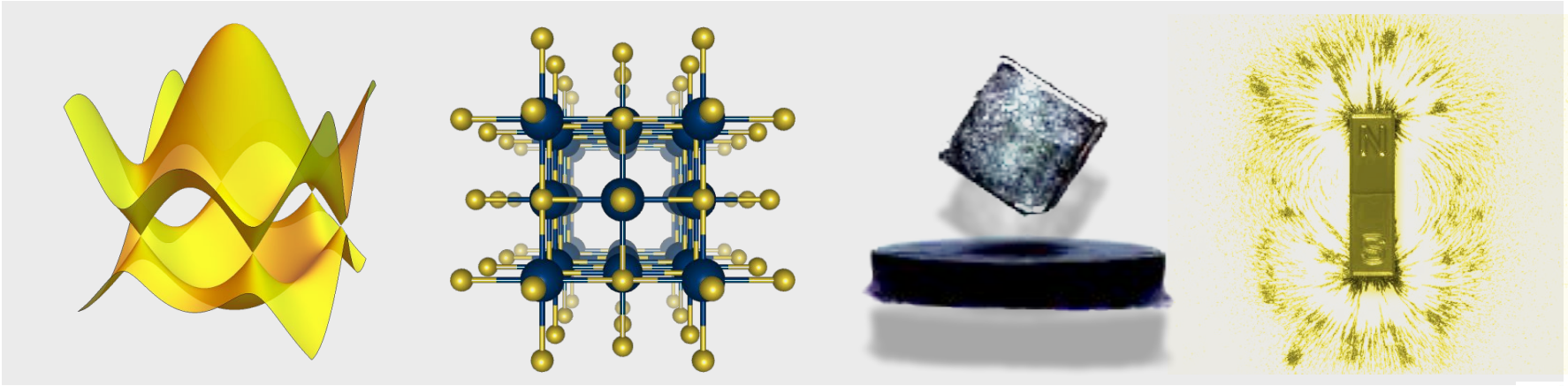
ESCOLA SÉRGIO MASCARENHAS DE FÍSICA DA MATÉRIA CONDENSADA

Hands-On 2 - Computational

Band Structure and Density of States



SBF

UFPE

Getting started

➔ Basic Unix Commands:

Unix Command	Description
ls	List directory contents
cp	Copy files
rm	Remove directory entries
which	Locate a program file in the user's path
diff	Find differences between two files
vi	Text editor
mv	Move and rename files
pwd	Print working directory name
cd	Change working directory
ln	Make a file link
mkdir	Make directories
rmdir	Remove directories
alias	Create a command alias

http://www.tech-faq.com/basic-unix-commands.html

Getting started

➔ SLURM (Simple Linux Utility for Resource Management) commands:

SLURM command	Sample command syntax	Meaning
scancel	scancel <jobid>	Cancel a job. `scancel` can also be used to kill job arrays or job steps.
sacct	sacct -j <jobid>	Check job accounting data. Running `sacct` is most useful for completed jobs.
scontrol	scontrol show job <jobid>	Look at a running job in detail. For more information about the job, add the `-dd` parameter.
scontrol	scontrol hold <jobid>	Pause a job
scontrol	scontrol release <jobid>	Release a held job (allow it to run)
sinfo	sinfo	See node and partition information. Use the `-N` parameter to see information per node.
srun	srun --pty -t 0-0:5:0 -p interactive /bin/bash	Start an interactive session for five minutes in the interactive queue.
sbatch	sbatch <jobscript>	Submit a batch job.
squeue	squeue -u <userid>	View status of your jobs in the queue. Only non-completed jobs will be shown.

https://wiki.rc.hms.harvard.edu/display/O2/Using+Slurm+Basic

Getting started

➔ Log in to SDummont:

```
>> ssh your_username@login.sdumont.lncc.br
```

➔ Loading packages:

```
>> module load python/3.9.12
```

➔ Go to your scratch area:

```
>> cd /scratch/efmc24/your_username
```

➔ Copy files to you user area:

```
>> cp -r /scratch/efmc24/HandsOn_Material/day2 .
>> cd day2
```

Today's goals

1. Calculate electronic band structure of YIn_3:
   - ↳ Input file
   - ↳ Choosing high symmetry points in the reciprocal space

2. Calculate Density of States (DOS) of YIn_3:
   - ↳ Self-consistent x non self-consistent calculations (scf x nscf).

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Band structure calculation: Workflow

Step 0:

Structural relaxation:

```
pw.x vc-relax.in > vc-relax.out
```

Step 1:

Generate charge density (scf):

```
pw.x scf.in > scf.out
```

Step 2:

Calculate eigenvalues:

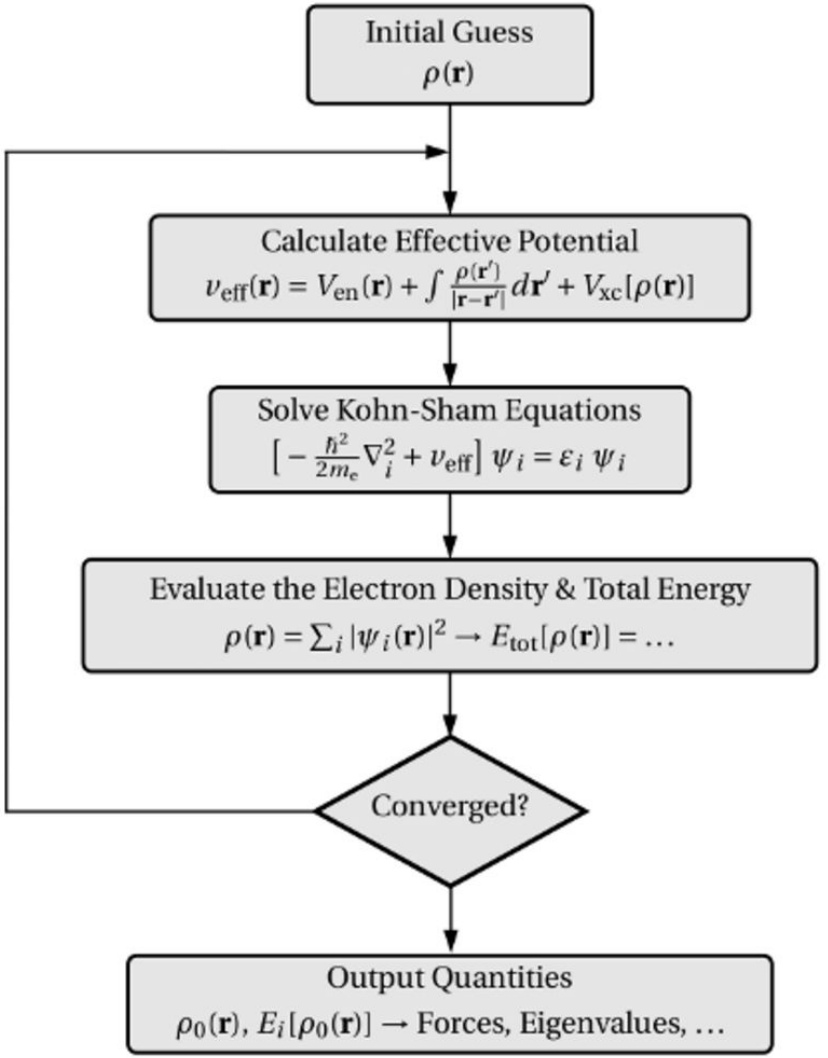
```
pw.x pw.bands.in > pw.bands.out
```

Step 3:

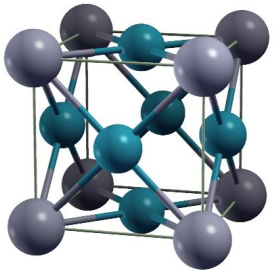
Post-processing and plot:

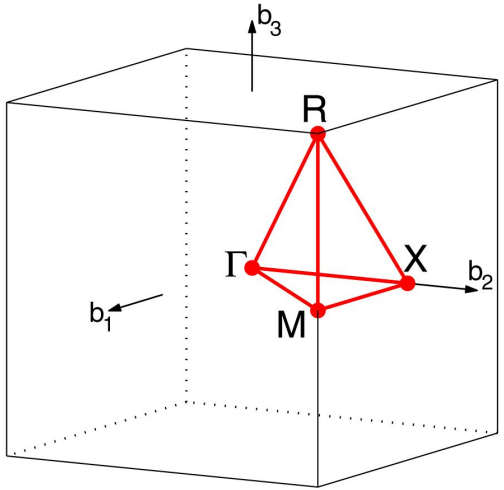
```
python qe_pp_bands.py
```

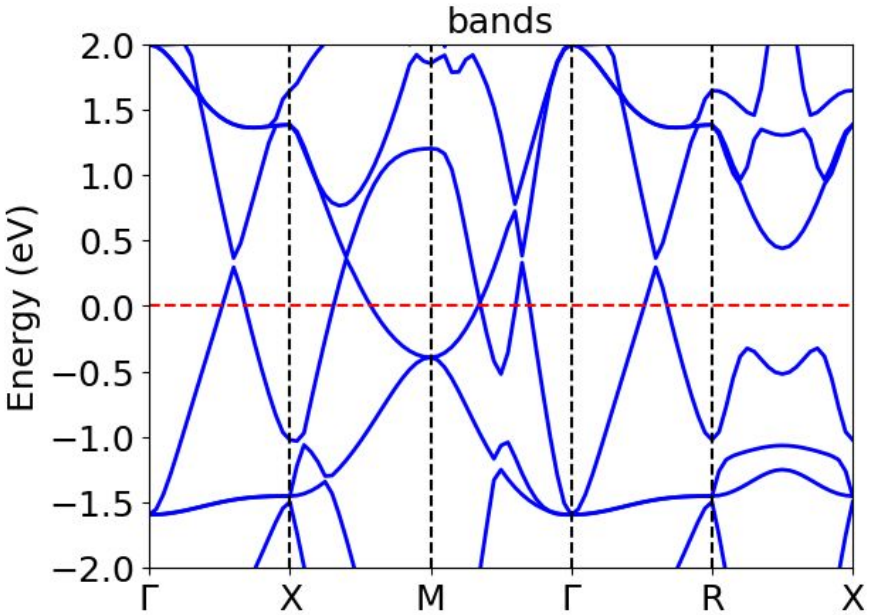
Ciclo auto-consistente



Electronic band structure: YIn_3







CUB path: Γ-X-M-Γ-R-X|M-R

Electronic band structure calculation.

1. Go to the working directory:

```
>> cd day2
```

We start from a scf calculation to generate the charge density: charge-density.dat.

2. Run!

```
>> sbatch sub.srm
```

3. Check if the calculation finished properly:

```
>> tail scf.out
….
=-----------------------------------
   JOB DONE.
=————————————————————————————————=
```

```
 &CONTROL
  calculation = 'scf'
  outdir = './'
  prefix = 'yin3'
  pseudo_dir =
'/scratch/efmc2024/HandsOn_Material/Pseudos/
/
&SYSTEM
  ecutwfc =   90
  ibrav = 0
  nat = 4
  ntyp = 2
/
&ELECTRONS
/
&IONS
/
&CELL
/

ATOMIC_SPECIES
Y      88.90  Y.pbe-spn-kjpaw_psl.1.0.0.UPF
In    114.82  In.pbe-dn-kjpaw_psl.1.0.0.UPF
```

Electronic band structure calculation.

4. Go to the directory 2_bands;

```
>> cd ../2_bands
```

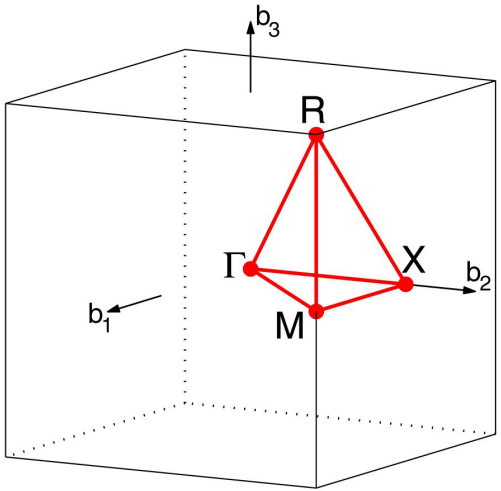
5. Have a look at the input file **pw.bands.in**.. What is different from the previous scf calculation?

```
&CONTROL
   calculation = 'bands'
   etot_conv_thr =   6.0000000000d-05
   forc_conv_thr =   1.0000000000d-04
   outdir = './'
   prefix = 'yin3'

…

K_POINTS crystal_b
6
   0.00   0.00   0.00   20   !$\GAMMA$
   0.00   0.50   0.00   20   !X
   0.50   0.50   0.00   20   !M
   0.00   0.00   0.00   20   !$\GAMMA$
   0.00   0.00   0.50   20   !R
   0.00   0.50   0.00   20   !X
```

Electronic band structure calculation.



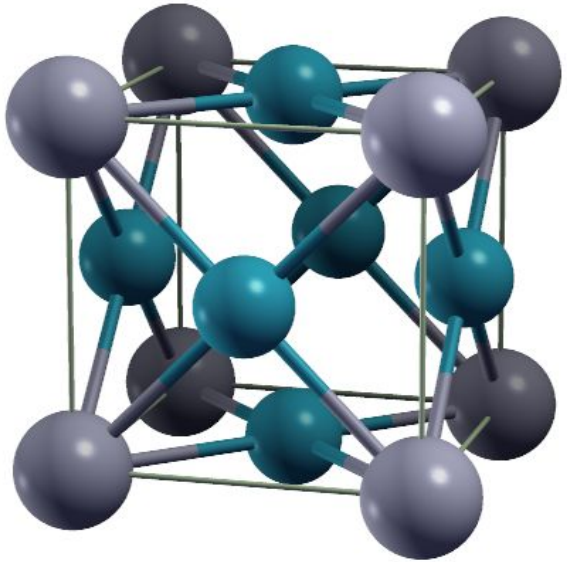
CUB path: Γ-X-M-Γ-R-X|M-R

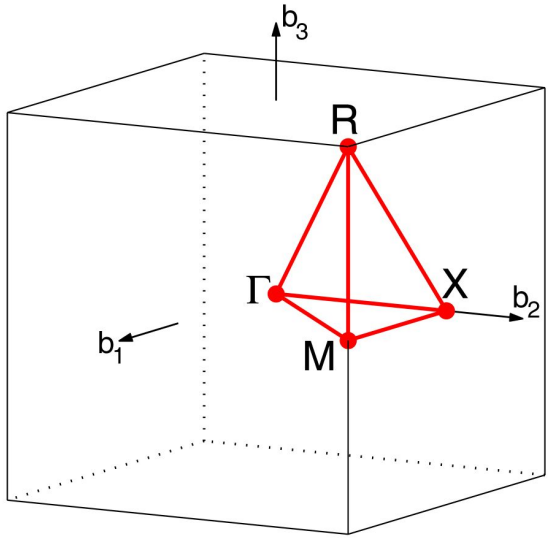
```
&CONTROL
   calculation = 'bands'
   etot_conv_thr =   6.0000000000d-05
   forc_conv_thr =   1.0000000000d-04
   outdir = './'
   prefix = 'yin3'

…


K_POINTS crystal_b
6
    0.00    0.00    0.00    20    !$\GAMMA$
    0.00    0.50    0.00    20    !X
    0.50    0.50    0.00    20    !M
    0.00    0.00    0.00    20    !$\GAMMA$
    0.00    0.00    0.50    20    !R
    0.00    0.50    0.00    20    !X
```

Real Space x Reciprocal Space





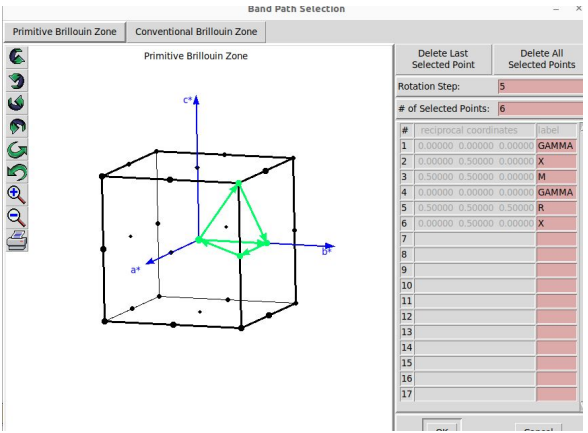
CUB path: Γ-X-M-Γ-R-X|M-R

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

Reciprocal Space data

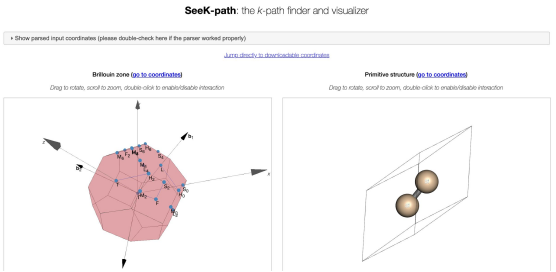
How to choose high symmetry points? .... Many different ways!
A few options:

From QE input file:



http://www.xcrysden.org/

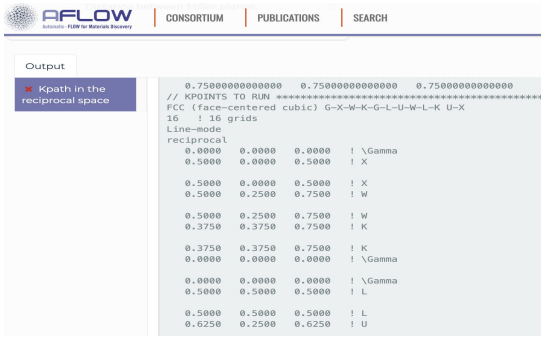
MATERIALSCLOUD



https://www.materialscloud.org/home

From POSCAR (VASP input file):

AFLOW
Automatic - FLOW for Materials Discovery



http://aflowlib.org/

Electronic band structure calculation.

4. Go to the directory 2-bands;

```
>> cd ../2_bands
```

5. Have a look at the input file **pw.bands.in**.. What is different from the previous scf calculation?

6. Create a link for the folder with the charge density file generated from the scf calculation:

```
>> ln -s ../1_scf/yin3.save .
```

```
&CONTROL
   calculation = 'bands'
   etot_conv_thr =   6.0000000000d-05
   forc_conv_thr =   1.0000000000d-04
   outdir = './'
   prefix = 'yin3'

…

K_POINTS crystal_b
6
   0.00   0.00   0.00   20   !$\GAMMA$
   0.00   0.50   0.00   20   !X
   0.50   0.50   0.00   20   !M
   0.00   0.00   0.00   20   !$\GAMMA$
   0.00   0.00   0.50   20   !R
   0.00   0.50   0.00   20   !X
```

Electronic band structure calculation.

4. Go to the directory 2-bands;

```
>> cd ../2_bands
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5. Have a look at the input file **pw.bands.in**.. What is different from the previous scf calculation?

6. Create a link for the folder with the charge density file generated from the scf calculation:

```
>> ln -s ../1_scf/yin3.save .
```

7. Run!

```
>> sbatch sub.srm
```

8. Check if the calculation finished properly:

```
>> tail pw.bands.out
….
=-----------------------------------
   JOB DONE.
=————————————————————————————————=
```

Electronic band structure plot.

9. Use your preferred tool to plot the band structure!
   ↳ In our tutorial we will use the **DFTtoolbox** package

https://github.com/pipidog/DFTtoolbox

```
>> python qe_pp_bands.py

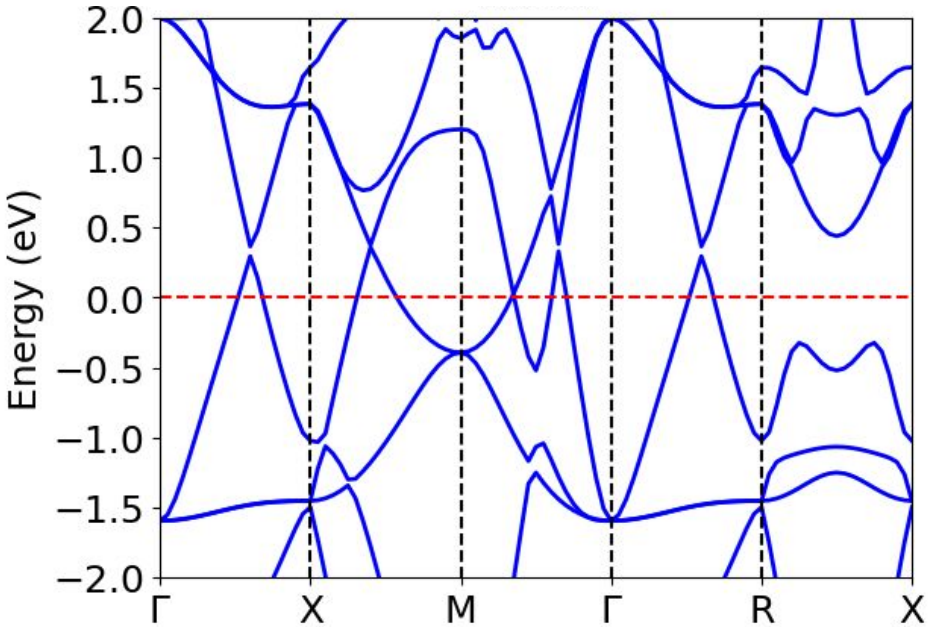
>> ls

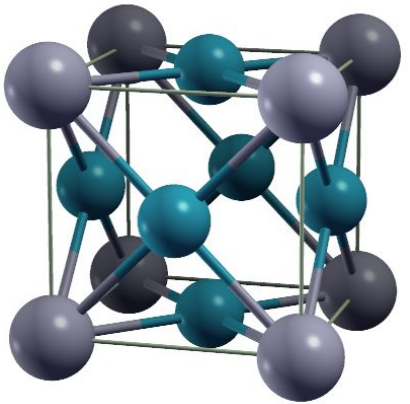
>> band.png  bands.in  pw.bands.out
```

10. To visualize the figure, you need to copy the file to your local machine:
    ↳ Go to another terminal.
    ↳ Type:

```
>> scp your_username@login.sdumont.lncc.br:/scratch/efmc24/your_username/…
…HandsOn/day2/2_bands/band.png .
```

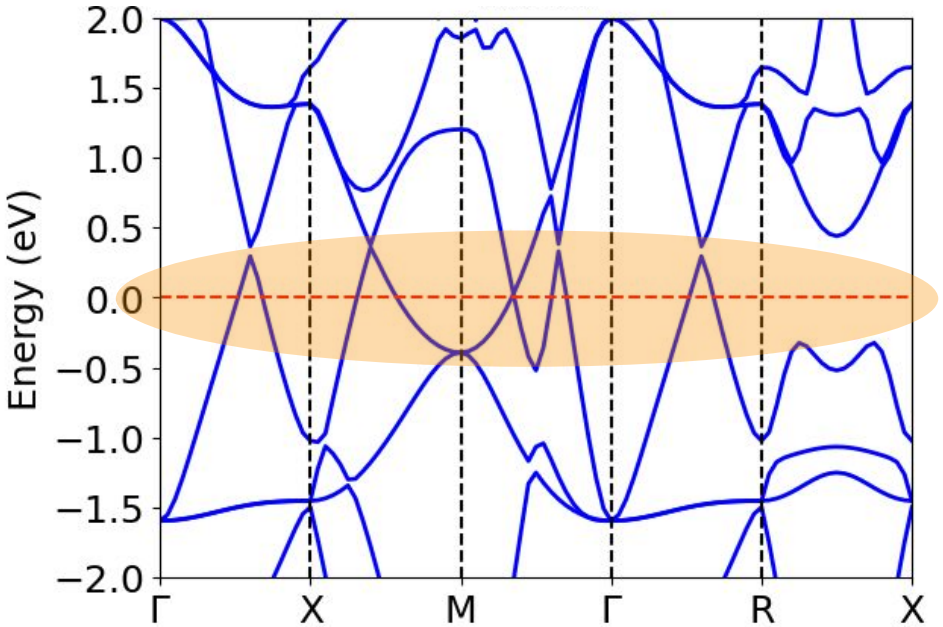
Electronic band structure plot: YIn_3.

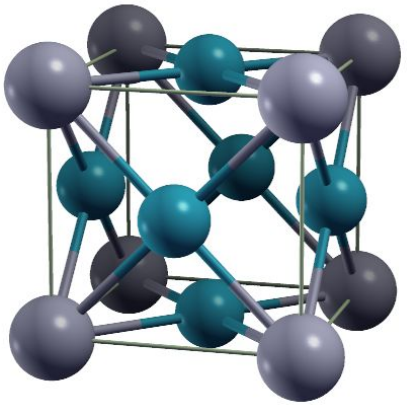




Voilà! You have calculated your first band structure.

Electronic band structure plot: YIn_3.

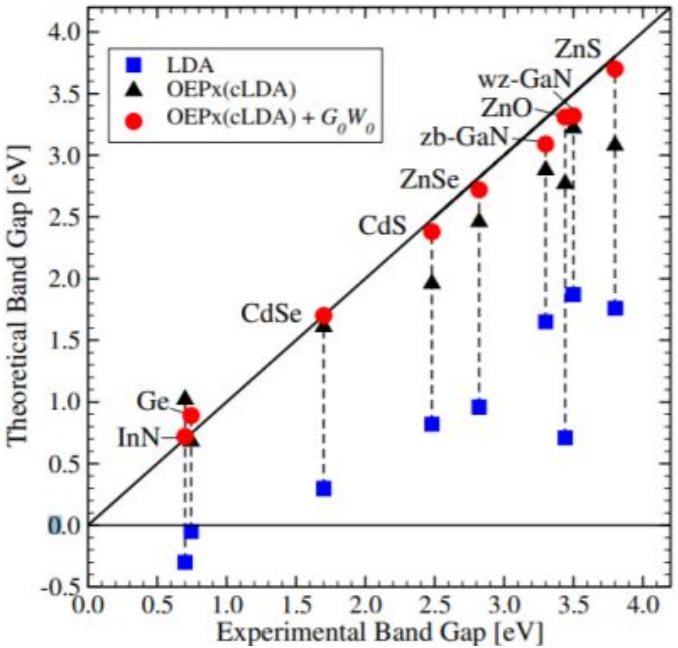




YIn_3 is a metal.

Voilà! You have calculated your first band structure.

DFT: Electronic band structure gap problem.



P. Rinke et al. New J. Phys. 7, 126 (2005), phys. stat. sol. (b) 245, 929 (2008) 2

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2. Calculate Density of States (DOS) of YIn_3:
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DOS calculation: Workflow

Step 0: Structural relaxation:

```
…/pw.x -in vc-relax.in > vc-relax.out
```

Step 1: Generate charge density (scf):

```
…/pw.x -in scf.in > scf.out
```

Step 2: Calculate eigenvalues (nscf):

```
…/pw.x -in pw.nscf.in > pw.nscf.out
```

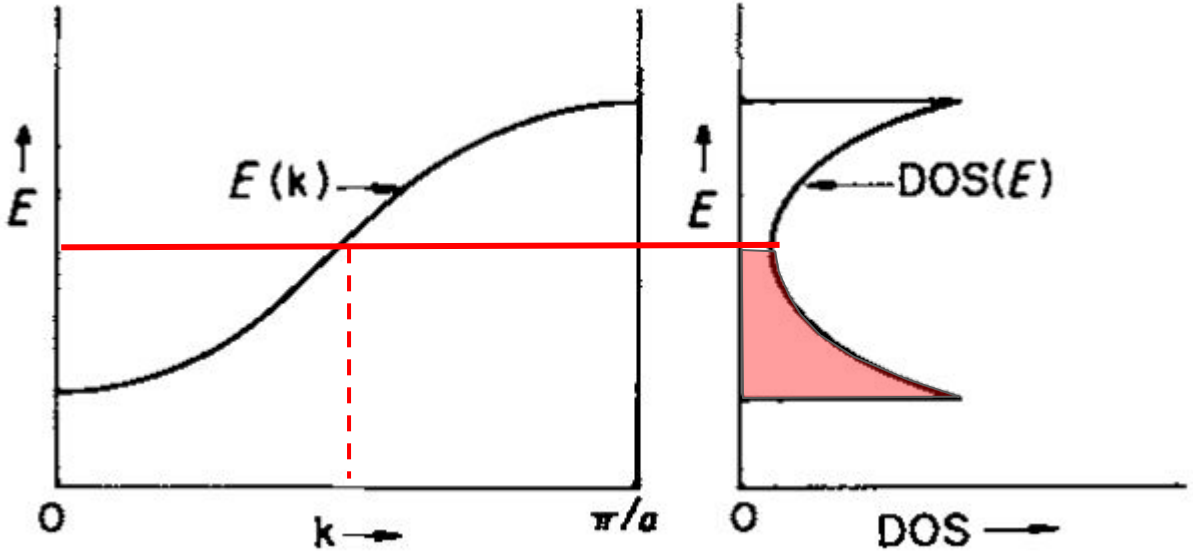
Step 3: Post-processing:

```
…/dos.x -in dos.in > dos.out
```

Step 4: Plot!

Density of States (DOS) calculation.

$\mathrm{DOS}(E)\,dE$ = number of levels between E and $E+dE$



Density of States (DOS) calculation.

1. Go to the working directory:

```
>> cd day2/3_dos
```

2. Have a look at the input file pw.nscf.in.

   ↳ What is different from the previous input files for scf and electronic bands calculations?

```
&CONTROL
  calculation = 'nscf'
  etot_conv_thr =   0.0000000000d-05
  forc_conv_thr =   1.0000000000d-04
  outdir = './'
  verbosity = 'high'

…
/
&SYSTEM
  degauss =   0.02
  ecutwfc =   100
  ibrav = 0
  celldm(1)= 17.4836462409963
  nat = 4
  ntyp = 2
  occupations = 'tetrahedra'
  smearing = 'gauss'
/

…

K_POINTS automatic
20 20 20 0 0 0
```

Density of States (DOS) calculation.

```
 &CONTROL
  calculation = 'nscf'
  etot_conv_thr =   0.0000000000d-05
  forc_conv_thr =   1.0000000000d-04
  outdir = './'
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…
/
&SYSTEM
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  nat = 4
  ntyp = 2
  occupations = 'tetrahedra'
  smearing = 'gauss'
/

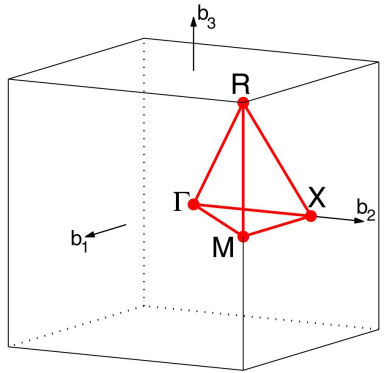
…

K_POINTS automatic
20 20 20 0 0 0
```

calculation = ‘nscf’,

occupations = ‘tetrahedra’,

We need a very dense grid here, to cover the whole BZ.



CUB path: Γ-X-M-Γ-R-X|M-R

Density of States (DOS) calculation.

3. Create a link for the folder with the charge density file generated from the scf calculation:

```
>> ln -s ../1_scf/yin3.save .
```

4. Post-processing: Have a look at the file dos.in.:

```
&dos
    ! prefix must be the same as in the band calculation
    prefix  = 'yin3'
    ! outdir must be the same as in the band calculation
    outdir='./'
    fildos = 'yin3.dat'
    DeltaE = 0.005
 /
```

5. Submit:

```
>> sbatch sub.srm
```

User guides

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

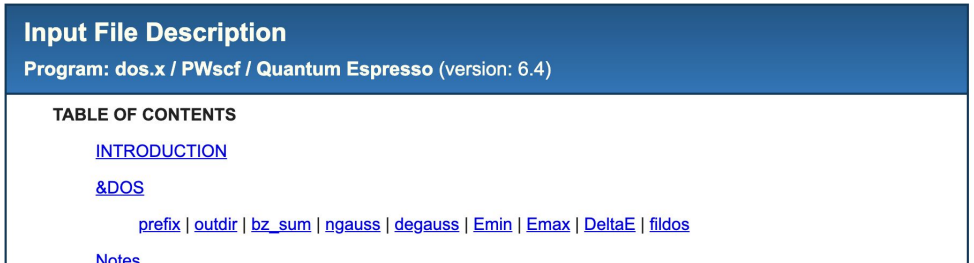
Executables:

pw.x

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

bands.x

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



dos.x

Density of States (DOS) calculation.

6. Have a look at the files:

```
>> ls
>> dos.out yin3_dos.dat
```

`yin3_dos.dat` contains the DOS data.

7. Use your preferred tool to plot the band structure!

   Example: python script **plot_dos.py**:

```
>> python3 qe_plotdos.py
```

Density of States (DOS) calculation.