QUANTUM ESPRESSO FOUNDATION

QUANTUMESPRESSO

MaX School on Advanced Materials and Molecular Modelling
with QUANTUM ESPRESSO

QE-2021: Hands-on session – Day-1

MAX

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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:

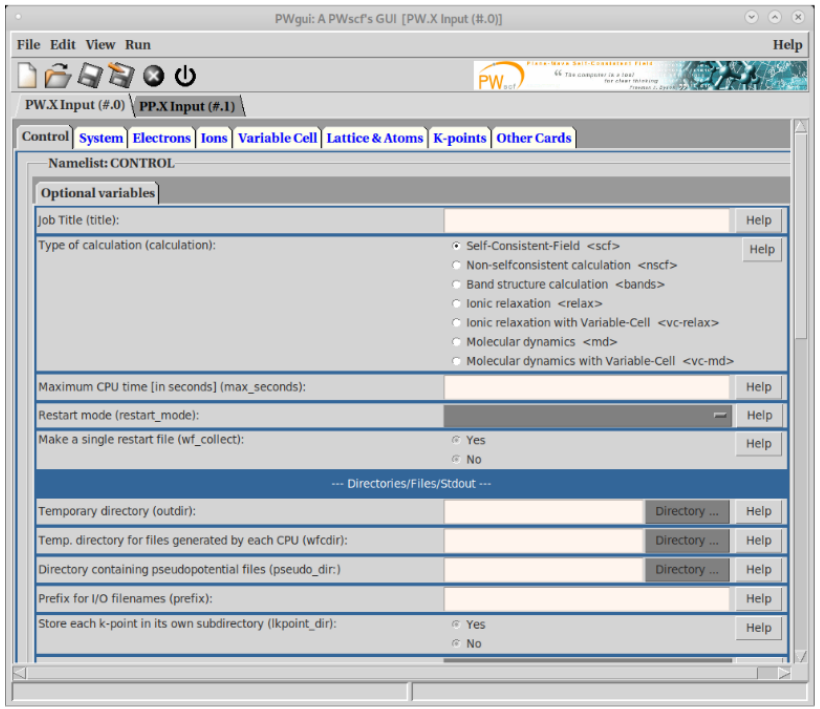
```
$ ./configure
$ make pw
```

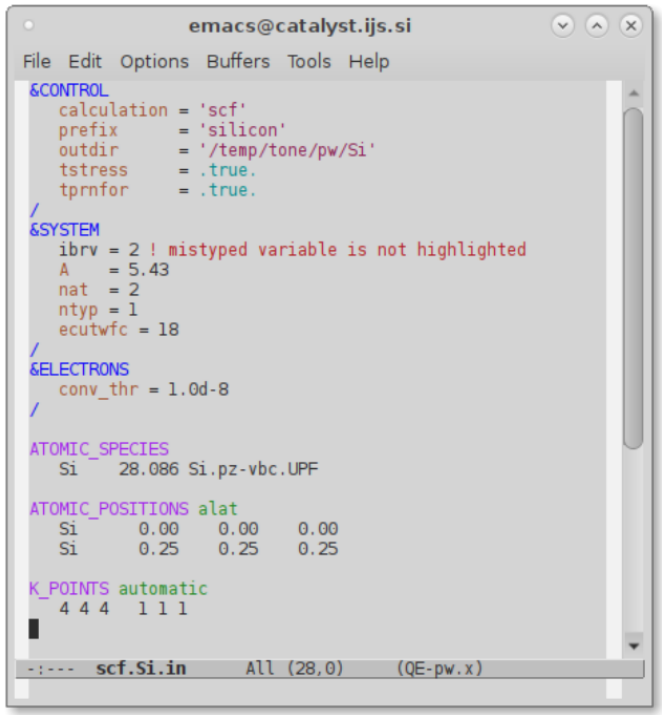
... and wait for a while as compilation takes some time. If all went OK, the compiled `pw.x` program (along with some other executables) is now located in `bin/` directory.

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:

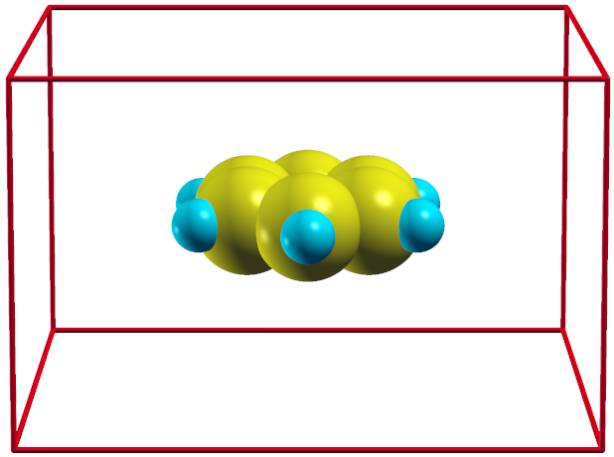
- Alt-x *prog*-insert-template – inserts a respective input file template
- Alt-x *prog*-*NAMELIST* – inserts a blank namelist named *NAMELIST*
- Alt-x *prog*-*CARD* – inserts a blank namelist named *CARD*
- Alt-x *prog*-*variable* – inserts a namelist variable named *variable*
- Alt-x *prog*-mode – 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 molecular orbitals of benzene (actually, $\mathrm{sign}(\psi(\boldsymbol{r}))|\psi(\boldsymbol{r})|^2$), 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,
 /
```

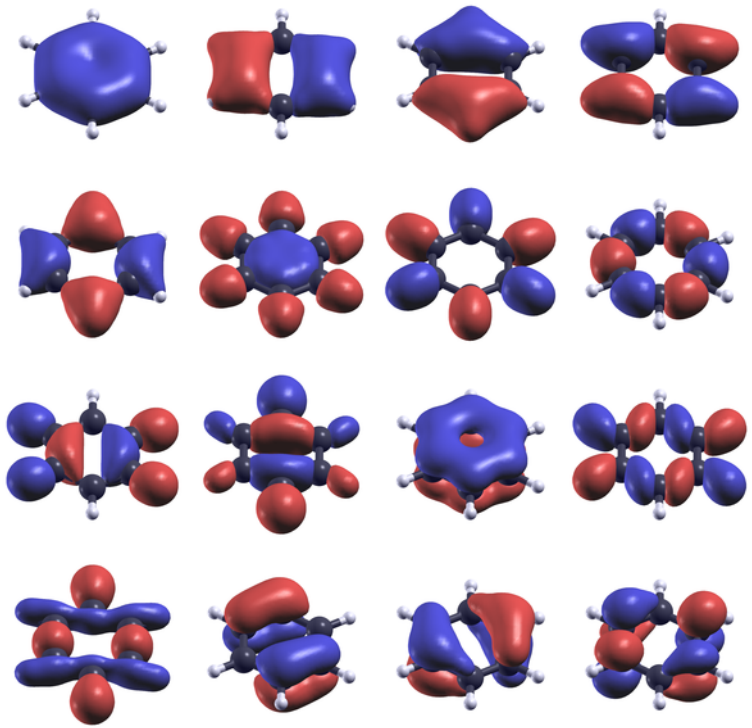
-:--- **pp.benzene.psi2.in** All (1,0) (QE-pp.x)

1. How to calculate and plot molecular orbitals

To plot molecular orbitals (actually the signed square modulus, $\mathrm{sign}(\psi(\boldsymbol{r}))|\psi(\boldsymbol{r})|^2$), 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., $\mathrm{sign}(\psi(\boldsymbol{r}))|\psi(\boldsymbol{r})|^2$) are written to `psi2.benzene_*.xsf`

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

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

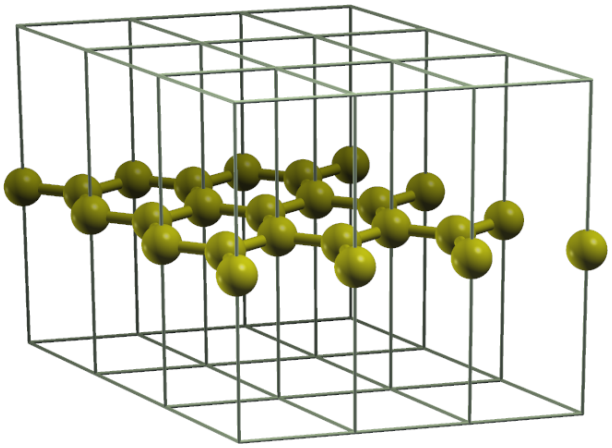
  and follow these instructions:
  - use the menu `Tools-->Data Grid`; a new window opens, press `[OK]`
  - an isosurface-control window appear; specify the `Isovalue`, say `0.005` and press `[Submit]`
  - click the `Render +/- isovalue` radiobutton and again press `[Submit]`
  - rotate and zoom the structure 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 9×9×1 grid, centered on $\mathbf{k} = (0, 0, 0)$)

2. Graphene: DOS and bands (spaghetti)

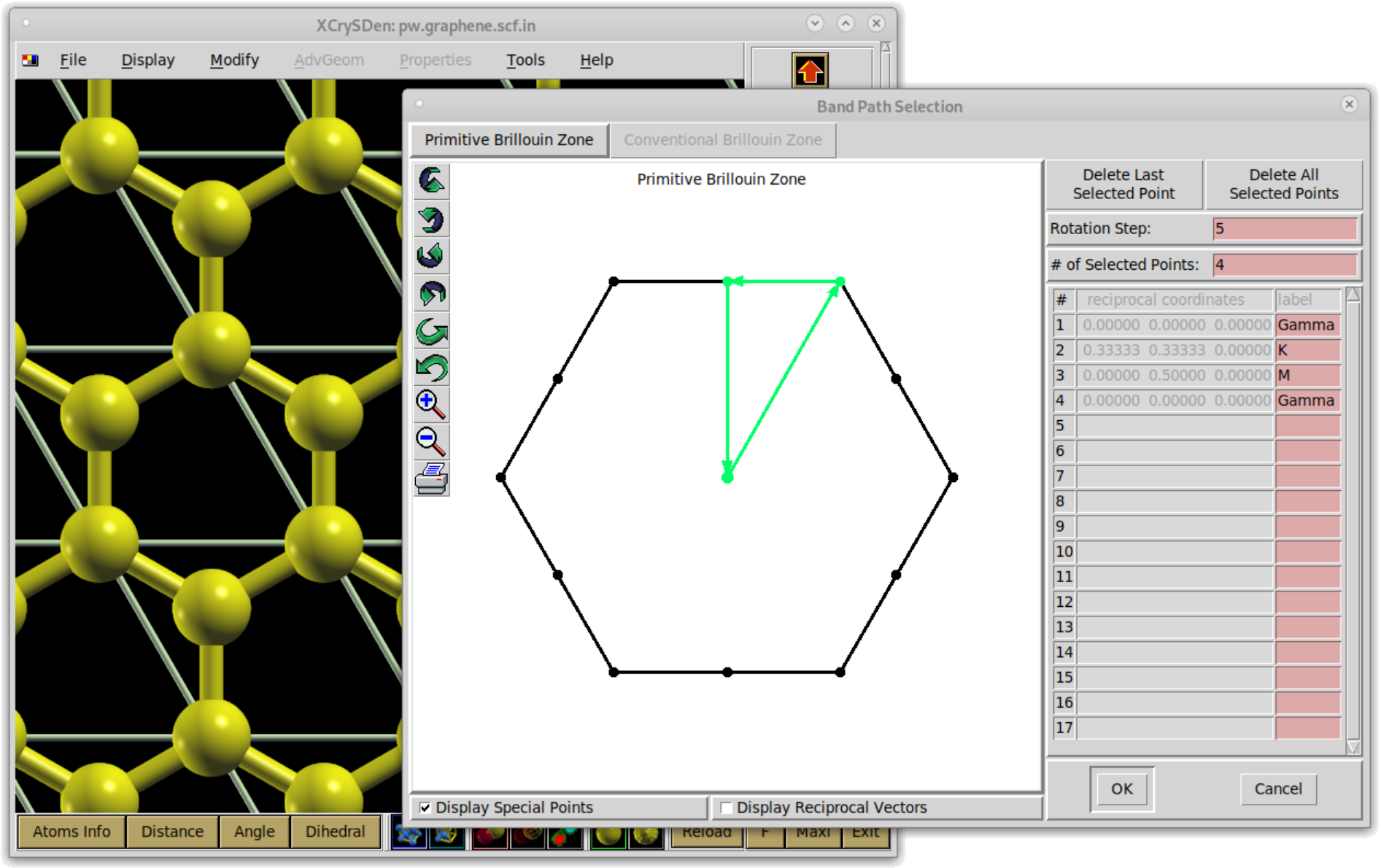
- DOS is typically calculated by a `pw.x` SCF calculation followed by a `pw.x` non-SCF calculation (`calculation = 'nscf'`) with a denser k-point grid, and finally using `dos.x` post-processing code.

- 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