PART 4

MATERIAL DESIGN

QUANTUM ESPRESSO INPUT PARAMETER

HANDS-ON #1

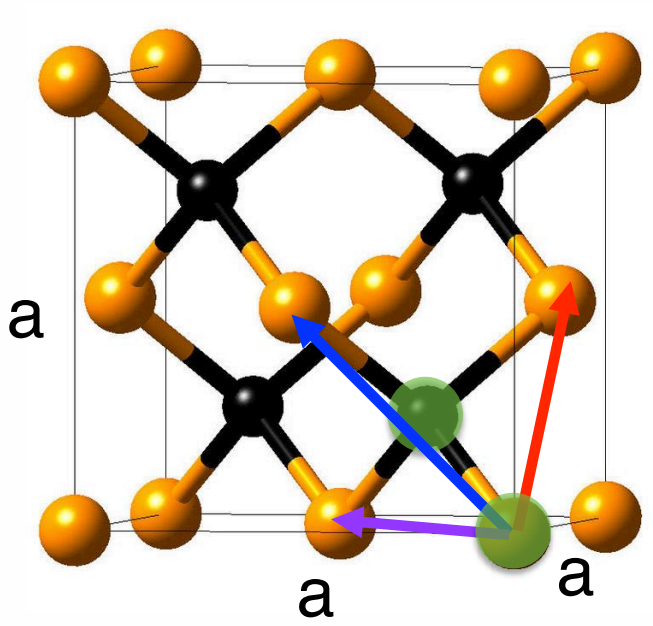
Structure of QE input file

```
&CONTROL
 calculation='scf',
 restart_mode='from_scratch',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&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
4 4 4 1 1 1
```

Silicon

Mass of Si

FCC structure



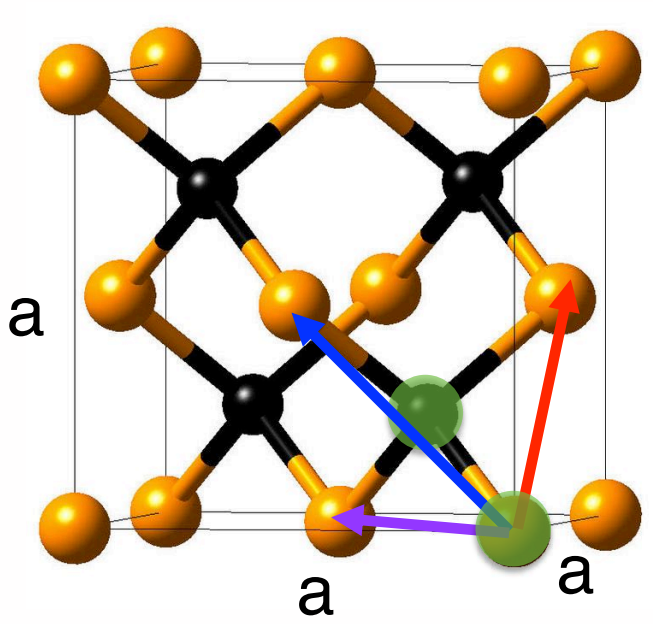
Pseudopotential

```
&CONTROL
 calculation='scf',
 restart_mode='from_scratch',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&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
4 4 4 1 1 1
```

PP file

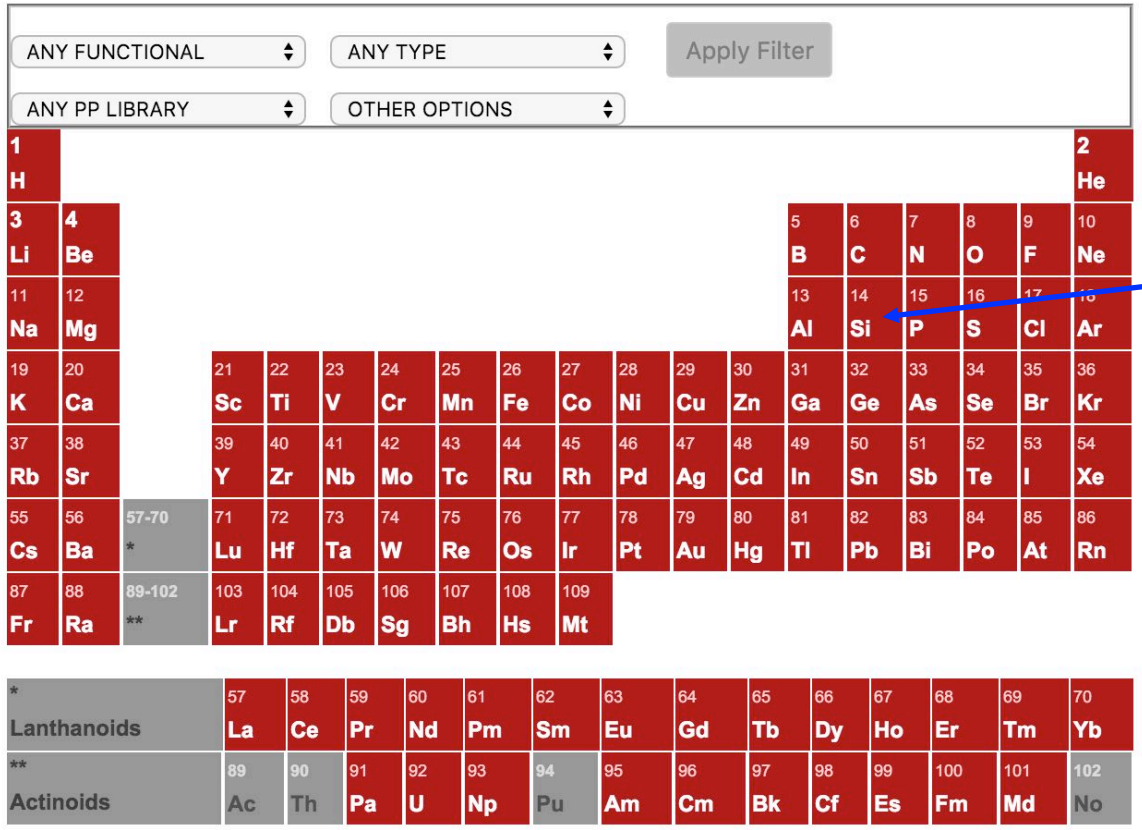
Name of the pseudopotential file

FCC structure



How to get pseudopotential

http://www.quantum-espresso.org/pseudopotentials/



PSEUDO SEARCH RESULTS

Pseudopotential File

Si.blyp-hgh.UPF

```
Pseudopotential type: NORMCONS
Method: Goedecker-Hartwigsen-Hutter-Teter
Functional type: Becke-Lee-Yang-Parr (BLYP) exch-corr
non relativistic

Origin: Hartwigsen-Goedeker-Hutter PP
Author: Goedecker/Hartwigsen/Hutter/Teter
Generated in analytical, separable form. Converted from CPMD format using cpmd2upf v.5.0.1.
Uploaded by marsamos
Classification unverified
```

Si.pbe-rrkj.UPF

```
Pseudopotential type: NORMCONS
Method: Rappe Rabe Kaxiras Joannopoulos
Functional type: Perdew-Burke-Ernzerhof (PBE) exch-corr
scalar relativistic

Origin: Original QE PP library
Author: Andrea Dal Corso
Generated by Andrea Dal Corso code (rrkj3)
Uploaded by Erica Vidal
Classification controlled by Paolo Giannozzi
```

Si.pbe-van_gipaw.UPF

```
Pseudopotential type: ULTRASOFT
Method: Rappe Rabe Kaxiras Joannopoulos
Functional type: Perdew-Burke-Ernzerhof (PBE) exch-corr
Is Gipaw
scalar relativistic

Origin: Original QE PP library
Generated by "atomic" code by A. Dal Corso (QE distribution)
Uploaded by Erica Vidal
Classification controlled by Paolo Giannozzi
```

Si.pbe-rrkj.UPF

- type of exchange-correlation functional
- type of pseudopotential

Pseudopotential

```
&CONTROL
 calculation='scf',
 restart_mode='from_scratch',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&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
4 4 4 1 1 1
```

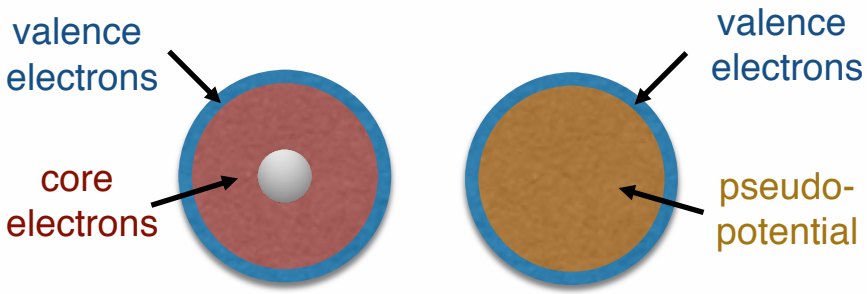
```
<PP_INFO>
Generated using Andrea Dal Corso code (rrkj3)
Author: Andrea Dal Corso   Generation date: unknown
Info:   Si PBE 3s2 3p2 RRKJ3
    0        The Pseudo was generated with a Non-Relativistic Calculation
  2.50000000000E+00    Local Potential cutoff radius
nl pn  l   occ               Rcut            Rcut US            E pseu
3S  1  0  2.00      2.50000000000      2.60000000000      0.00000000000
3S  1  0  0.00      2.50000000000      2.60000000000      0.00000000000
3P  2  1  2.00      2.50000000000      2.70000000000      0.00000000000
3D  3  2  0.00      2.50000000000      2.50000000000      0.00000000000
</PP_INFO>
<PP_HEADER>
   0                    Version Number
  Si                    Element
   NC                   Norm - Conserving pseudopotential
    F                   Nonlinear Core Correction
 SLA  PW   PBE  PBE     PBE  Exchange-Correlation functional
   4.00000000000       Z valence
  -7.47480832270       Total energy
  0.0000000  0.0000000 Suggested cutoff for wfc and rho
   2                    Max angular momentum component
  883                   Number of points in mesh
   2    3               Number of Wavefunctions, Number of Projectors
 Wavefunctions          nl  l   occ
                        3S  0  2.00
                        3P  1  2.00
</PP_HEADER>
<PP_MESH>
  <PP_R>
  1.77053726905E-04  1.79729551320E-04  1.82445815642E-04  1.85203131043E-04
  1.88002117930E-04  1.90843406086E-04  1.93727634813E-04  1.96655453076E-04
  1.99627519645E-04  2.02644503249E-04  2.05707082721E-04  2.08815947154E-04
  2.11971796056E-04  2.15175339506E-04  2.18427298316E-04  2.21728404189E-04
  …
```

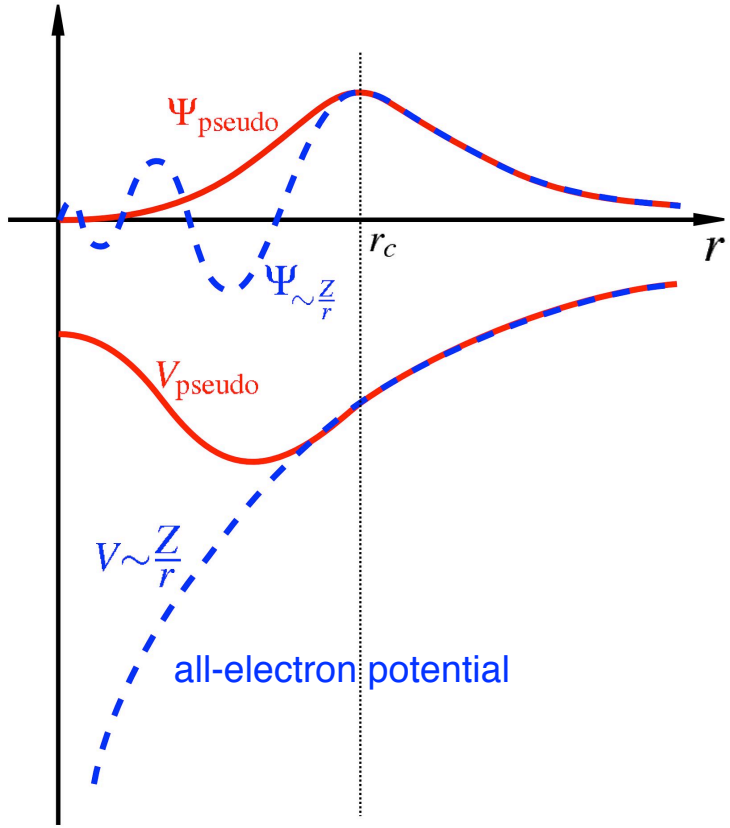
Pseudopotential

Electrons experience a Coulomb potential due to the nuclei with simple form:

$$V_{ion} = -\frac{Z}{r}$$

But this leads to computational problems!





Pseudopotential (PP):

Replace the strong Coulomb potential of the nucleus and tightly bound core electrons by an effective ionic potential acting on the valence electrons.

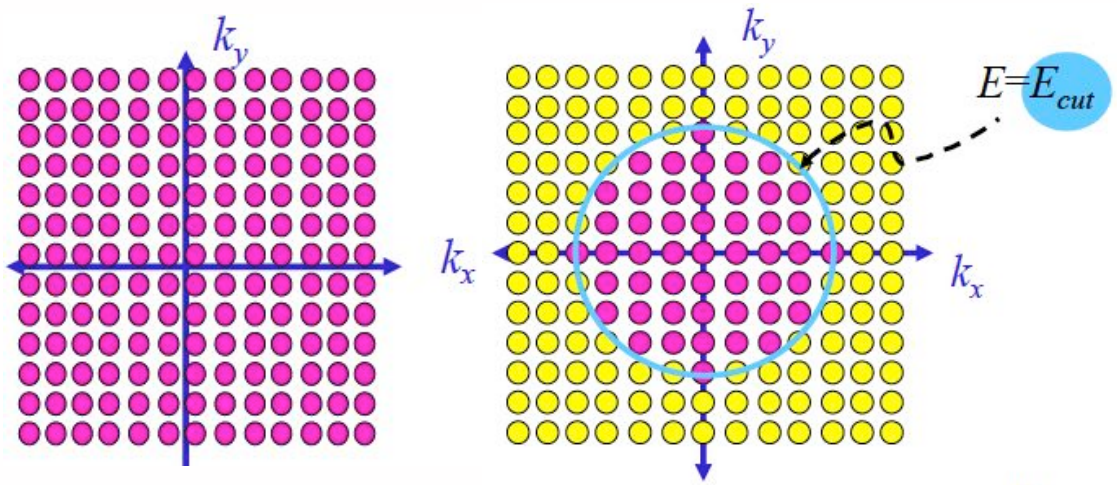
Plane wave expansion

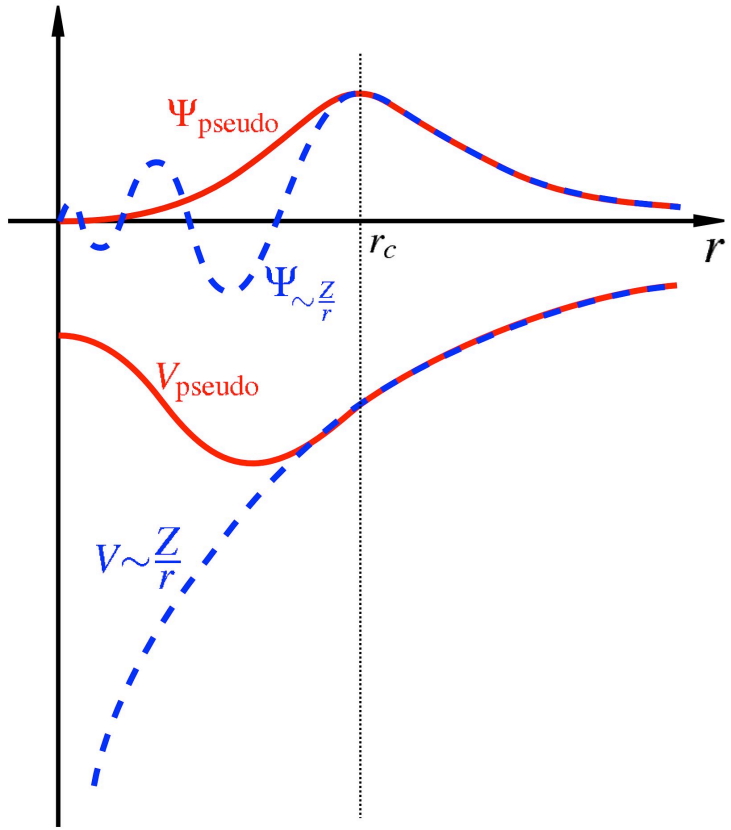
In a periodic system we can write the KS states as a superposition of plane waves:

$$\Psi_{k,n}(r) = \frac{1}{\Omega}\sum_{G} c_{k,n}^{G} e^{i(k+G)\cdot r}$$

G are vectors in reciprocal space.
The sum, in principle infinite, can be truncated:

$$\frac{\hbar^2}{2m}|k+G|^2 \leq E_{cut}$$





Plane wave expansion

```
&CONTROL
 calculation='scf',
 restart_mode='from_scratch',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&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
4 4 4 1 1 1
```

$$\frac{\hbar^2}{2m}|k+G|^2 \leq E_{cut}$$

Units: Ry (1 Ry = 0.5 Ha = 13.6057 eV)
For ultrasoft pseudopotentials we have also:
ecutrho = usually 8-12 × ecutwfc

Sampling of the Brillouin zone

Many quantities we need to compute involve an integral over the BZ:

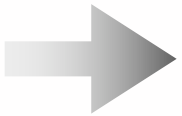
$$\bar{A} = \frac{1}{\Omega_{BZ}} \int_{BZ} A(k) d(k)$$

An example is the electronic density n(r):

$$n(r) = \frac{1}{\Omega_{BZ}} \sum_i \int_{BZ} |\Psi_{i,k}(r)|^2 f(\epsilon_{i,k} - \epsilon_F) d(k)$$

In practice the integral is discretized:

$$\frac{1}{\Omega_{BZ}} \int_{BZ} d(k) \rightarrow \sum_k \omega_k$$



How do we choose the k points to include in the sum???

Monkhorst and Pack (1976)

Example: square 2D lattice

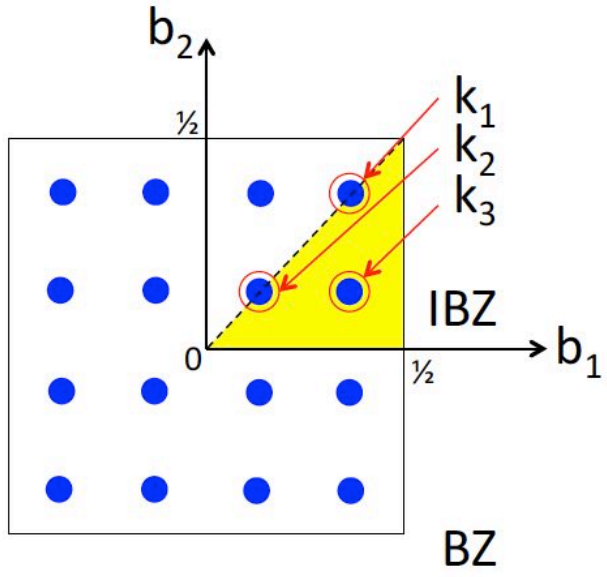
4×4 k-points grid (16 points)

3 inequivalent point (IBZ)

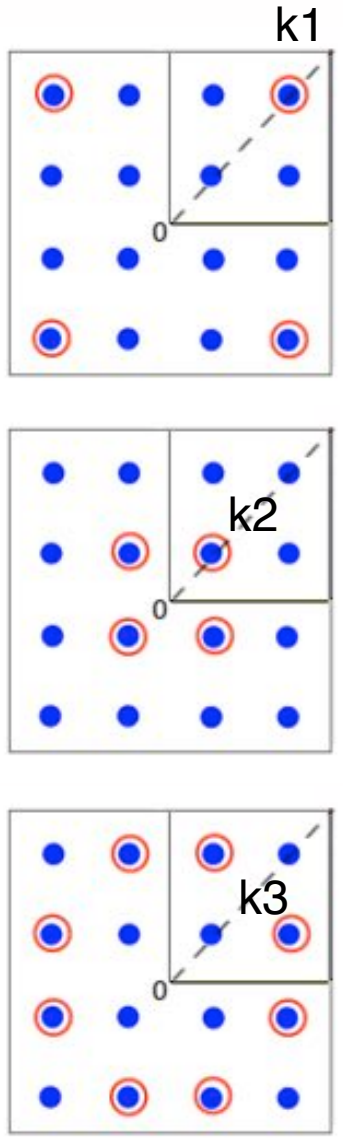
$$4 \times k_1 \rightarrow \omega_1 = 4/16 = 1/4$$

$$4 \times k_2 \rightarrow \omega_2 = 4/16 = 1/4$$

$$8 \times k_3 \rightarrow \omega_3 = 8/16 = 1/2$$

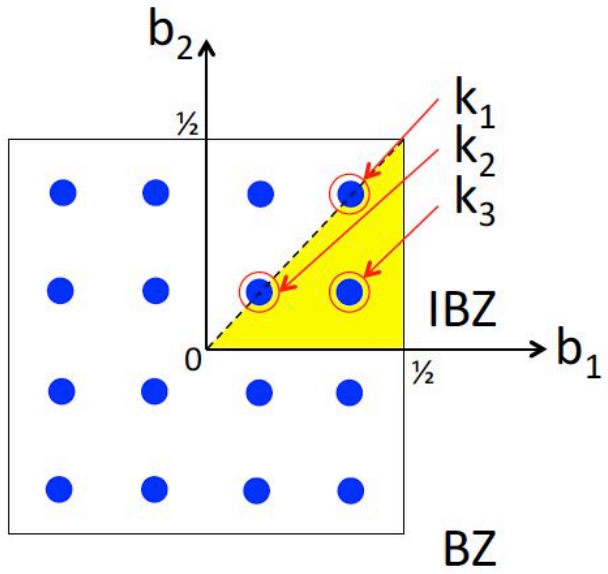


$$\frac{1}{\Omega_{BZ}} \int_{BZ} A(k)d(k) \simeq \frac{1}{4}A(k_1) + \frac{1}{4}A(k_2) + \frac{1}{2}A(k_3)$$



Sampling of the Brillouin zone

```
&CONTROL
 calculation='scf',
 restart_mode='from_scratch',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&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
4 4 4 1 1 1
```



K_POINTS automatic
nk1, nk2, nk3, k1, k2, k3

nk1, nk2, nk3 as in Monkhorst-Pack grids k1, k2, k3 must be 0 (no offset) or 1 (grid displaced by half a grid step in the corresponding direction)

Construct structure