

# Quantum Espresso Quick Start

## Introduction

Quantum Espresso (<http://www.quantum-espresso.org/>) is a sophisticated collection of tools for electronic structure calculations via DFT using plane waves and pseudopotentials. A variety of codes are available within the distribution for the calculation of material properties eg., phonon dispersion, NMR shifts and band structure to name a few. Quantum Espresso is available as a module on most Lion clusters at PSU.

### Citation :

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### Online Guide for QE :

[http://www.quantum-espresso.org/user\\_guide/user\\_guide.html](http://www.quantum-espresso.org/user_guide/user_guide.html)

### FAQ for QE :

[http://www.quantum-espresso.org/user\\_guide/node57.html](http://www.quantum-espresso.org/user_guide/node57.html)

## First Step : Identifying Pseudopotentials

### Readily available Pseudopotentials :

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

Before a DFT calculation for an extended system can proceed, pseudopotentials for constituent atoms must exist within a library directory, constructed using the same exchange-correlation functional to be applied later. A pseudopotential (PP) drastically reduces the number of plane waves required in a calculation by using an approximation to the core region; Quantum Espresso (QE) supports both norm-conserving (NCPP) and ultrasoft (USPP) types. Considerations of which electrons are to be treated as valence and thus explicitly is generally dictated by transferability, or the ability of the PP to describe an atom in a variety of different chemical environments. As a rule of thumb, more valence electrons amount to better transferability and longer computation time. If the pseudopotential(s) available to you are unsuitable for whatever reason, they may be constructed using the atomic facilities within QE. The following is a simple input file to the program `ld1.x`, for Ti, which is passed in via stdin :

```
&input
  atom='Ti', dft='PBE', config='[Ar] 3d2 4s2 4p0',
  rlderiv=2.90, eminld=2.0, emaxld=2.0, delld=0.01, nld=3,
  iswitch=3
```

```

/
&inputp
pseudotype=1, nlcc=.true., lloc=0,
file_pseudopw='Ti.pbe-n-rrkj.UPF'
/
3
4P  2    1    0.00 0.00 2.9  2.9
3D  3    2    2.00 0.00 1.3  1.3
4S  1    0    2.00 0.00 2.9  2.9

```

The first input line gives the form of the DFT functional (PBE), electronic configuration, atomic label and `iswitch=3` requesting a PP calculation. The second line refers to (`nld`) 3 logarithmic derivatives at (`rlderiv`) 2.9 a.u. from the origin, the energy range (`eminld`) -2.0 Ry to (`emaxld`) 2.0Ry, in energy steps of (`deld`) 0.01 Ry. These parameters simply refer to points of wavefunction logarithmic derivatives, which are dumped to files, for subsequent inspection, to be discussed shortly. The constructed PP is stored in the file specified via `file_pseudopw`.

The second section (`inputp`) specifies single projector, NCPP (`pseudotype=1`), with non-linear core correction (`nlcc=.true.`) and the  $l=0$  channel as local (`lloc=0`). The former attempts to account for the nonlinearity introduced via the exchange-correlation potential. The latter refers indirectly to the Kleinman-Bylander transformation, by which the PP is separated into local and non-local components, for greater computational tractability. Inappropriate choice of channel (in particular) may lead to introduction of ghost states.

Finally, the electronic orbitals to be pseudized (total number first eg., 3) must be specified in detail, with the local channel last. Column one gives the label, column two principle quantum number (1 for lowest S and increment if necessary, 2 for lowest P etc), column three angular momentum number, followed by occupation number in column four. Column five contains the energy used to pseudize the corresponding state; 0.0 should only be used for bound states. Finally, columns six and seven refer to matching radii for NCPP and USPP respectively.

The process of constructing a PP is fairly involved; the final product must certainly be able to reproduce established properties eg., lattice parameters in model systems, before being used in the target system. One must also test for the presence of (and eliminate by parameter adjustment where applicable) ghost states by examination of the output to `stdout`; at a bare minimum there should be good correspondence between all-electron and pseudo-wave functions and their logarithmic derivatives. As mentioned, this data is available after execution in text files `ld1ps.wfc` and logarithmic data in `ld1ps.dlog` and `lpd1.dlog`; the contents of the first file are displayed in figure 1. The reader is encouraged to read Paolo Giannozzi's "Notes on Pseudopotential Generation" for further information.

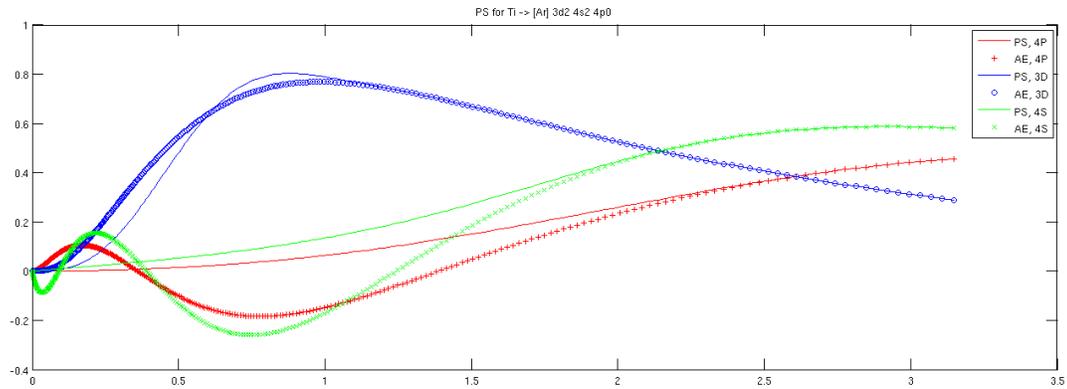


Figure 1: All-electron and pseudo orbital wavefunctions for Ti

### Online Reference for `ld1.x` :

[http://www.quantum-espresso.org/input-syntax/INPUT\\_LD1.html](http://www.quantum-espresso.org/input-syntax/INPUT_LD1.html)

## Main Step : Performing DFT for Target System

The DFT code (`pw.x`) within QE is derived directly from the PWScf development community. In addition, Car-Parinello dynamics are available via `cp.x`. Before embarking on hand-editing input files for either code supplied as input via `stdin`, the user may wish to consider using `pwgui`, a graphical means for constructing input. However, for posterity, the following is a brief overview of the critical sections of the input file, in this case for `pw.x` :

```
&CONTROL
  calculation='scf',
  restart_mode='from_scratch',
  prefix='silicon',
  pseudo_dir='/gpfs/home/wjb19/scratch/pseudo/',
  outdir='/gpfs/home/wjb19exit
  /scratch/tmp'
/
```

This input namelist specifies location for pseudopotential(s), temporary output, as well as calculation type and the nature of a possible restart. The calculation field string may take on a variety of values, the most common being `bands`, `scf` and `md`.

This section is followed immediately by a specification of the target system :

```
&SYSTEM
 ibrav=2, celldm(1)=10.20, nat=2, ntype=1, ecutwfc=18.0,
/
```

The total number of atoms (`nat`) must be specified, as well as the number of different types (`ntype`)

and energy cutoff for wavefunctions. The Bravais lattice index is given in `ibrav`, whose value is related to numerical cell dimensions given via `celldm` parameters OR via more traditional `a=...`, `b=...`, `c=...` specifications; all these parameters are described in the following matrix, including correspondence between `celldm`, `a/b/c` etc and applicability to symmetry specified via `ibrav`.

	<b>celldm</b> →	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>
<b>ibrav</b>	<b>Description</b>	<b>a</b>	<b>b</b>	<b>c</b>	<b>cosab</b>	<b>cosac</b>	<b>cosbc</b>
0	Read unit cell parameters from CELL_PARAMETERS (ie., specified later file)						
1	Cubic P (SC)	*					
2	Cubic F (FCC)	*					
3	Cubic I (BCC)	*					
4	Hexagonal and Trigonal P	*		*			
5	Trigonal R	*			*		
6	Tetragonal P (ST)	*		*			
7	Tetragonal I (BCT)	*		*			
8	Orthorhombic P	*	*	*			
9	Orthorhombic base-centered (BCO)	*	*	*			
10	Orthorhombic face-centered	*	*	*			
11	Orthorhombic body-centered	*	*	*			
12	Monoclinic P	*	*	*	*		
13	Monoclinic base-centered	*	*	*	*		
14	Triclinic P	*	*	*	*	*	*

Again, one may specify `celldm` parameters or `a, b, c` (in angstrom) etc but not both; if the former, `celldm(1)` is the lattice parameter `a` in bohr units; `celldm(2)` and `celldm(3)` are scaled by `a` ie., expressed in pure units. If specifying `ibrav=0`, then cell parameters appear in a final input field comprising lattice vectors and description of symmetry (note; not preceded with ampersand '&'):

```
CELL_PARAMETERS symmetry_class
  a(1,1) a(2,1) a(3,1)
  a(1,2) a(2,2) a(3,2)
  a(1,3) a(2,3) a(3,3)
```

where `symmetry_class` may be either cubic or hexagonal; if `celldm(1) ≠ 0`, lattice vectors are given in these units, otherwise lattice vectors are given in bohr and the length of the first lattice vector is equivalent to the lattice parameter. The namelist directly following `&SYSTEM` pertains to numerical algorithmic details of the DFT calculation:

```
&ELECTRONS
  diagonalization='david'
  mixing_mode = 'plain'
  mixing_beta = 0.7
```

```
conv_thr = 1.0d-8
/
```

There are several matrix diagonalization options available; Davidson (`david`) is default and is fast, 'cg' is conjugate gradient-like and slower but uses less memory. Mixing parameters and `conv_thr` affect the rate of convergence as one might expect. There are several options in particular for the nature of the mixing, the user is encouraged to experiment with these, paying close attention to numerical accuracy. If performing molecular dynamics, these namelists are accompanied by `&IONS` and `&CELL`, please consult the reference at the end of this section for further information on these and all namelists.

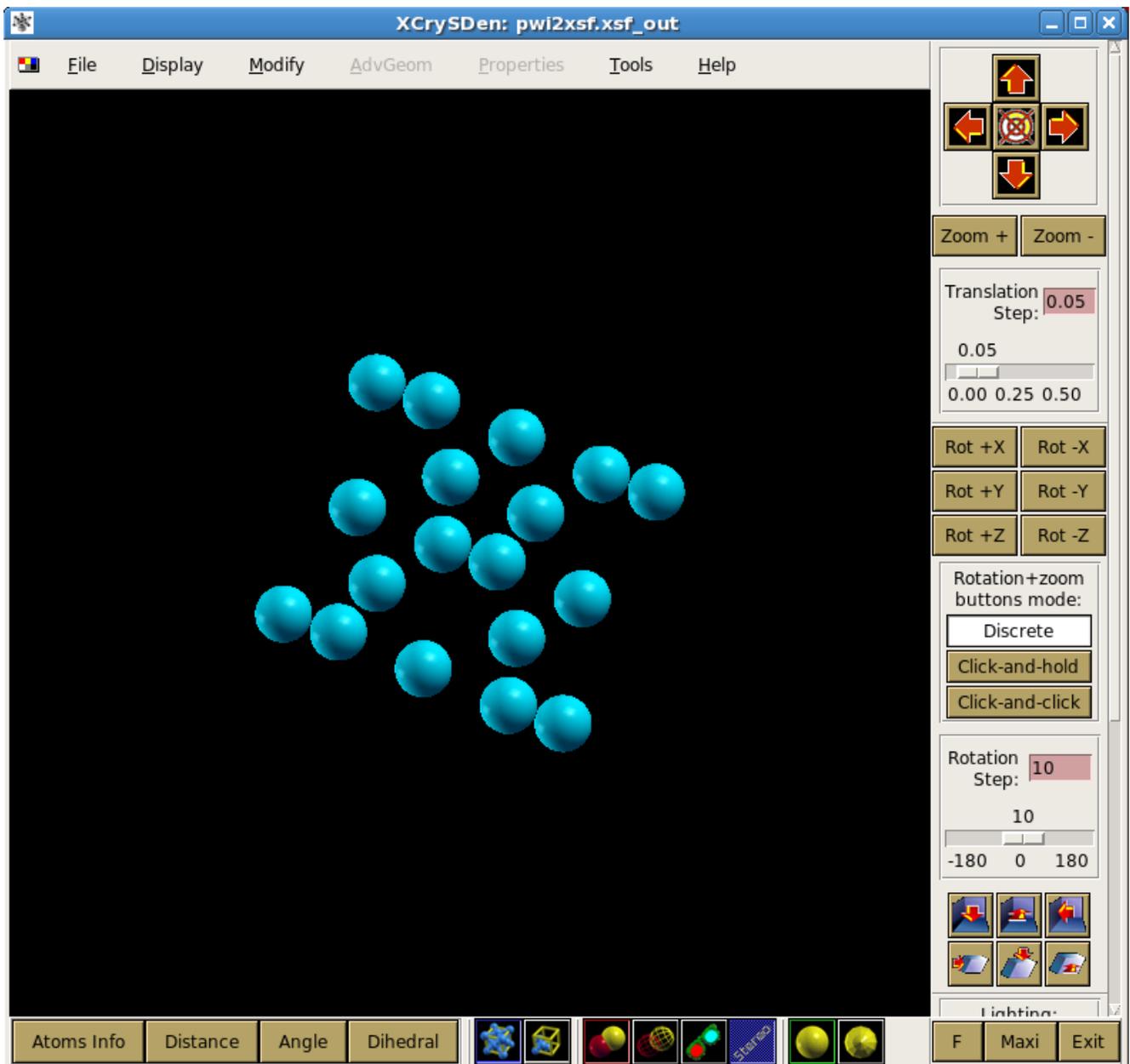
After all the namelists have been specified, a number of other fields are necessary in order to describe constituent atoms and positions, eg.,

```
ATOMIC_SPECIES
Si 28.086 Si.pz-vbc.UPF
ATOMIC_POSITIONS
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
```

The first section must give atomic label, mass, and the name of the pseudopotential to be used in the calculation, one line per unique atom. This section is directly followed by details of the unit cell, and finally the k-points within the Brillouin zone must be specified eg.,

```
K_POINTS
10
0.1250000 0.1250000 0.1250000 1.00
0.1250000 0.1250000 0.3750000 3.00
0.1250000 0.1250000 0.6250000 3.00
0.1250000 0.1250000 0.8750000 3.00
0.1250000 0.3750000 0.3750000 3.00
0.1250000 0.3750000 0.6250000 6.00
0.1250000 0.3750000 0.8750000 6.00
0.1250000 0.6250000 0.6250000 3.00
0.3750000 0.3750000 0.3750000 1.00
0.3750000 0.3750000 0.6250000 3.00
```

There are a number of ways to specify this data, here the default is used which gives x/y/z and weight in column four. Additionally, there is a gui utility `xcrysden` which provides a useful aid in examining input (as well as output) structure, by loading `pw.x` files; figure 2 contains a screenshot for the silicon example given here, and available as `example01` in the quantum espresso examples directory.



**Figure 2: screenshot of silicon in xcrsden**

**Online Reference for px.x :**

[http://www.quantum-esspresso.org/input-syntax/INPUT\\_PW.html](http://www.quantum-esspresso.org/input-syntax/INPUT_PW.html)

The following resource has many useful structures.

**American Mineralogist Database :**

<http://rruff.geo.arizona.edu/AMS/amcsd.php>

# Final Step(s)

There are many useful post-processing options available, including :

- Plotting
- Band structure
- Density of States
- Wannier Functions
- Normal Phonon modes
- NMR parameters

## Summary

- Select or create Pseudopotentials for constituent atoms
  - If creating new files, use `ld1.x` tool, test rigorously against various AE configurations using the `&test` namelist
  - Test using a simple system
- Create an input file for the target system; write by hand or use `pwgui`
  - Remember to use one OR other convention for symmetry, pay close attention to units
  - Must specify k-points, pseudopotentials and atomic species with positions in unit cell
- Post-process if desired
- 

## References

“Pseudopotentials that work: From H to Pu”, G.B.Bachelet, D.R.Hamann, M.Schluter, Phys Rev B, 4199-4228, 26(8), 1982

“Projector augmented wave method”, P. Blochl, Phys Rev B , 17953-17979, 50(24), 1994

“Efficient pseudopotentials for plane-wave calculations”, N.Troullier, J.L.Martins, Phys Rev B, 1993-2006, 43(3), 1991

“Soft Self-Consistent Pseudopotentials in a Generalized Eigenvalue Formalism”, D.Vanderbilt, Phys Rev B, 41, 7892, 1991