
MAX School on Advanced Materials and Molecular Modelling
with **QUANTUM ESPRESSO**

QE-2021: Hands-on session – Day-1
(Basic SCF + post-processing calculations)

QE-2021: Hands-on session – Day-1



Topics of Day-1 hands-on session:

1. Installation/compilation of Quantum ESPRESSO ([example0.QE-compilation/](#))
2. How to run basic PWscf (`pw.x`) calculations
3. How to run post-processing calculations to plot molecular-orbitals and charge-density (`pp.x`), DOS (`dos.x`), and band-structure (`bands.x`)
4. How to calculate low-dimensional systems ([example1.benzene/](#) and [example2.graphene/](#))

About Quantum ESPRESSO



More info about Quantum ESPRESSO can be found in:

- <https://www.quantum-espresso.org/>
- Quantum ESPRESSO (QE) documentation:
 - on-line manuals at www.quantum-espresso.org/resources/users-manual
 - [Doc/](#) sub-directories in the QUANTUM ESPRESSO distribution
 - input data description: most programs contained in QE have their own input file description in the form of hyperlinked **INPUT_***.html** files (where *** stands for the name of the program)

Hands-on material

Hands-on material for each day is contained within its own directory:

- `Day-1/` – hands-on exercises for Day-1
- `Day-2/`, `Day-3/` ... `Day-10/` – hands-on exercises for Day-2 to Day-10

Please go to the `Day-1/` directory and execute: `git pull`
this will update the hands-on exercises to the latest version from the GitLab.

- All directories contain a `README.md` file with instructions how to run exercise(s)
- Naming of files is described in `README-filenames.md` (in `Day-1/`).
- To help recognizing for which program a given input file is intended, the filename starts with the name of the program, i.e.:
 - `pw.*.in` – input file for `pw.x` program
 - `pp.*.in` – input file for `pp.x` program
 - etc.

Disclaimer: *many examples use lousy convergence thresholds to speed-up calculations*

0. Compilation of Quantum ESPRESSO



Please go to the `Day-1/` directory, then execute:

```
$ cd example0.QE-compilation/  
$ tar zxvf qe-6.7-ReleasePack.tgz  
$ cd qe-6.7/
```

Now read the `INSTALL.md` file therein. It contains installation (compilation) instructions. In essence, compilation consists of:

```
$ ./configure [options]  
$ make target
```

(remark: `make` alone prints a list of acceptable targets)

Today we will only compile `pw.x` program (for the sake of time constraint), hence:

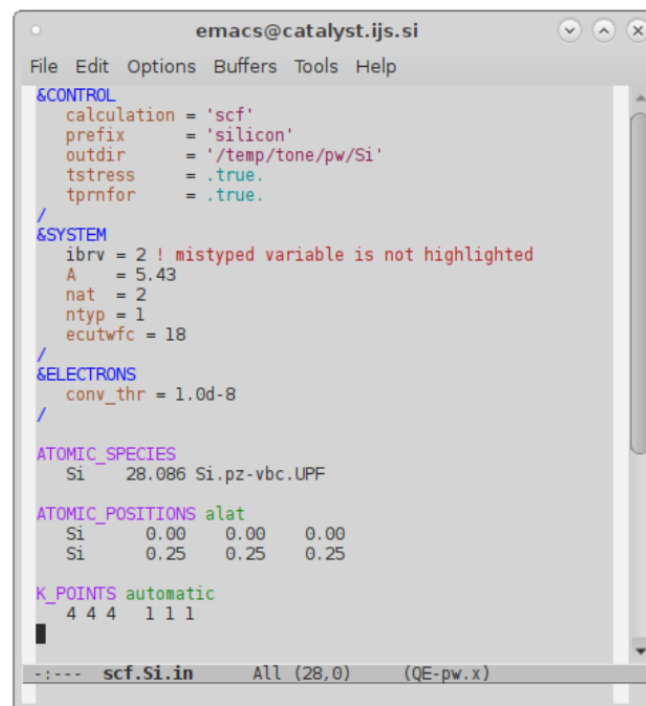
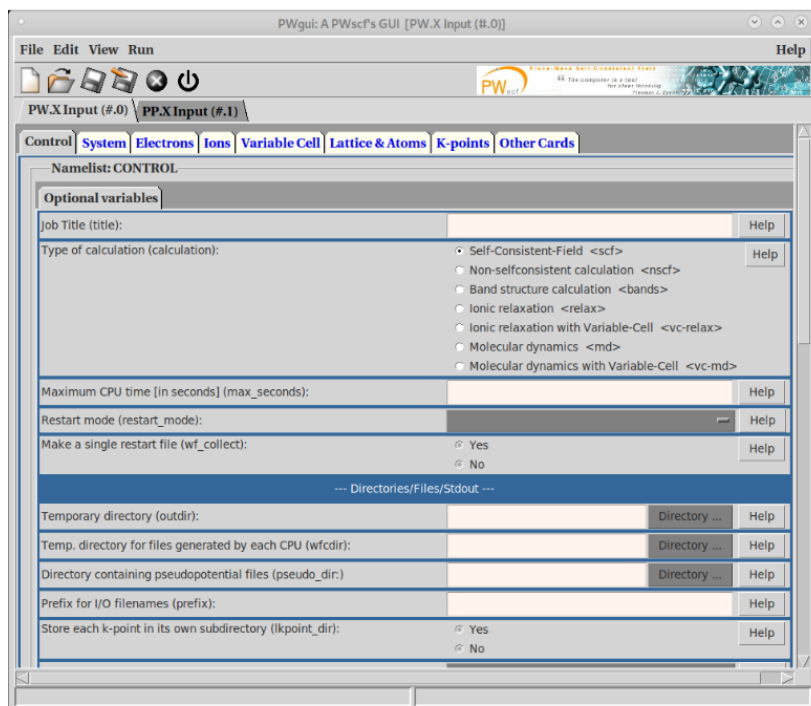
```
$ ./configure  
$ make pw
```

and wait for a while as compilation takes some time. If all went OK, the compiled `pw.x` program (along with some other executables) is now located in `bin/` sub-directory.

Preparation of Quantum ESPRESSO input files

A few tools are available that aid at editing Quantum ESPRESSO input files:

- **PWgui** – a QE input file builder GUI (**pwgui**)
- **QE-emacs-modes** – makes editing of input files easier with **emacs** editor. It provides syntax highlighting, basic auto-indentation, and several utility commands; its manual is available in the QE sub-directory [GUI/QE-modes/Doc/user_guide.pdf](#)



About QE-emacs-modes

QE-emacs-modes package provides syntax highlighting, auto-indentation, and several utility commands, in particular:

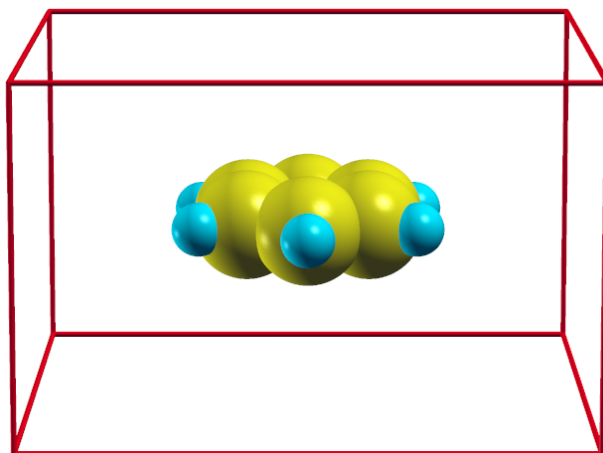
- **Alt-x** *prog-insert-template* – inserts a respective input file template
- **Alt-x** *prog-NAMELIST* – inserts a blank namelist named *NAMELIST*
- **Alt-x** *prog-CARD* – inserts a blank namelist named *CARD*
- **Alt-x** *prog-variable* – inserts a namelist variable named *variable*
- **Alt-x** *prog-mode* – toggles the respective mode
- **Alt-x** *indent-region* – indents region

where

- *prog* is one of *qe*, *pw*, *neb*, *cp*, *ph*, *ld1*, or *pp* (these stands for *pw.x*, *neb.x*, ... Quantum ESPRESSO (QE) programs)
- *NAMELIST* is the uppercase name for a given QE namelist
- *CARD* is the uppercase name for a given QE card
- *variable* is the lowercase name for a given namelist variable

1. How to describe a molecule with Quantum ESPRESSO

With Quantum ESPRESSO we can describe a molecule by putting it in a big box.

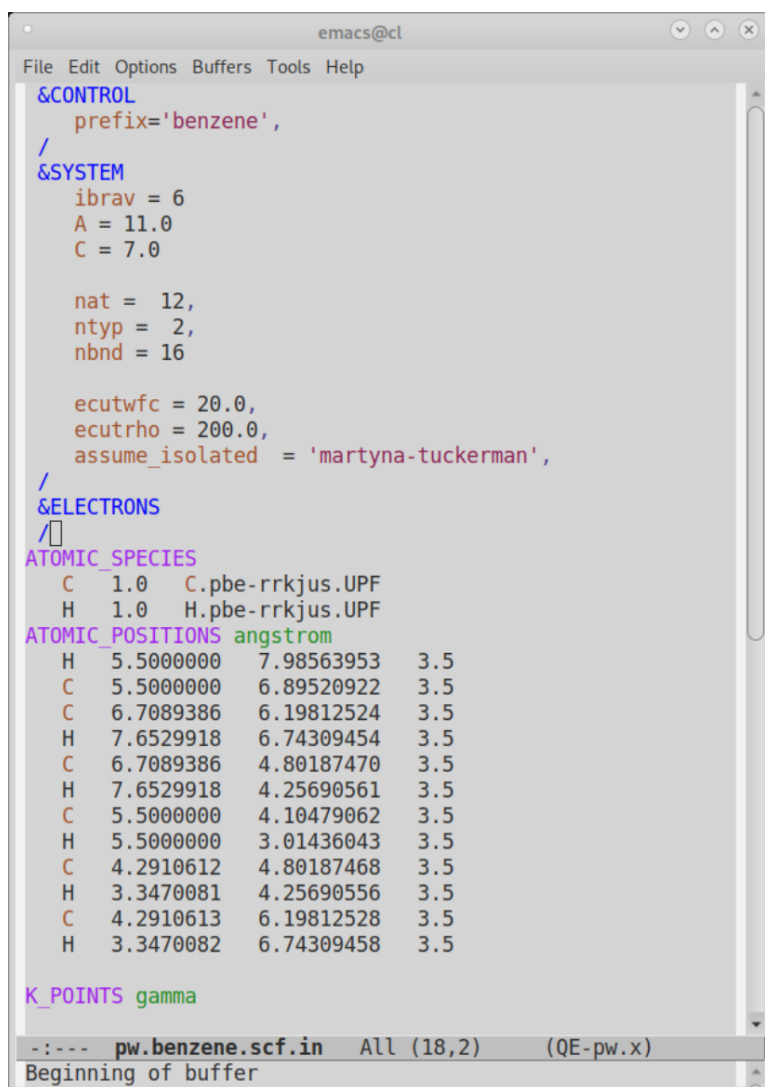


- move to `Day-1/example1.benzene/` directory
- look at the input file `pw.benzene.scf.in`. It is composed of three “namelists” `&CONTROL` (note that `calculation = 'scf'` is the default value), `&SYSTEM`, `&ELECTRONS`, followed by three “cards” `ATOMIC_SPECIES`, `ATOMIC_POSITIONS`, `K_POINTS`
- instructions for how to run the example are in `README.md`

Disclaimer: *the box used in this example is very small as to speed-up calculations*

1. How to calculate and plot molecular orbitals

Here are the two needed input files for calculation of signed molecular-orbital densities of benzene (i.e., $\text{sign}(\psi_i(\mathbf{r}))|\psi_i(\mathbf{r})|^2$), opened with **emacs** using **QE-emacs-modes**:



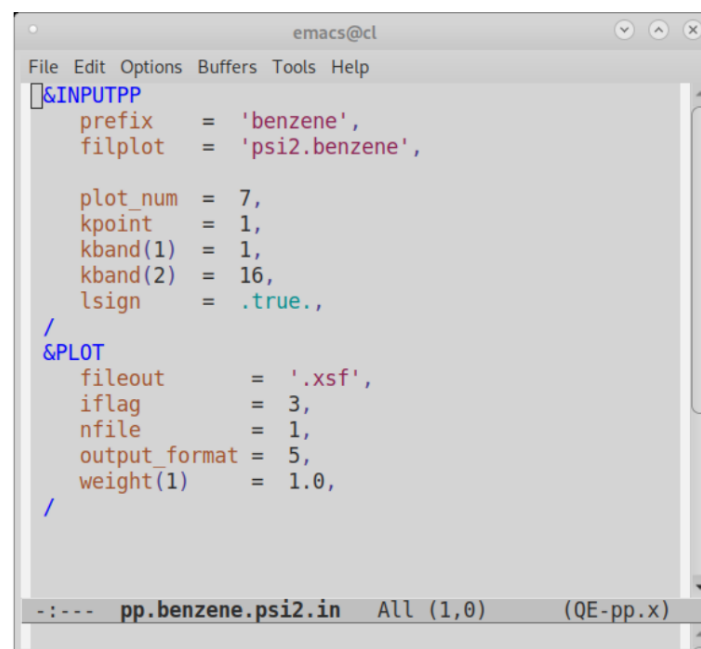
```
emacs@cl
File Edit Options Buffers Tools Help
&CONTROL
  prefix='benzene',
/
&SYSTEM
 ibrav = 6
  A = 11.0
  C = 7.0

  nat = 12,
  ntyp = 2,
  nbnd = 16

  ecutwfc = 20.0,
  ecutrho = 200.0,
  assume_isolated = 'martyna-tuckerman',
/
&ELECTRONS
/
ATOMIC_SPECIES
C 1.0 C.pbe-rrkjus.UPF
H 1.0 H.pbe-rrkjus.UPF
ATOMIC_POSITIONS angstrom
H 5.5000000 7.98563953 3.5
C 5.5000000 6.89520922 3.5
C 6.7089386 6.19812524 3.5
H 7.6529918 6.74309454 3.5
C 6.7089386 4.80187470 3.5
H 7.6529918 4.25690561 3.5
C 5.5000000 4.10479062 3.5
H 5.5000000 3.01436043 3.5
C 4.2910612 4.80187468 3.5
H 3.3470081 4.25690556 3.5
C 4.2910613 6.19812528 3.5
H 3.3470082 6.74309458 3.5

K_POINTS gamma

-:--- pw.benzene.scf.in All (18,2) (QE-pw.x)
Beginning of buffer
```



```
emacs@cl
File Edit Options Buffers Tools Help
&INPUTPP
  prefix = 'benzene',
  filplot = 'psi2.benzene',

  plot_num = 7,
  kpoint = 1,
  kband(1) = 1,
  kband(2) = 16,
  lsign = .true.,
/
&PLOT
  fileout = '.xsf',
  iflag = 3,
  nfile = 1,
  output_format = 5,
  weight(1) = 1.0,
/

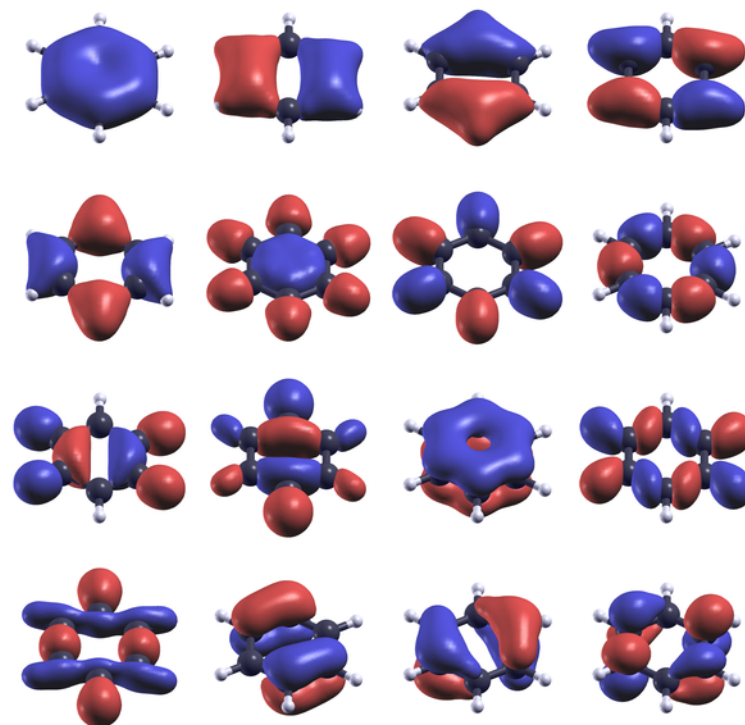
-:--- pp.benzene.psi2.in All (1,0) (QE-pp.x)
```

1. How to calculate and plot molecular orbitals

To plot signed molecular-orbital densities ($\text{sign}(\psi_i(\mathbf{r}))|\psi_i(\mathbf{r})|^2$), we need to:

- calculate Kohn-Sham states with `pw.x` (i.e. make an SCF calculation)
- instruct `pp.x` to write them in a suitable format to specified files
- plot orbitals with `xcrysden`

See [README.md](#) for detailed instructions.



1. How to plot molecular orbitals with xcrysden

- Execute in the terminal:

```
$ pw.x < pw.benzene.scf.in > pw.benzene.scf.out
```

```
$ pp.x < pp.benzene.scf.in > pp.benzene.scf.out
```

The resulting molecular orbitals (i.e., $\text{sign}(\psi(\mathbf{r}))|\psi(\mathbf{r})|^2$) are written to `psi2.benzene_*.xsf`

- Plot one of the generated XSF files with `xcrysden`, e.g.:

```
$ xcrysden --xsf psi2.benzene_K001_B006.xsf
```

and follow these instructions:

- use the menu `Tools-->Data Grid`; a new window opens, press [OK]
- an isosurface-control window appear; specify the `Isovalue`, say 0.005 and press [Submit]
- click the `Render +/- isovalue` radiobutton and again press [Submit]
- rotate and zoom the structure according to your preference
- save the displayed *state* via the menu `File-->Save Current State` (e.g., save to `my-display.xcrysden`)
- try this with other orbitals, e.g.:

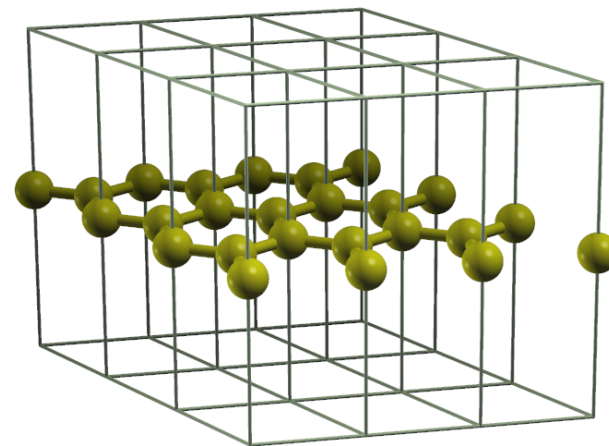
```
$ xcrysden --xsf psi2.benzene_K001_B005.xsf --script my-display.xcrysden
```

- To plot all orbitals, execute: `./plot-psi2.sh`

2. How to calculate a 2D-periodic system: graphene

A 2D-periodic system (e.g., a graphene sheet) is modelled by adding a vacuum layer in the 3rd direction.

- move to `Day-1/example2.graphene/` directory
- look at the input file `pw.graphene.scf.in`; graphene has a 2-atom hexagonal unit cell in the xy plane:
`ibrav=4`, `celldm(1)=4.654`,
`celldm(3)=some suitably large value, e.g. 3.0`;



(remember: `celldm(1)` in Bohr radii, `celldm(3)=c/a`; alternatively: $A=2.463$, $C=7.388$ in Å)

- atomic positions:

ATOMIC_POSITIONS (alat)

```
C 0.000000 0.000000 0.000000
C 0.000000 0.5773503 0.000000
```

or, equivalently:

ATOMIC_POSITIONS (crystal)

```
C 0.000000 0.000000 0.000000
C 0.333333 0.666667 0.000000
```

- k-points: use a dense grid in the xy plane only, e.g.

K_POINTS (automatic)

```
9 9 1 0 0 0
```

(a uniform $9 \times 9 \times 1$ grid, centered on $\mathbf{k} = (0, 0, 0)$)

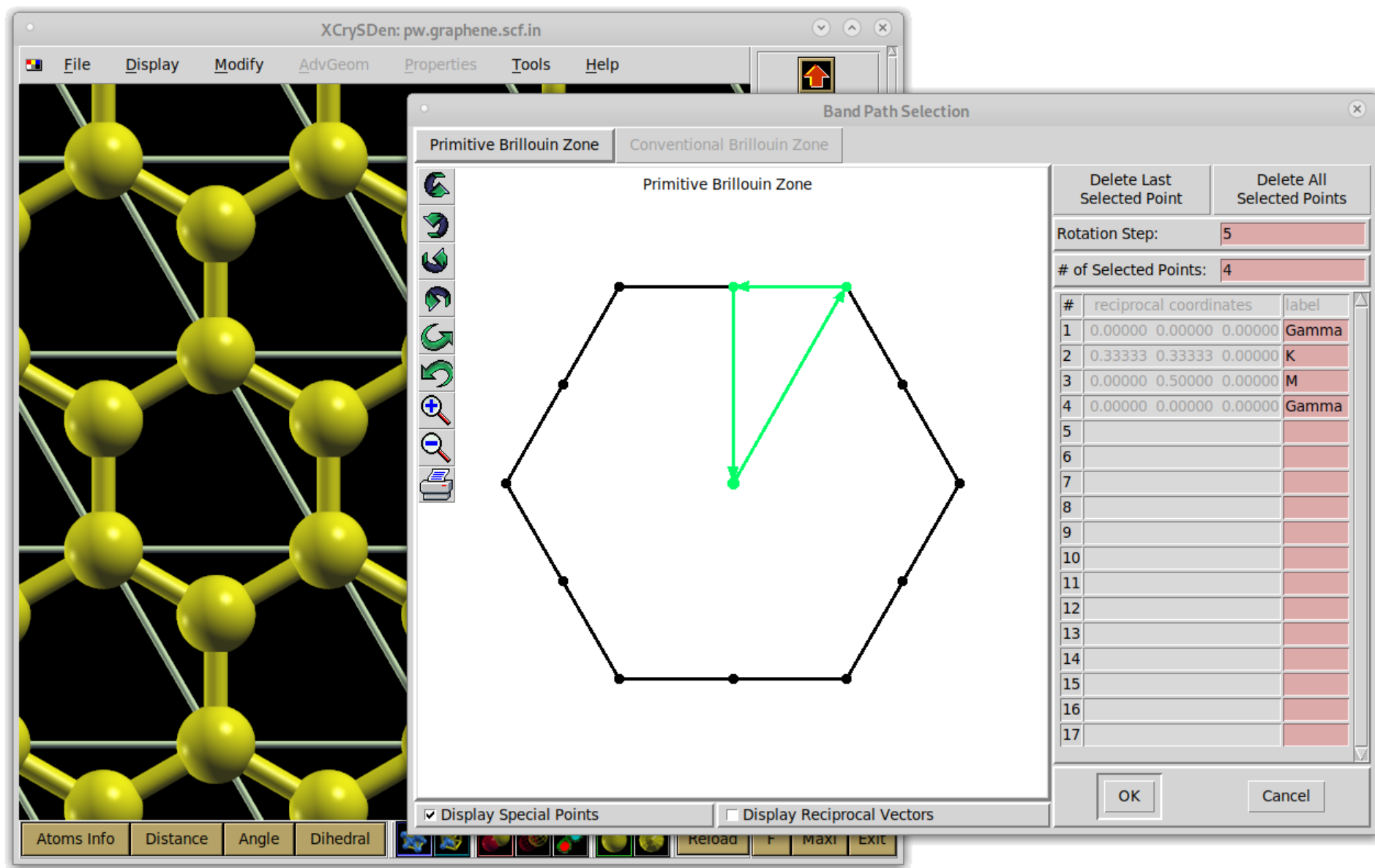
2. Graphene: DOS and bands (spaghetti)

- DOS is typically calculated by a `pw.x` SCF calculation followed by a `pw.x` non-SCF calculation (`calculation = 'nscf'`) with a denser k-point grid, and finally using `dos.x` post-processing code.
- to calculate the bands (spaghetti plot), the `pw.x` SCF calculation is followed by a `pw.x` “bands”-type non-SCF calculation (`calculation = 'bands'`), for which we need a suitable path of k-points. The most difficult (?) part is to figure out a suitable path of k-points.

You may either use the “k-path selection” tool of `xcrysden` or the `SeeK-path` web site at <http://materialscloud.org/tools/seekpath>.

- instructions for how to calculate DOS and bands are in `README.md`

K-path selection tool of xcrysden



(important: to save k-path in Quantum ESPRESSO format, explicitly specify the *.pwscf extension)

SeeK-path @ <http://materialscloud.org/tools/seekpath>

