PART 6

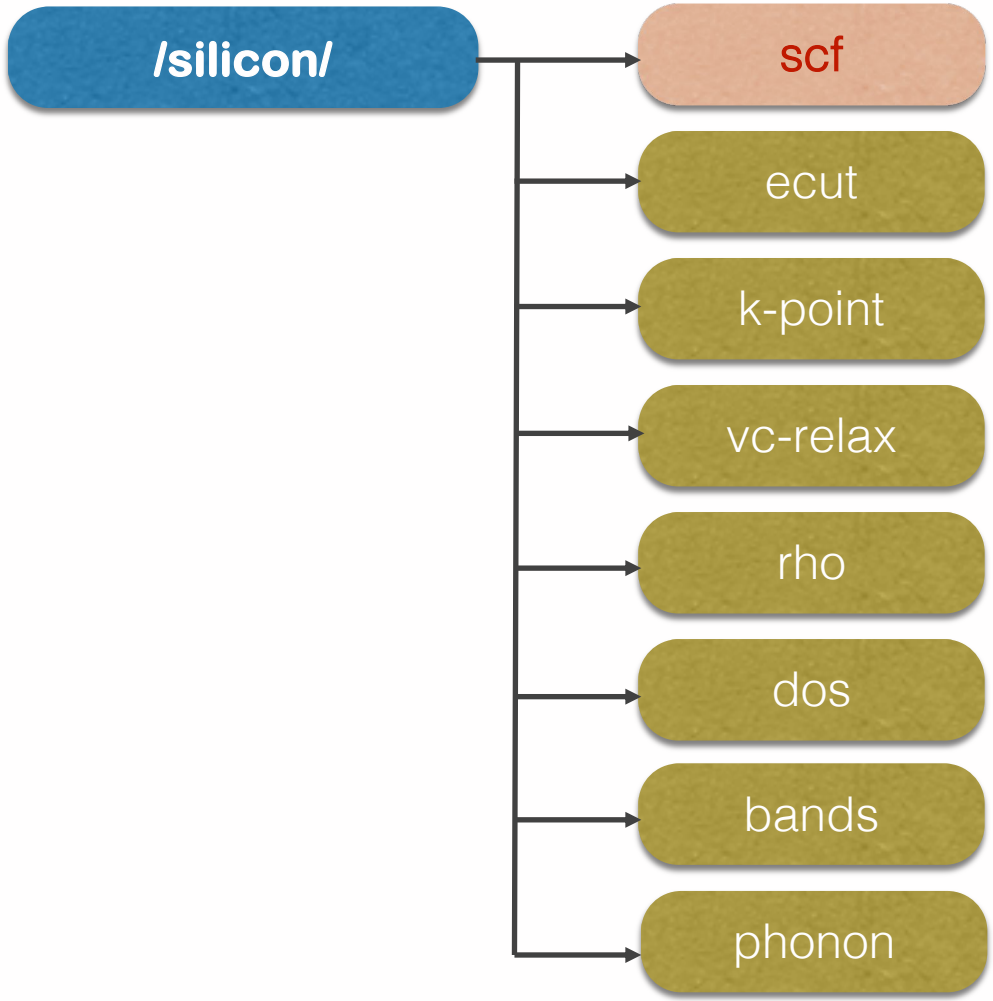
MATERIAL DESIGN

QUANTUM ESPRESSO CONVERGENCY

HANDS-ON #1

SCF

Files for self consistent calculation



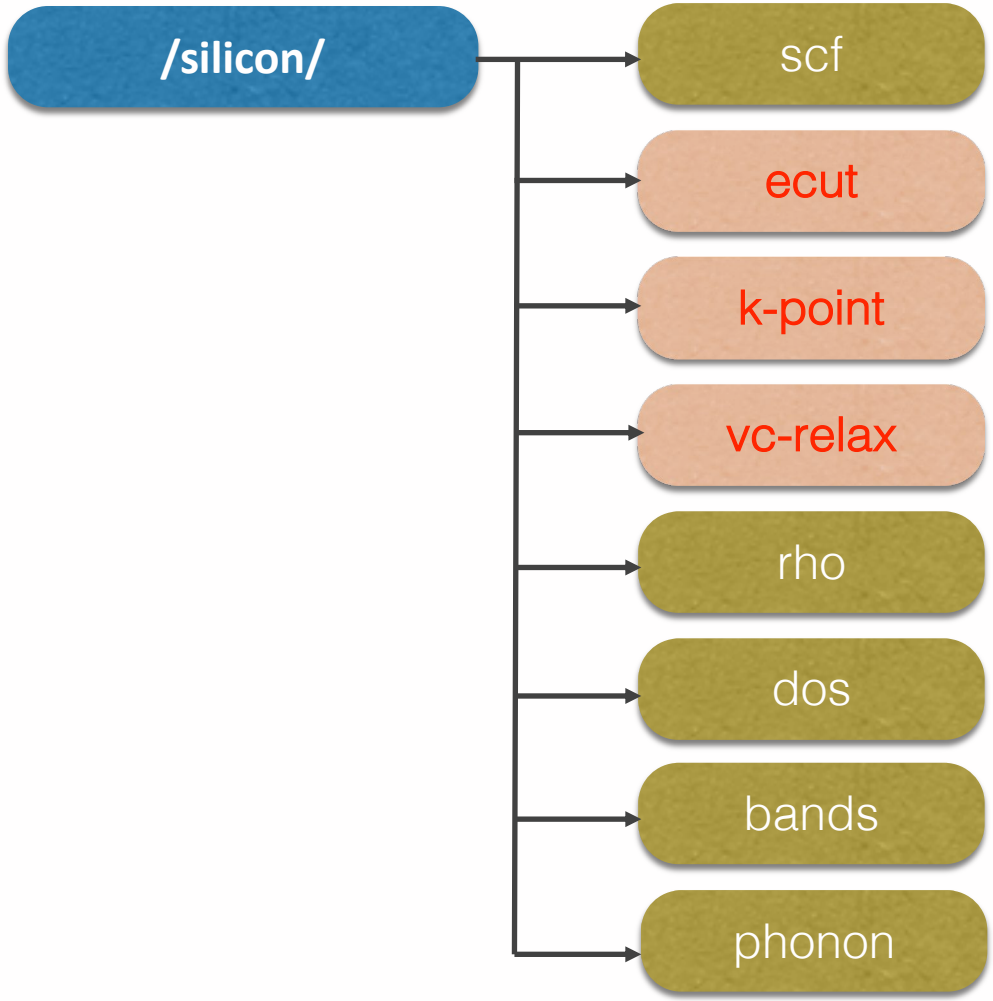
- Basic self consistent calculation (**scf**)

Command:

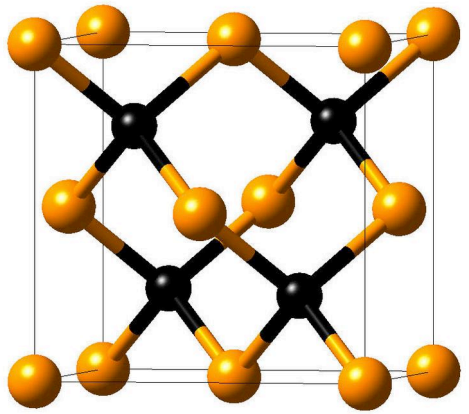
```
$ pw.x <Si.scf.in> Si.scf.out
```

```
     highest occupied level (ev):     5.9399

!    total energy              =     -15.74122935 Ry
     Harris-Foulkes estimate   =     -15.74122935 Ry
     estimated scf accuracy    <          8.8E-09 Ry

     The total energy is the sum of the following terms:

     Parallel routines
     fft_scatter  :      0.16s CPU      0.24s WALL (    2061 calls)

     PWSCF        :     1.96s CPU         4.47s WALL


   This run was terminated on:  19: 3:24  14Feb2016

=------------------------------------------------------------------------------=
   JOB DONE.
=------------------------------------------------------------------------------=
```

Hands-on #1 Total energy & Relaxation for Silicon



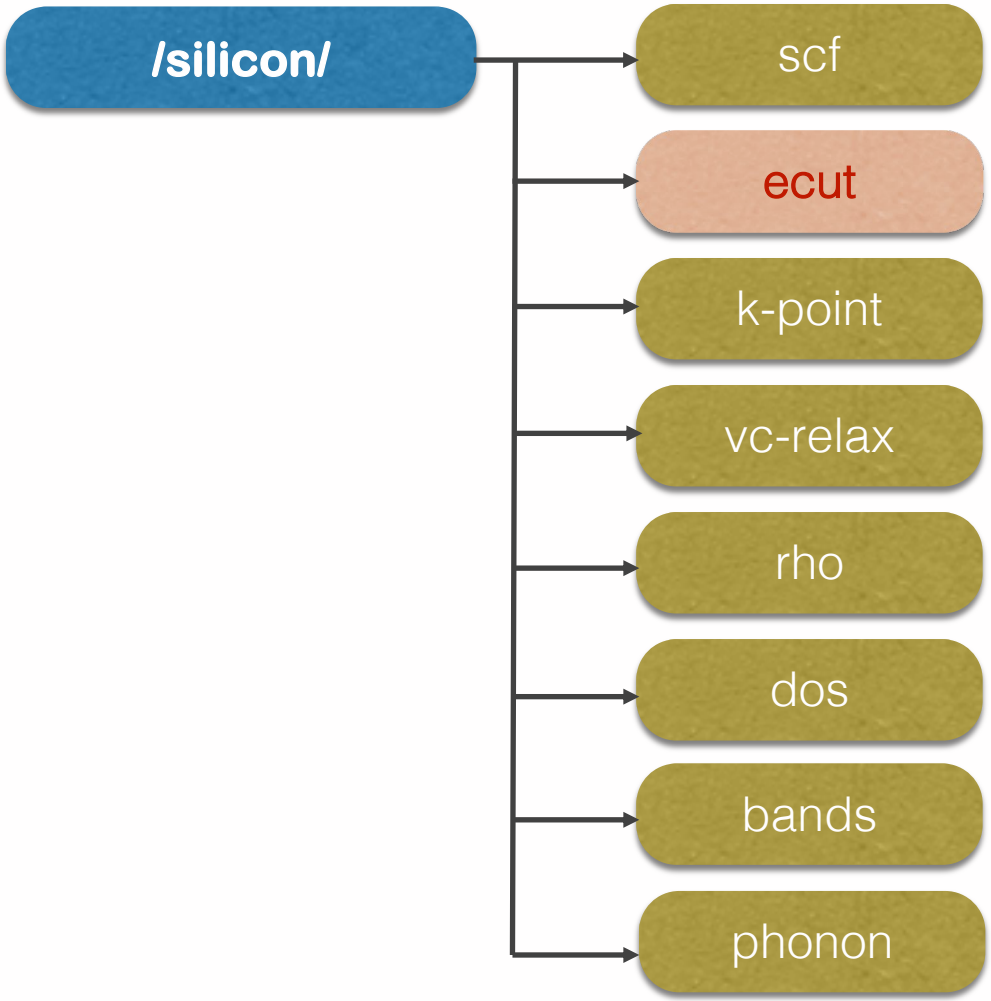
- Basic self consistent calculation (**scf**)
- Convergence of total energy & plane waves cut-off (**ecut**)
- Convergence of total energy & BZ sampling (**k-point**)
- Lattice constant (**vc-relax**)



Silicon

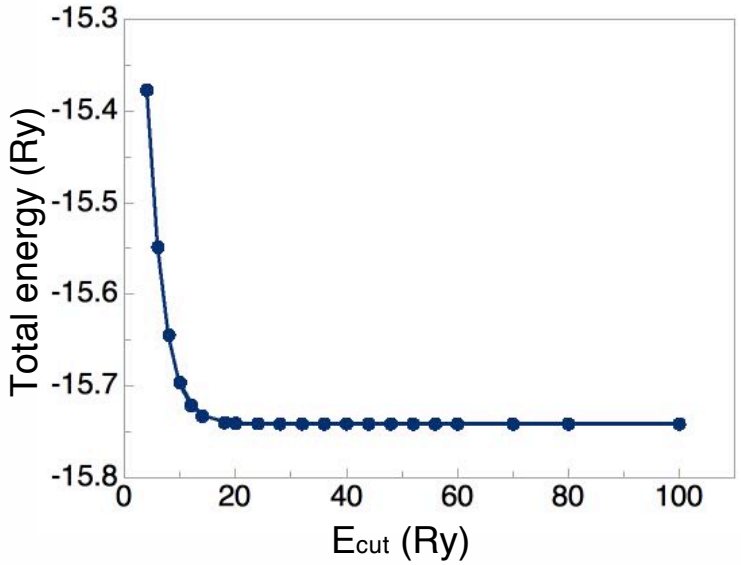
ECUT

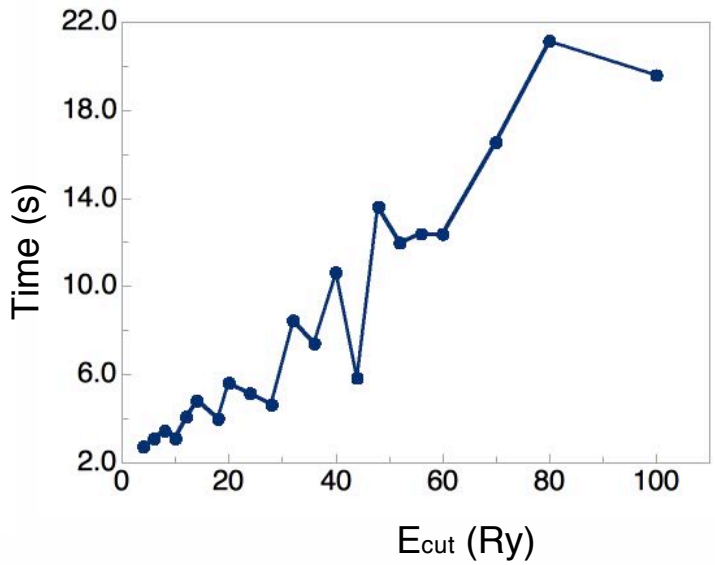
Files for cutoff energy



- Convergence of total energy & plane waves cutoff (**ecut**)

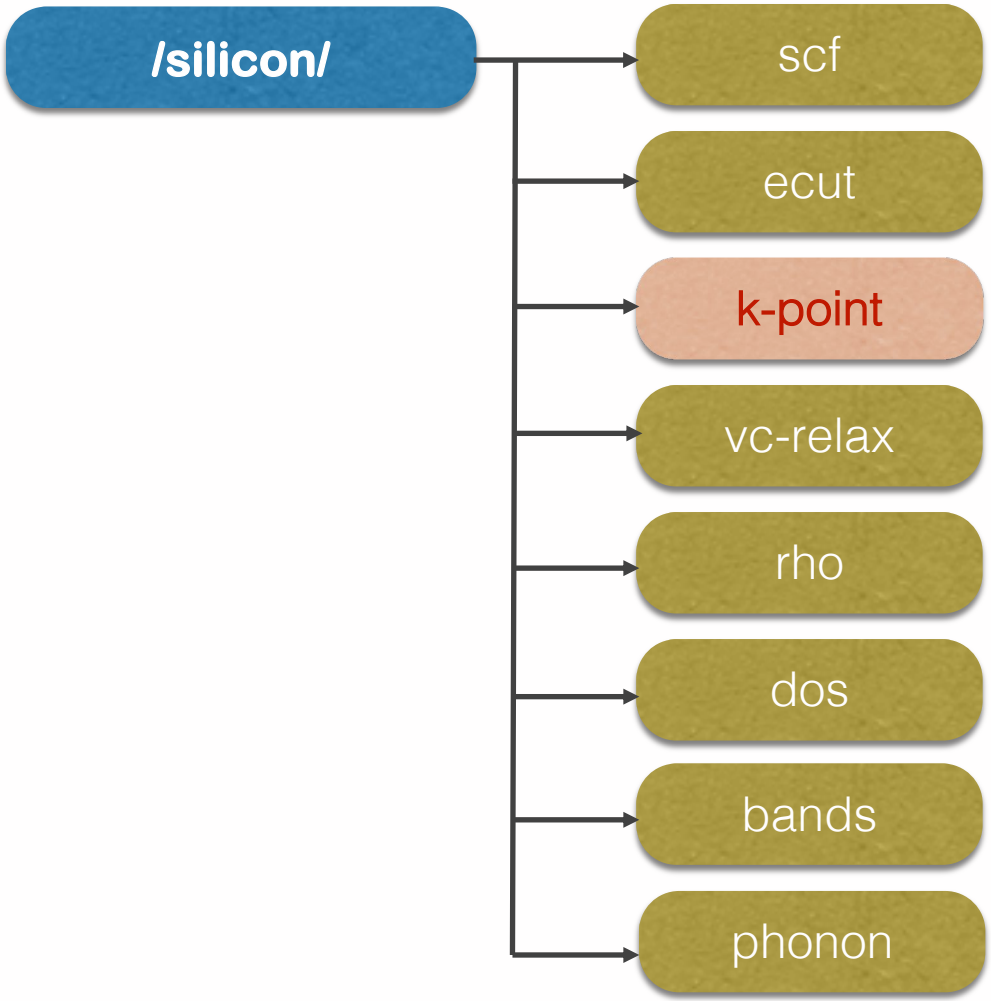
```
Command:
$ pw.x <Si.ecut.#.in> Si.ecut.#.out
```





K-POINT

Files for k-point sampling



- Convergence of total energy & BZ sampling (**k-point**)

```
Command:
$ pw.x <Si.k-point.#.in> Si.k-point.#.out
```