PART 10

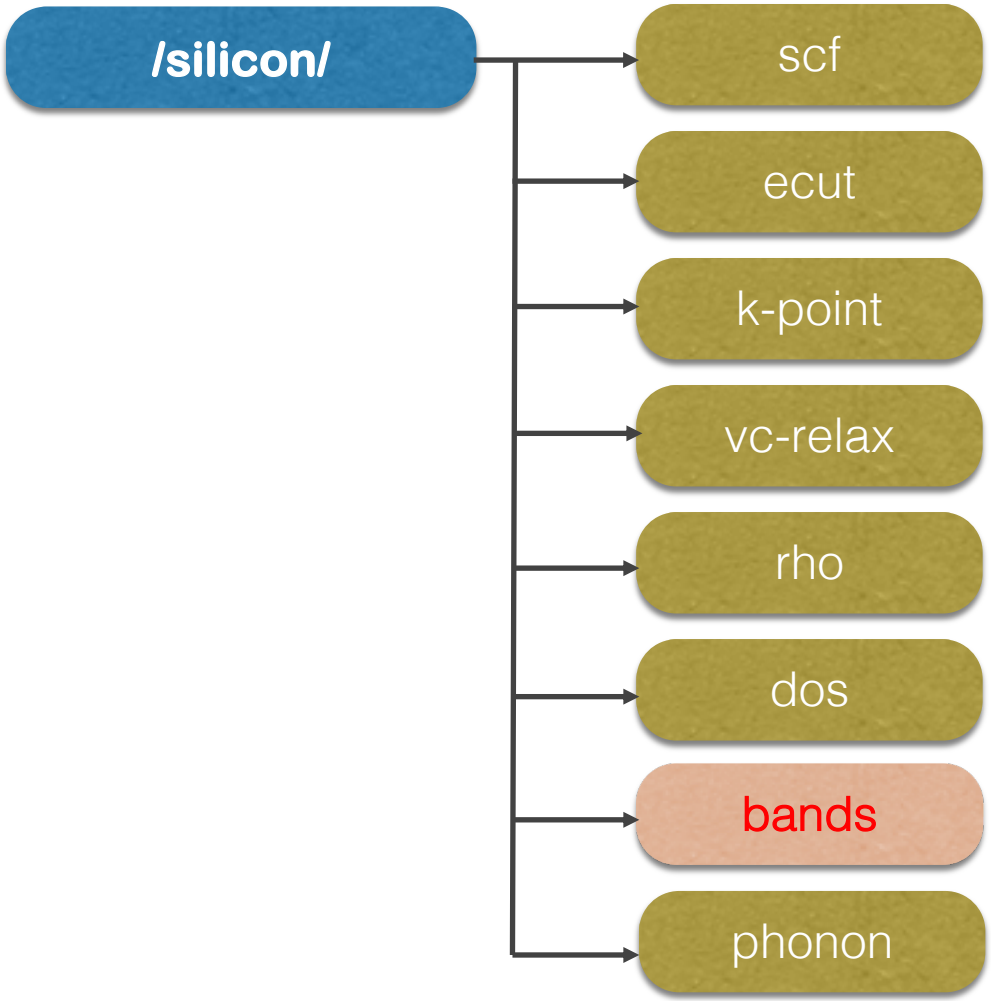
MATERIAL DESIGN

QUANTUM ESPRESSO BANDS STRUCTURE

HANDS-ON #2

Band structure

Files for band structure



Step 1: SCF calculation (Hands-on #1)
Step 2: Non-SCF calculation
Step 3: Data of bands structure
Step 4: Plot band structure

Command:

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

Band structure

Si.nscf.in

```
&CONTROL
 calculation='bands',
 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,
/
&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 {crystal_b}
5
   0.0000000000   0.0000000000  -0.5000000000  20
   0.0000000000   0.0000000000   0.0000000000  30
  -0.5000000000   0.0000000000  -0.5000000000  10
  -0.3750000000   0.0000000000  -0.6250000000  30
   0.0000000000   0.0000000000   0.0000000000  20
```

non-SCF calculation

Selected special k-point coordinates

L
Γ
X
U
Γ

Step 1: SCF calculation (Hands-on #1)
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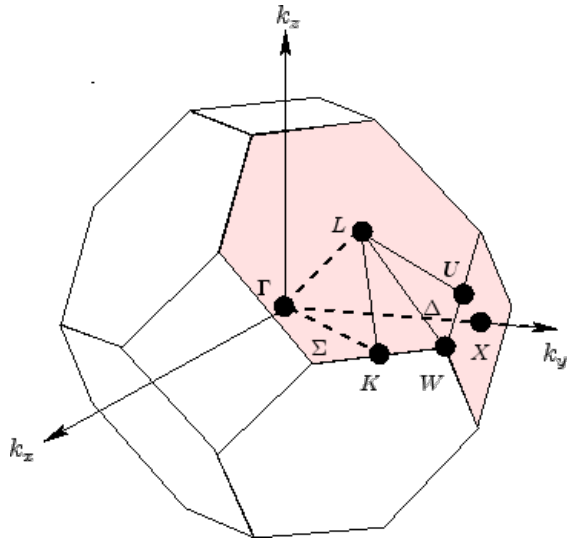
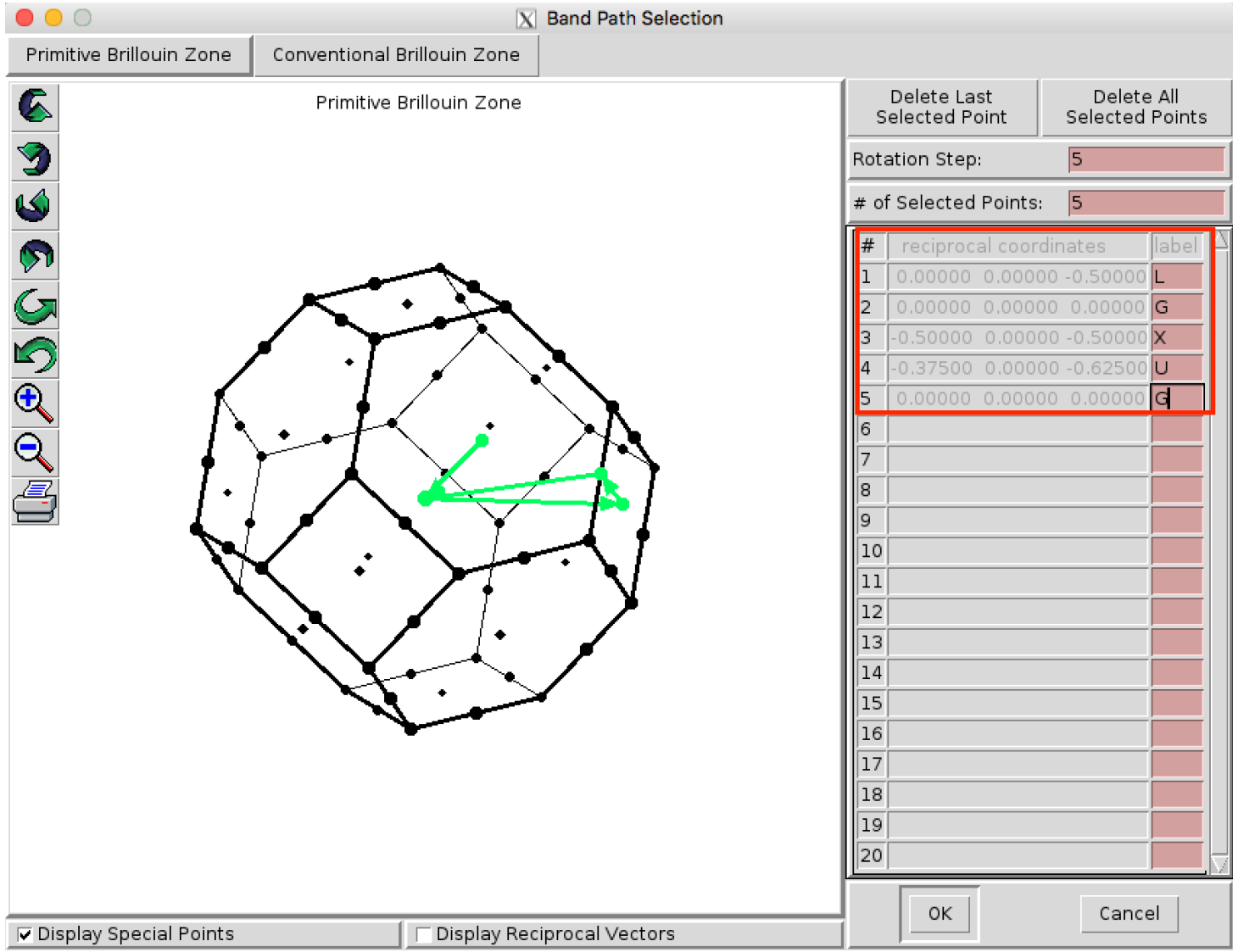
Command:

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



XCrySDen k-path

XCrySDen: http://www.xcrysden.org



Band structure

Si.bands.in

```
&BANDS
 outdir='../tmp/',
 prefix='si',
 filband='si.bands',
/
```

Name of data file

Step 1: SCF calculation (Hands-on #1)
Step 2: Non-SCF calculation
Step 3: Data of bands structure
Step 4: Plot band structure

Command:

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

Band structure

Step 1: SCF calculation (Hands-on #1)
Step 2: Non-SCF calculation
Step 3: Data of bands structure
Step 4: Plot band structure

Si.bands.in

```
&BANDS
 outdir='../tmp/',
 prefix='si',
 filband='si.bands',
/
```

→ Name of data file

Si.plotband

```
si.bands
-6.0 10
si.bands.xmgr
si.bands.ps
6.255
1.0 6.255
```

← Data file

Command:

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