

このホームページは **WIX.com** を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)



Computational Physics Course

Learn to use software packages

Home

More

Quantum Espresso

Let us use the package "Quantum espresso" to learn what we can do with DFT.

Why QE?

Quantum espresso was called PWscf before. With PWscf, one can do a DFT calculation using the plane wave basis set and the pseudopotential. This software package has been extended by including many subroutines and was renamed as Quantum espresso. There have been continuous efforts to distribute this package to general users and this has become one of the most popular packages. Detailed documents and tutorials are available; from this viewpoint, QE is the most suitable for learners.

Let us learn from the tutorial

Quantum Espresso Tutorial

Hands-on Session #1

First steps with QE: total energy and relaxations

Let me acknowledge Prof. Piccinin

Simone Piccinin
CNR – Institute of Materials (IOM), Trieste (Italy)
piccinin@iom.cnr.it

QE can be obtained from this site.

このホームページは **WIX.com** を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)



<http://www.quantum-espresso.org/>

HOME PROJECT DOWNLOAD RESOURCES PSEUDOPOTENTIALS CONTACTS NEWS & EVENTS

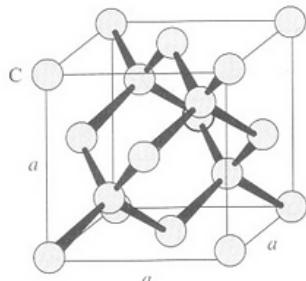
SEARCH



Forum

Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 1 1 1
```



Suppose we want to calculate the crystalline silicon of diamond structure.

One need to prepare the input file indicating

1. How to approach the problem
 2. Information on the cell
 3. Number of atoms and elements
 4. Number of basis functions
 5. How to achieve self-consistency
- and then
1. Element information (mass, pseudopotential)
 2. Position of each atom
 3. Mesh used for the Brillouine zone integration

The Kohn-Sham problem

KS eqns: $\left[-\frac{1}{2} \nabla^2 + V_{nucl}(r) + V_H[n] + V_{xc}[n] \right] \Psi_i(r) = \epsilon_i \Psi_i(r)$

SCF: $\Psi_i(r) \longrightarrow n(r) \longrightarrow H[n]$

QE solves the Schrödinger type equation, called Kohn-Sham equation. Because of the nonlinearity, it needs to be solved iteratively by assuming a form for the electron density $n(r)$ and correcting the assumption afterwards.

Iterative solution of KS equations

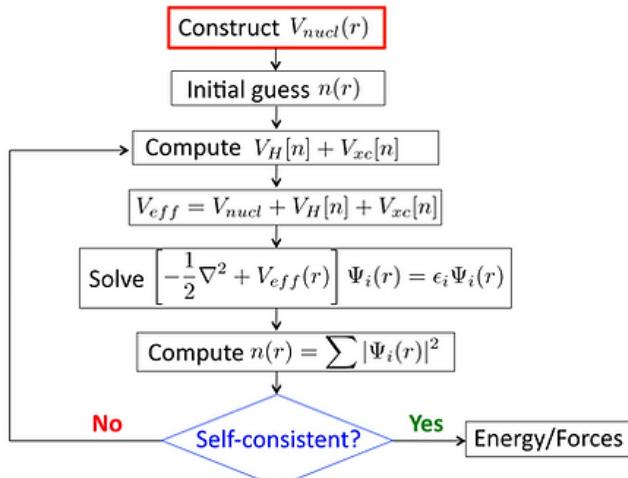
Structure of QE input file

```
&control
  calculation = 'scf', ← = 'scf', 'nscf', 'relax', 'md', ...
/
&system
  ibrav = 2,
  cellm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```

Coming back to the input file, we notice that there are several ways for approach:

1. scf: self-consistently solve the KS equation
2. nscf: non-self-consistently solve it using a guess for $n(r)$
3. relax: optimize the nuclear position according to the atomic force obtained from the solution of the KS equation.
4. md: run a molecular dynamics simulation using the atomic force

Iterative solution of KS equations



There are some comments on constructing the Coloumb potential originated from the nuclear charge.

In QE, we apply the periodic boundary condition unless otherwise specified. So, the atoms in a unit cell is repeated three-dimensionally.

このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)

Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```

ibrav= 1: simple cubic
 ibrav= 2: fcc
 ibrav= 4: hexagonal
 ...

simple cubic:
 $v1 = a(1,0,0)$, $v2 = a(0,1,0)$, $v3 = a(0,0,1)$

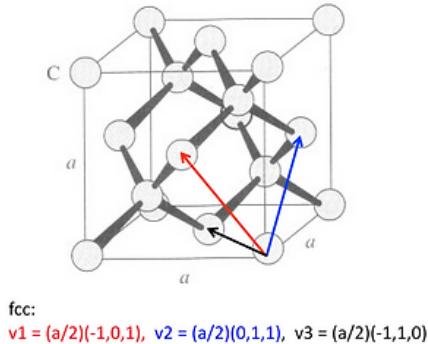
fcc:
 $v1 = (a/2)(-1,0,1)$, $v2 = (a/2)(0,1,1)$, $v3 = (a/2)(-1,1,0)$

hexagonal:
 $v1 = a(1,0,0)$, $v2 = a(-1/2,sqrt(3)/2,0)$, $v3 = a(0,0,c/a)$

Therefore we need to specify the unit cell. For this, we have to provide the type Bravais lattice (ibrav), length of the cell, and so on.

Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```



For silicon, which has a fcc unit cell, we need to specify the Bravais lattice type and the cell dimension a.

Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26, ← Units: bohr (1 bohr = 0.529177 Å)
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```

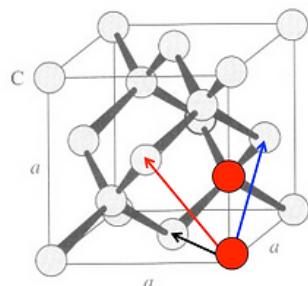
We have two silicon atoms in the

このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)

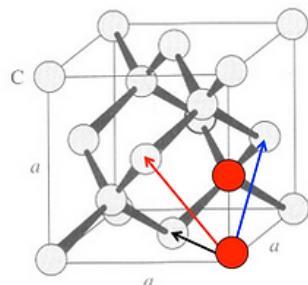
Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
```



Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```



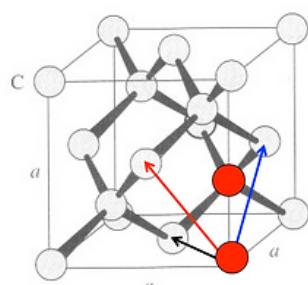
We have only one element, "silicon".

We have to specify the species, mass, and the pseudopotential (PP). The PP is specified by the name of the file that contains information on PP.

PP will be explained later.

Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```



NB: If PP files are in a separate directory then specify:
 &control
 pseudo_dir='/where/my/pseudos/are'
 /

The PP file is stored in a directory specified by "pseudo_dir"

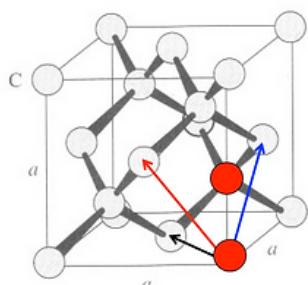
Position of atoms is given in unit of a . It can be alternatively given in unit of Bohr or Angstrom.

このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

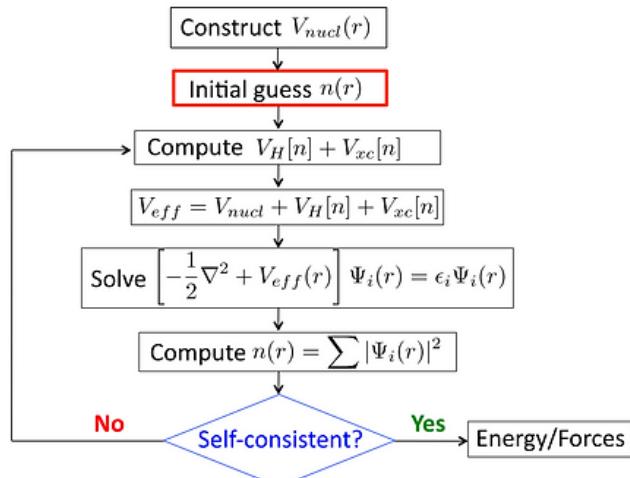
[今すぐはじめる](#)

Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
```



Iterative solution of KS equations



Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```

startingwfc = 'atomic' (DEFAULT)
= 'random'
= 'file'

First of all, we need to assume a form for the electron density $n(r)$. It is automatically assumed on the basis of the atomic charge stored in PP file, but you can alternatively give a randomly generated density or specify a file that store the information of $n(r)$.

As written above, we normally use the plane wave as the basis function. We then need to specify the number of the functions. This is done by indicating the threshold value. Normally we use the cut-off energy for the kinetic energy.

このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)

Plane wave expansion

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

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

Plane wave expansion

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

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

\mathbf{G} 's are vectors in reciprocal space.

The sum, in principle infinite, can be truncated:

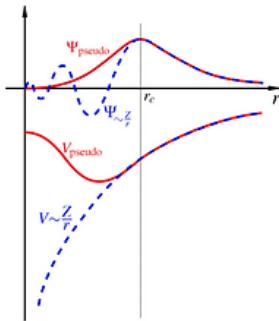
$$\frac{\hbar^2}{2m} |\mathbf{k} + \mathbf{G}|^2 \leq E_{cut}$$

Problems:

- 1) Core electrons are localized
- 2) Valence electrons have nodes close to the nucleus

An all-electron calculation would require high E_{cut}

Pseudopotentials: The choice of E_{cut} depends on the PP



Here I comment on the pseudopotential (PP). PP is necessary for the plane wave because the localized nature of the core electrons cannot be described using unrealistically large number of plane waves. So, effect of core is described by introducing an effective potential for valence electrons; core electrons are not treated explicitly. The valence electrons are then made node-less in the core region. PPs are constructed by smoothly extrapolating the potential inside the cut-off radius.

There are various methods for constructing PP and the constructed PPs are available on the internet.

Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20 ←
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```

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

Units: Ry (1 Ry = 0.5 Ha = 13.6057 eV)

For ultrasoft pseudopotentials we have also:
ecutrho = usually 8-12 * ecutwfc

このホームページは **WIX.com** を使って作成されました。あなたも無料で作ってみませんか？

今すぐはじめる

Structure of QE input file

Pseudopotentials

You can construct your PP using the code provided by QE. Here is the input file for the PP generation calculation.

Here we show a download site for the PP provided by QE.

<http://www.qe-forge.org/gf/project/pslibrary/>

このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)

Structure of QE input file

```

&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1

```

point mesh used for the Brillouine zone (BZ) integration.

Sampling of the Brillouin zone

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

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

An example is the electronic density $n(\mathbf{r})$:

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

In practice the integral is discretized:

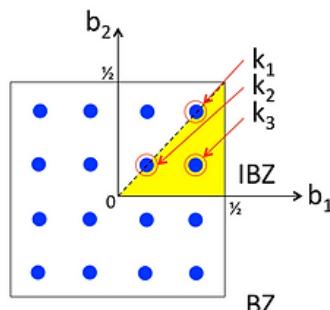
$$\frac{1}{\Omega_{BZ}} \int_{BZ} d\mathbf{k} \rightarrow \sum_{\mathbf{k}} \omega_{\mathbf{k}}$$

How do we choose the \mathbf{k} points to include in the sum?

We discretize inside the BZ and apply the trapezoidal rule or the tetrahedron method for the BZ integration.

Sampling of the Brillouin zone

- example: square 2D lattice
- 4x4 k-points grid (16 points)
- 3 inequivalent points (IBZ)



$$\frac{1}{\Omega_{BZ}} \int_{BZ} A(\mathbf{k}) d\mathbf{k} \simeq \frac{1}{4} A(\mathbf{k}_1) + \frac{1}{4} A(\mathbf{k}_2) + \frac{1}{2} A(\mathbf{k}_3)$$

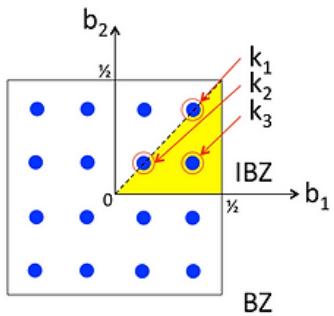
This figure assumes 4 4 4 1 1 1, differently from the example.

このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)

Structure of QE input file

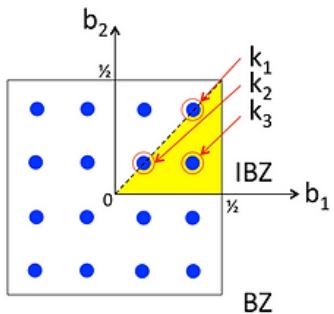
```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
```



then the k-points include the origin, called gamma point.

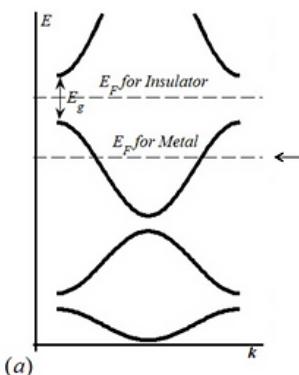
Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```



Nk1, NK2, NK3, shift1, shift2, shift3
shift: 0 or 1

Sampling of the Brillouin zone



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

- a) $f(x) = \Theta(x) = \begin{cases} 1 & \text{for } x \leq 0 \\ 0 & \text{for } x > 0 \end{cases}$
 b) $f(x) = \text{smooth function of } x/\sigma$
 (i.e. partial occupations)

σ : dimensions of energy,
 controls the broadening of the Fermi surface
 "smearing" of the Fermi surface

We normally use different BZ integration method for metals and insulators. The BZ for metals is demanding. The simplest one is to apply the trapezoidal rule with the Fermi surface smeared by introducing

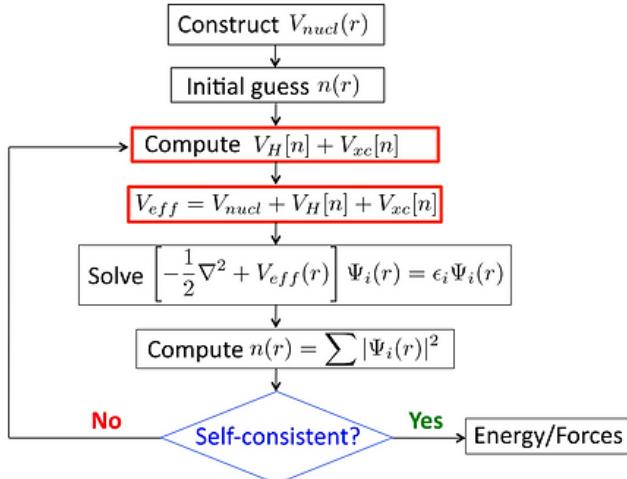
このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)

Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
```

Iterative solution of KS equations



Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 1 1 1
```

← Name of the PP file: Si.pbe-rrkj.UPF

By default the XC functional is chosen based on the information contained in the PP file.

ntyp > 1 --> XC must be consistent (or overwritten)

We need to specify the functional form for the exchange-correlation. This is put implicitly in the PP file. In the sample input, a semi-local functional of generalized gradient approximation (GGA) type is used. PBE refers to those who developed the functional.

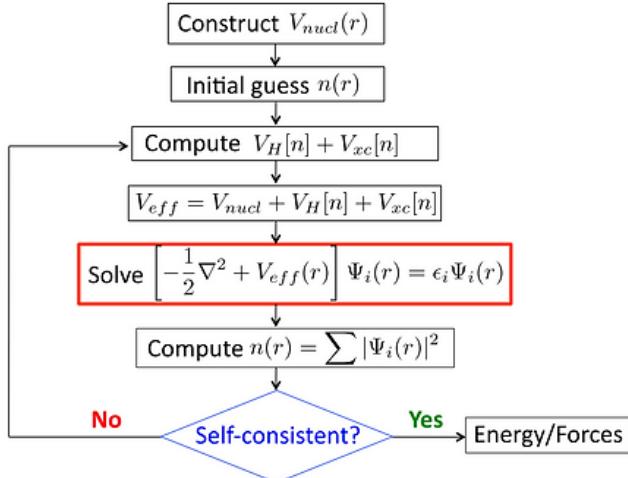
Popular GGA functionals include RPBE, PZ, B3LYP, and so on.

このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)

Structure of QE input file

Iterative solution of KS equations



Structure of QE input file

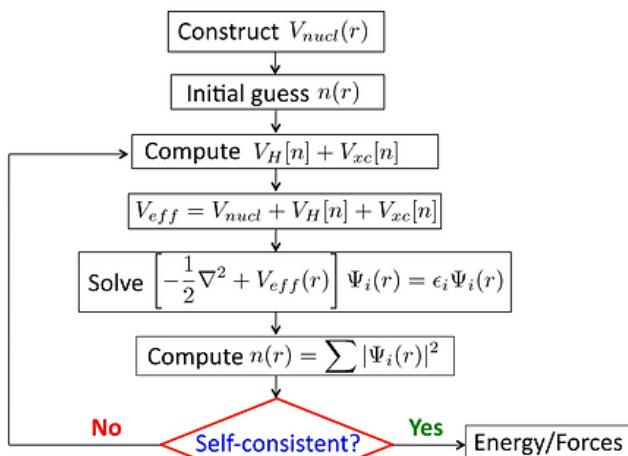
```

&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.08 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
  
```

A portion of a Quantum Espresso input file is shown. It includes sections for control parameters (&control), system properties (&system), and electronic configurations (&electrons). The &electrons section specifies a mixing beta of 0.7. The ATOMIC_SPECIES section lists silicon (Si) with a pseudopotential file 'Si.pbe-rrkj.UPF'. The ATOMIC_POSITIONS section provides atomic coordinates in alat units. The K_POINTS section indicates a 6x6x6 grid of k-points for the Brillouin zone.

There are a few ways to solve the Shroedinger type differential equation. Davidson method and the conjugate gradient (CG) are the most popular.

Iterative solution of KS equations



このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)

Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```

If the input density and the output density are the same within the given threshold, self-consistency is achieved and QE proceeds to calculate the total energy and the force.

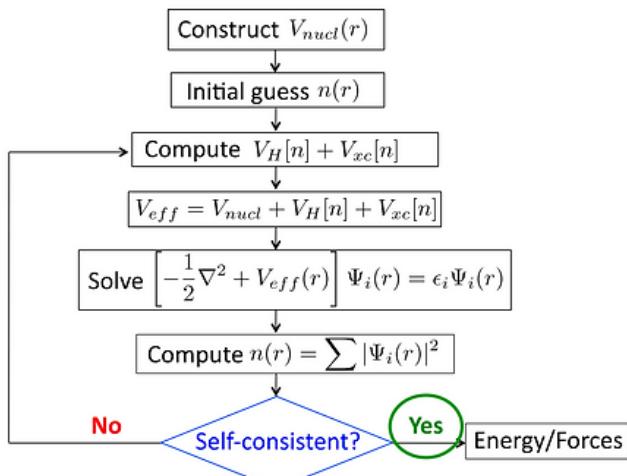
Mixing

```
&control
  calculation = 'scf',
  prefix = 'Si_excl',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```

- Mix new and old density
- 0.7 = 70% of the new density and 30% of old at first step, then use Broyden scheme

It is known for a long time that the self-consistency can be generally achieved by mixing the input density with the output density. This parameter depends significantly on the electronic structure. In some cases we need take 0.05!

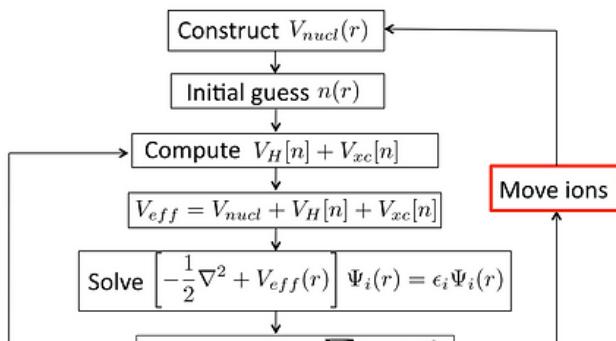
Iterative solution of KS equations



このホームページは WIX.com を使って作成されました。あなたも無料で作ってみませんか？

[今すぐはじめる](#)

Iterative solution of KS equations



Structure of QE input file

```

&control
  calculation = 'relax',
  nstep=50,
  etot_conv_thr = 1.d-4
  forc_conv_thr = 1.d-3
  ...
  ...
  &electrons
    conv_thr = 1.d-7
  ...
  /
  &ions
    ion_dynamics      = "bfgs",
    pot_extrapolation = "second_order",
    wfc_extrapolation = "second_order",
    upscale           = 100,
  /
  ...
  
```

(or 'damp', 'verlet', 'langevin')
 (DEFAULT: 'none')
 (DEFAULT: 'none')
 (DEFAULT: 10)

To relax the atomic structure, we need to specify other parameters as well.

Report (1) deadline is 13th December

The Quantum Espresso (QE) community provides excellent tutorial not only for beginners but also more advanced users. Here we follow the tutorial given by Prof. Madhura Marathe to solve the Kohn-Sham equation of crystalline silicon and plot the band dispersion along lines connecting symmetric points in the Brillouine zone.

Using the obtained plot, let us estimate the effective mass of the electrons and holes. By comparing the result with experiment, let us consider the reason for the discrepancy, which is due to approximations made in the calculation.

Report the results. This is a first step toward more complicated calculations. Try to understand what you are doing.

[PDF](#)


このホームページは **WIX.com** を使って作成されました。あなたも無料で作ってみませんか？ [今すぐはじめる](#)



Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso

The University of Tokyo

© 2016 by Osamu Sugino

HO

OH