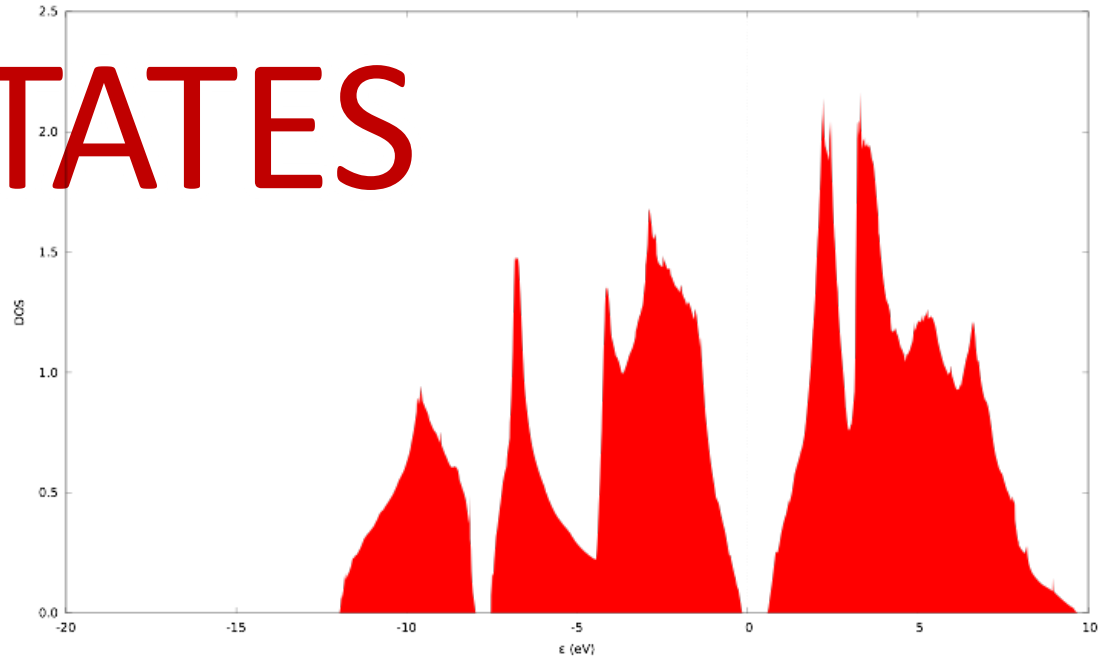
PART 9

MATERIAL DESIGN

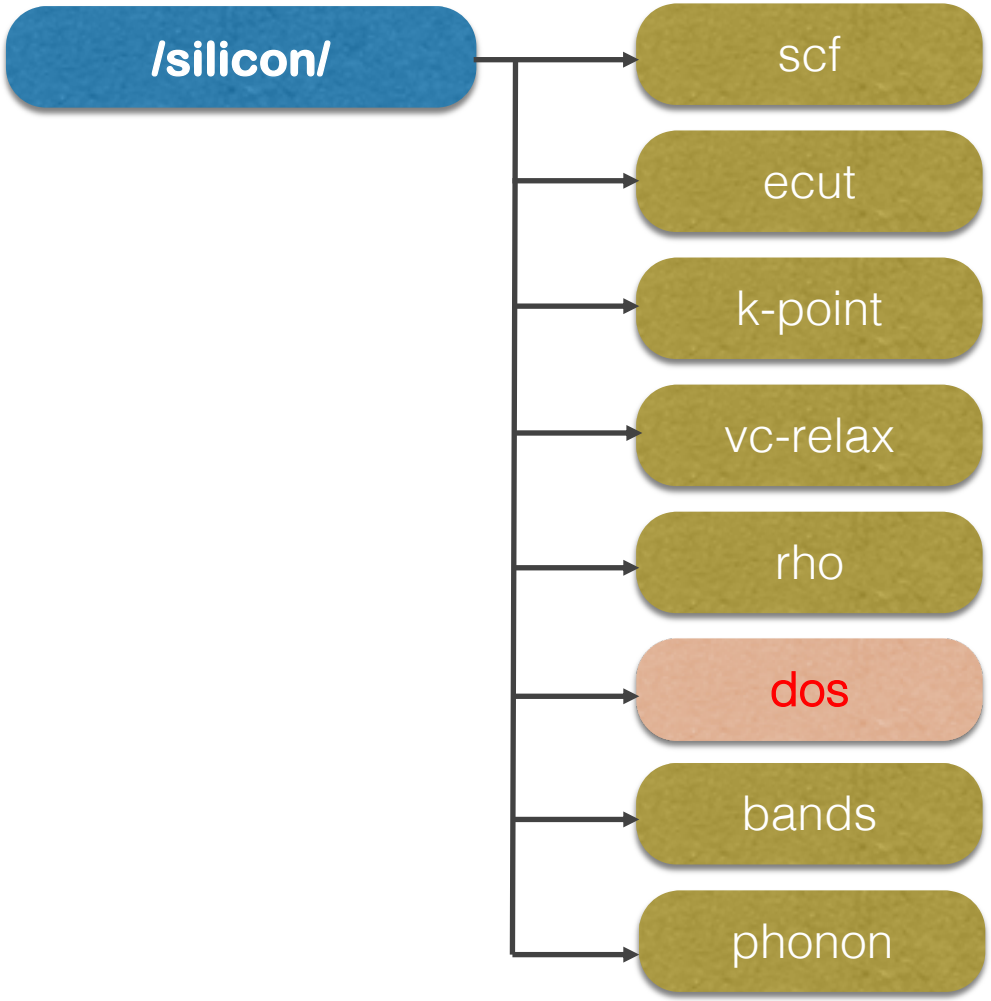
QUANTUM ESPRESSO DENSITY OF STATES

HANDS-ON #2



Density of states (DOS)

Files for density of states



Step 1: SCF calculation (Hands-on #1)
Step 2: Non-SCF calculation
Step 3: Plot DOS

Command:

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

Density of states (DOS)

Si.nscf.in

```
&CONTROL
 calculation='nscf',
 verbosity = 'high',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
 nbnd=8,
 occupations='tetrahedra',
/
&ELECTRONS
 mixing_beta=0.7,
 conv_thr=1d-8,
/
ATOMIC_SPECIES
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si  0.00  0.00  0.00
Si  0.25  0.25  0.25
K_POINTS automatic
12 12 12 1 1 1
```

non-SCF calculation

Linear tetrahedron method

High density k-point

Step 1: SCF calculation (Hands-on #1)
Step 2: Non-SCF calculation
Step 3: Plot DOS

Command:

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

Density of states (DOS)

Step 1: SCF calculation (Hands-on #1)
Step 2: Non-SCF calculation
Step 3: Plot DOS

Si.dos.in

```
&DOS
  prefix='si',
  outdir='../tmp/',
  fildos='si.dos'
  emin=-9.0,
  emax=16.0,
/
```

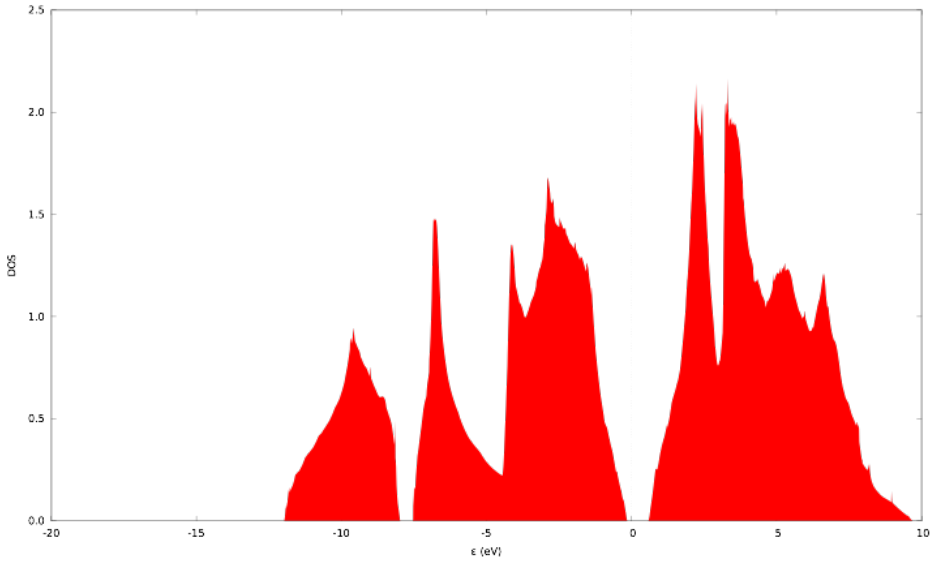
→ Data file of DOS (state/eV)

Command:

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

Command:

```
$ gnuplot < si_dos.gnu
```



Projected Density of States (PDOS)

Step 1: SCF calculation (Hands-on #1)
Step 2: Non-SCF calculation
Step 3: Plot PDOS

Si.projwfc.in

```
&projwfc
  prefix='si',
  outdir='../tmp/',
  degauss = 0.01,
/
```

Command:

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

Command:

```
$ gnuplot < si_pdos.gnu
```