

MATERIAL DESIGN

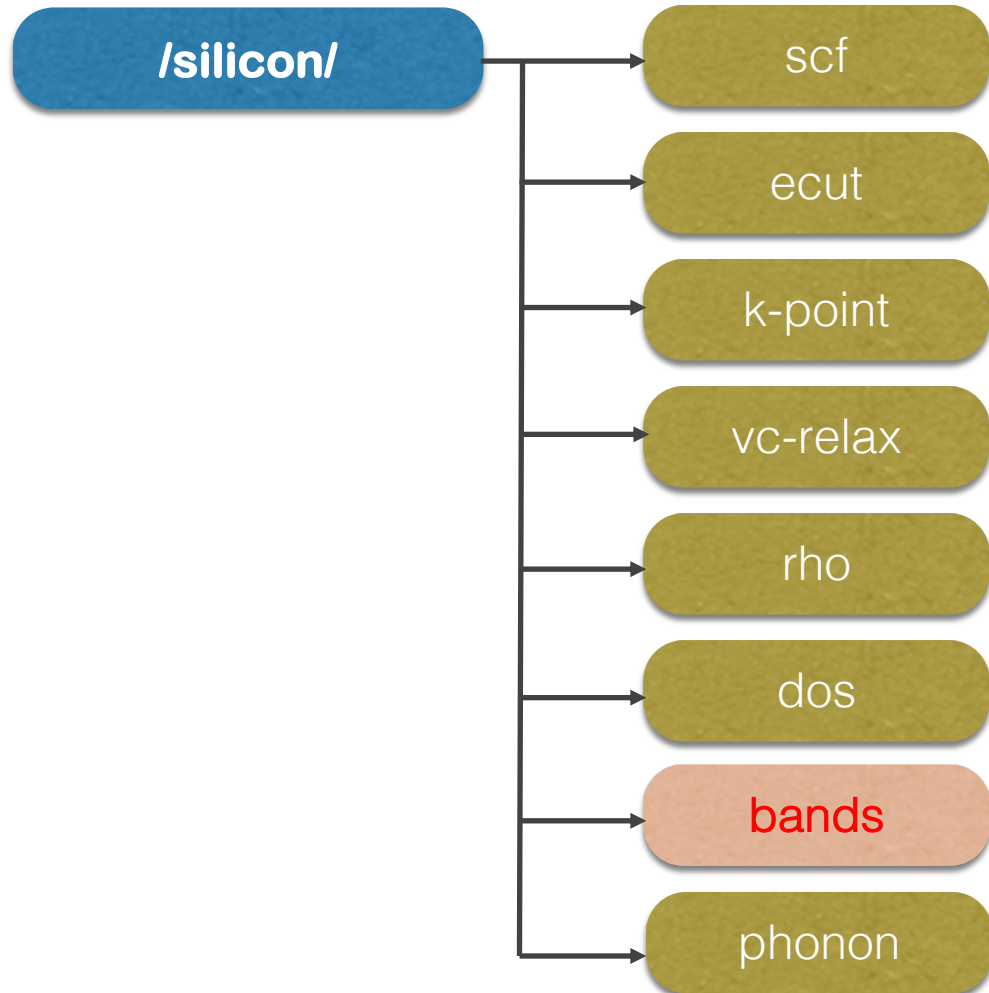
QUANTUM ESPRESSO BANDS STRUCTURE

HANDS-ON #2

PART 10

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	← L
	0.0000000000	0.0000000000	0.0000000000	30	← Γ
	-0.5000000000	0.0000000000	-0.5000000000	10	← X
	-0.3750000000	0.0000000000	-0.6250000000	30	← U
	0.0000000000	0.0000000000	0.0000000000	20	← Γ

non-SCF calculation

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
```

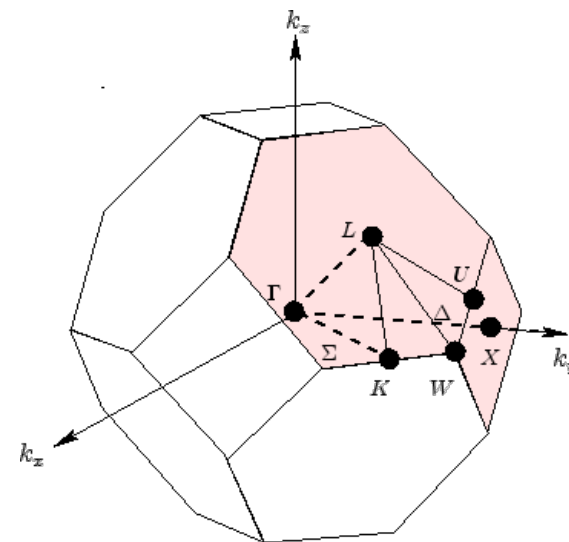
Step 1: SCF calculation (Hands-on #1)

Step 2: Non-SCF calculation

Step 3: Data of bands structure

Step 4: Plot band structure

Selected special k-point coordinates



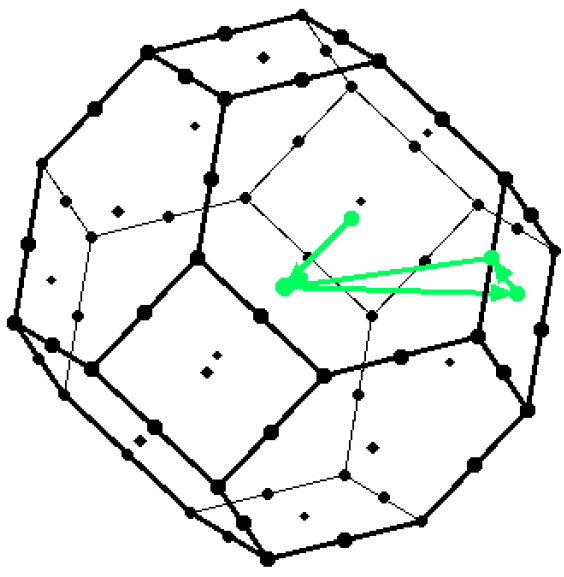
XCrySDen k-path

XCrySDen: <http://www.xcrysden.org>

Band Path Selection

Primitive Brillouin Zone Conventional Brillouin Zone

Primitive Brillouin Zone



Delete Last Selected Point Delete All Selected Points

Rotation Step: 5

of Selected Points: 5

#	reciprocal coordinates	label
1	0.00000 0.00000 -0.50000	L
2	0.00000 0.00000 0.00000	G
3	-0.50000 0.00000 -0.50000	X
4	-0.37500 0.00000 -0.62500	U
5	0.00000 0.00000 0.00000	Γ
6		
7		
8		
9		
10		
11		
12		
13		
14		
15		
16		
17		
18		
19		
20		

☒ Display Special Points ☐ Display Reciprocal Vectors

OK Cancel

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

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

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
```

