

three major keywords in the QE input file

1. exchange-correlation functional

In the lectures of this course, you learned that the only essential approximation in DFT is the choice made for the exchange-correlation functional (XC-functional, for short). Therefore, how do you tell QE which XC-functional you want to use? That's pretty straightforward. In the input file for QE, you have in &SYSTEM block a line like this:

```
input_dft='LDA',
```

That's where you choose the XC-functional. The line above selects the Local Density Approximation. In order to take the Perdew-Burke-Ernzerhof function (a popular GGA XC-functional), use

```
input_dft='PBE',
```

Warning: pseudopotentials are made for a particular XC-functional. QE automatically takes the XC-functional to be identical to the one for the pseudopotentials you list in ATOMIC_SPECIES. That value is overwritten, however, by input_dft. Therefore, either make sure that you use the pseudopotentials for the XC-functional you want to have, or don't use input_dft at all. It is never a good idea to use a pseudopotential for another XC-functional than the one it is designed for.

2. reciprocal space sampling (k-mesh)

Many properties in a DFT code are obtained from an integral over the first Brillouin zone (in case you are not familiar with reciprocal space and Brillouin zones: we'll introduce that later – just think about an integral over some domain, for now). In order to solve that integral numerically, it is replaced by a sum over a few sampling points. The integrand needs to be evaluated for the sampling points only. The more sampling points, the better the numerical solution approximates the exact solution. Therefore, for every DFT-calculation it is mandatory to verify whether you used a sufficient number of sampling points. You can do this by plotting calculated quantities as a function of the number of sampling points. When this plot saturates, you know your sampling is good enough.

The number of sampling points is expressed as a three-dimensional grid in reciprocal space ("k-mesh"), and is set in &ELECTRONS block with the K_POINTS keyword. To set a 3x3x3 mesh, use

```
K_POINTS {automatic}  
  3 3 3 0 0 0
```

To use a 5x5x5 mesh, use

```
K_POINTS {automatic}  
  5 5 5 0 0 0
```

All details about the K_POINTS keyword (much more than you need) can be found [here](#).

3. basis set size

Many DFT codes use a 'basis set': the Kohn-Sham orbitals are expressed in a basis of infinite dimensionality (just as you can express any periodic function in an infinite basis of cosine functions, for instance). In a computer, such an infinite set has to be truncated somewhere. That will limit the precision of your calculation. Ideally, you should truncate the basis set only after the point where adding more basis functions does not notably influence your result any longer.

In QE, the basis set size is specified by the `ecutwfc` keyword in the `&SYSTEM` block:

```
ecutwfc=30.0d0,
```

Technically spoken, this determines the basis set size for describing the wave functions. In order to describe the density, another basis set is used, the size of which is determined by `ecutrho`. By default, `ecutrho` is 4x `ecutwfc`. As you can read [here](#), this factor 4 might need to be somewhat larger for PAW pseudopotentials, and much larger (8-12) for ultrasoft pseudopotentials. A good strategy is to test which value of `ecutwfc` you need (keeping `ecutrho` 4 times as large), and afterwards, once you have found your final `ecutwfc`, to increase that factor further until nothing changes any longer.

This text is informative/descriptive. The next document on convergence testing is an important exercise, where you can use the information hereabove.