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Density Functional Theory with Quantum Espresso

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I/O Structure of QE, Part 1

https://www.quantum-espresso.org/

Key Features:

- DFT, time-dependent DFT, and many-body perturbation theory.
- Supports periodic systems, slab geometries, and isolated systems.
- Highly scalable and suitable for parallel computing.
- Band structure, phonon dispersion, magnetic properties, NMR, FTIR, Raman, XPS, and many more properties.

I/O Structure of QE, Part 1

The QE code suite consists of many distinct executables:

- `pw.x:` Main executable, electronic calculation, geometry optimization
- `pp.x:` Postprocessing utilities such as band structure, charge density
- `ph.x:` Phonon calculation
- `neb.x:` Nudged elastic bands
- `bands.x:` Prepare the bands for plotting
- And many more...

I/O Structure of QE, Part 1

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pw.x

- The input file is divided in section called CARDS
- Mandatory QE Cards
  - `CONTROL`: General information about the logistics of the run.
  - `SYSTEM`: Specify the physical properties of your system.
  - `ELECTRONS`: Parameters for the electronic scf calculation.
  - `ATOMICS_SPECIES`: The pseudopotential le
  - `ATOMIC_POSITIONS`: The positions of the atoms
  - `K_POINTS`: The Monkhorst-Pack grid size

I/O Structure of QE, Part 1

```
  &CONTROL
  ! What kind of calculation? scf/relax etc
  calculation='scf'
  ! Do you want to restart from an interrupted run?
  restart_mode='from_scratch'
  ! The location of the pseudopotential files?
  pseudo_dir = './pseudo/'
  ! Where the wavefunctions should be written.
  outdir='./tempdir/'
  ! Prefix for the wavefunctions etc.
  prefix='cu'
/
```

I/O Structure of QE, Part 1

```
&SYSTEM
! Crystal symmetry: ibrav=0-14
ibrav = 2
! Lattice constants and/or angles: celldm(1-6)
celldm(1) =6.73
! Total number of atoms in the sim cell
nat= 1
! Number of elements
ntyp= 1
! Kinetic energy cutoff in Rydberg
ecutwfc = 25.0
! Cutoff for density in Rydberg
ecutrho = 300.0
! Smearing for metals
occupations='smearing'
! Type of smearing: mv, fd, g
smearing='marzari-vanderbilt'
! Width of the smearing functions
degauss=0.02
```

I/O Structure of QE, Part 1

```
 &ELECTRONS
 ! Diagonalization algorithm for the scf run
 diagonalization='cg'
 ! Break condition on the total energy
 conv_thr = 1.0e-8
 ! Density mixing level.
 mixing_beta = 0.7
/
```

I/O Structure of QE, Part 1

```
! The pseudopotential
ATOMIC_SPECIES
Cu 63.55 Cu.pz-d-rrkjus.UPF
! Atomic position in terms of the lattice constant
ATOMIC_POSITIONS alat
Cu 0.0 0.0 0.0
! The MP grid size
K_POINTS (automatic)
8 8 8 0 0 0
```

Next: I/O Structure of QE, Part 2

This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101101903. The JU receives support from the Digital Europe Programme and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Türkiye, Republic of North Macedonia, Iceland, Montenegro, Serbia

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I/O Structure of QE, Part 2

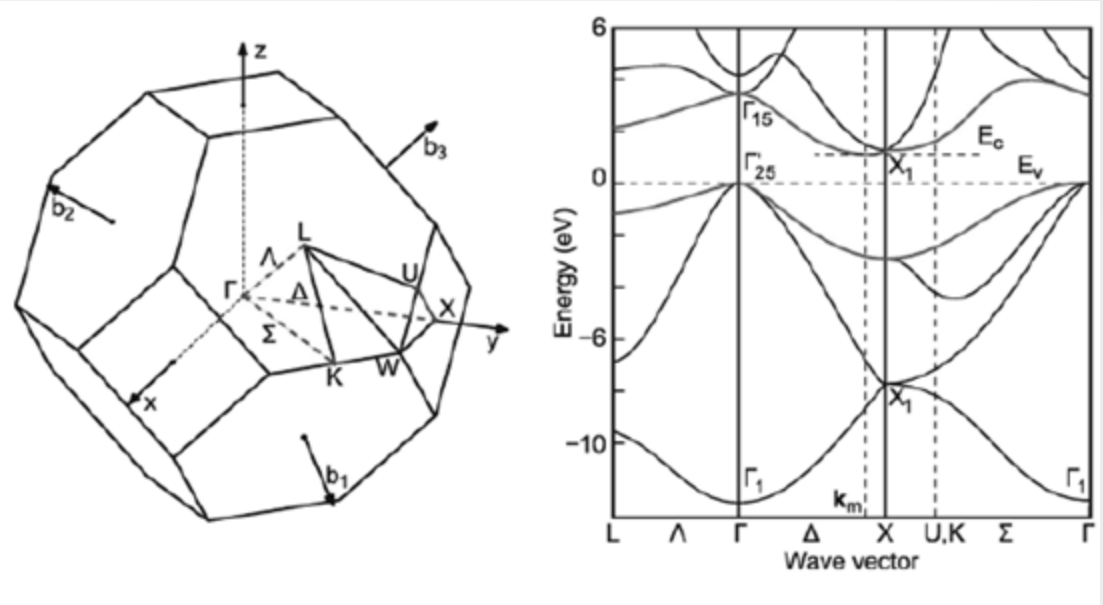
Postprocessing

- Several utility tools for analysis, usually performed following a self-consistent energy calculation.
- The main executable is `pp.x`, which extracts data from various output files and prepares it for analysis.
- Some of the most frequently used utility executables are
  - bands.x
  - plotbands.x
  - plotrho.x

I/O Structure of QE, Part 2

Postprocessing - Band Structure

- Energy as a function of the k vector along high-symmetry directions in the Brillouin Zone



I/O Structure of QE, Part 2

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Postprocessing – Band Structure

The band structure calculation is performed in a few steps.

Step 1: First, conduct an electronic minimization (`pw.x`)
Step 2: Run a non-self-consistent calculation to calculate the energies along high-symmetry directions within the Brillouin zone (`pw.x`)
Step 3: Run a PP calculation to extract data and prepare it for plotting (`bands.x`)
Step 4: Finally run a plotband calculation to produce the plot (`plotband.x`)

I/O Structure of QE, Part 2

```
 &control
    calculation='bands'
    pseudo_dir = './pseudo/',
    outdir='./tempdir/',
    prefix='si'
/
....
....
....
K_POINTS crystal_b
5
 0.0000 0.5000 0.0000 20   !L
 0.0000 0.0000 0.0000 30   !G
-0.500 0.0000 -0.500 10    !X
-0.375 0.2500 -0.375 30    !U
```

- This is a regular input file that is to be run with `pw.x`.
- The most significant difference is the K_POINTS card, which is not uniform, but k-points are chosen along the high symmetry directions between special points in the Brillouin zone.
- `crystal_b` means that the k points are given in fractional coordinates in terms of $\mathbf{b}_i$

I/O Structure of QE, Part 2

```
&bands
    ! The same prefix as the one in in.band
    prefix  = 'si'
    ! Where to get the result of in.band from
    outdir = './tempdir/'
    ! The output file
    filband = 'sibands.dat'
    ! Classify the bands with respect to irreps
    lsym=.true.,
 /
```

- This input file is to be run using `bands.x`

I/O Structure of QE, Part 2

```
! The output of the bands.x calculation
sibands.dat
! The range of energies
-6.0 10
! XMGrace output
sibands.xmgr
! PS otuput
sibands.ps
! The Fermi energy
6.255
! Energy increment and the zero of the plot
1.0 6.255
```

- This input file is to be run using `plotbands.x`
- The Fermi energy is obtained from the initial electronic minimization calculation.

I/O Structure of QE, Part 2

Charge Density

```
&inputpp
prefix  = 'si'          ! Usual prefix
outdir = '~/tmpdir'     ! Usual storage directory
filplot = 'sicharge'    ! Which file to save
plot_num= 0             ! What to save in filplot (0: density)
/
&plot
nfile = 1                 ! How many densities to superpose
filepp(1) = 'sicharge'    ! Where to read the file to plot
weight(1) = 1.0           ! Coefficient of the density
iflag = 3                 ! Dimensionality
output_format = 2         ! Which software (5: XCrysDen)
fileout = 'si.rho.xsf'    ! Output for plotting
/
```

- The charge density is stored at the end of a regular run on a real space grid.
- The XSF format can be visualized by using the software `XCrysDen`.
- Instead of a single file difference densities can also be subtracted from one another.

Next: Exercise 1 & 2

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