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Basics of Quantum Espresso

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Presentation Summary

- Intro to Quantum Espresso (QE)
- Input files structure
- Pseudopotential approach, Plane waves, Cutoff, SOC
- Structure visualization with VESTA
- DFT band structure calculation
- PBE0 or HSE scf calculation
- Phonon calculation
- Slurm input files

Quantum Espresso (QE) for DFT calculations

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



- *Open-source* code within the plane-wave and pseudopotential (also PAW) approaches
- Highly parallel linear algebra libs (MKL) tested on Intel, AMD, Cray XC HPC machines
- Widely used, suits well with most EuroHPC architectures.
- Refs: P. Giannozzi et al., [J. Phys.: Condens. Mat., 39, 21,\(2009\)](#) (citations: 33250),
P. Giannozzi et al., [J. Phys.: Condens. Mat., 46, 29, \(2017\)](#) (citations: 9595)

Download and compile QE

```
# 1a. Get the latest QE source (v7.5)
$ git clone https://github.com/QEF/q-e.git
$ cd q-e

# 1b. OR download from: https://www.quantum-espresso.org/download-page/
# you need to register first, then download QE 7.5, and extract (untar)
$ cd q-e

# 2. Quick auto-detect build (CPU-only is fine) and compile
$ ./configure          # add flags if needed, e.g. MPIF90=mpif90
$ make -j pw pp ph     # build main executables

# 3. Test run from the QE source tree:
$ cd examples/example01
$ ./run\_example      # or: pw.x -in si.in
```

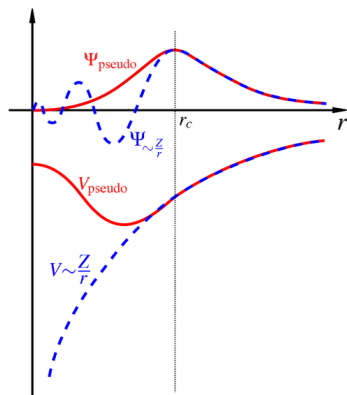
QE modules / capabilities

- `pw.x` Ground state DFT, SCF, Charge Density, Forces And Stresses, Geometry Optimization, Band structure
- `cp.x` *Ab initio* Molecular Dynamics, Structural Evolution in time
- `ph.x` Phonons, Dielectric Constants, Electron-Phonon Matrix, Infrared/Raman spectra
- `pp.x` Post-processing tool, Band Structure and Phonon Dispersion Plotting, DOS, Charge Density Visualization
- `neb.x` Nudged Elastic Band, Reaction Barrier, Atomic Migration
- `epsilon.x` Dielectric Functions, Absorption, Independent Particle Approx.
- `epw.x` Electron-Phonon Coupling (EPC), Dense Grids by Wannier Interp., Mobilities, Conductivity, Superconductivity, Ultrafast Dynamics, Phonon Linewidths, Polarons
- `ZG.x` Finite temperature DFT simulations, Anharmonicity, Nonperturbative EPC

Input structure for pw.x - I, [link](#)

```
&control
  calculation = 'scf' ! calc. type, 'nscf', 'bands', 'relax', 'vc-relax'
  restart_mode = 'from_scratch' ! if 'restart' starts from interrupted run
  prefix = 'scf' ! for output files
  pseudo_dir = '/path_to_pseudo/' ! directory to pseudopot. files
  outdir = './' ! output files are found in this directory
  tprnfor=.true. ! to calculate and print forces
  disk_io = 'low' ! Specifies the amount of output
/
&system
  ibrav = 2 ! Bravais-lattice index, 1 --> SC, 2 --> FCC, 3 --> BCC ...
  celldm(1) = 10.20, ! Lattice parameter "a" (in BOHR)
  nat = 2 ! number of atoms in the unit cell
  ntyp = 1 ! number of types of atoms in the unit cell --> ATOMIC_SPECIES
  ecutwfc = 50.00 ! kinetic energy cutoff (Ry) for wavefunctions
/
...
```

The pseudopotential approach



- Libraries: [SSSP](#), [SG15 ONCV](#), [PseudoDojo ONCV](#), [GBRV US](#)

- Replaces core electrons → not in chemical bonding
- Core electrons with the nucleus form ionic core
- Focuses on valence electrons → less KS states
- Pseudo-wavefunctions are smoother, fewer nodes compared to the true wavefunctions, making them easier and faster to handle (match above a radius r_c).
- Allows for more complex systems to be studied efficiently than would not be possible with “all-electron” methods
- PPs examples: Norm-Conserving by [Troullier and Martins](#), Ultrasoft (US) by [Vanderbilt](#), Optimized Norm-Conserving Vanderbilt (ONCV) by [Haman](#)
- An alternative to the PP method is [PAW](#)

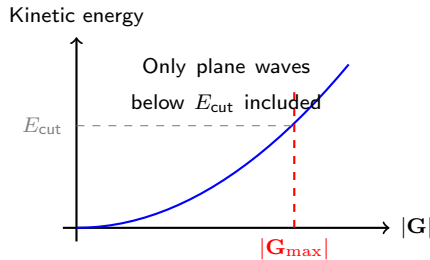
Plane-Wave Cutoff Energy

Kohn–Sham orbitals in plane-wave DFT:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{n\mathbf{k}}(\mathbf{G}) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

Infinite recip. latt. vectors $\mathbf{G} \Rightarrow$ need a **cutoff**:

$$E_{\text{cut}} = \frac{\hbar^2}{2m_e} |\mathbf{k} + \mathbf{G}_{\text{max}}|^2$$



Only plane waves with kinetic energy $\leq E_{\text{cut}}$ are included.

- Higher $E_{\text{cut}} \Rightarrow$ higher accuracy, Lower $E_{\text{cut}} \Rightarrow$ faster but less accurate.
- E_{cut} depends on pseudopotential type (harder potentials need higher cutoff).

Note: Converge E_{cut} by testing total energy/forces until changes $<$ few meV/atom.
(see hands-on)

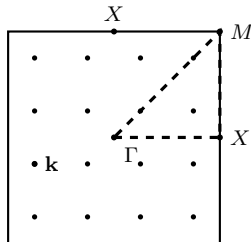
Input structure for pw.x - II, [link](#)

```
&electrons
  diagonalization = 'david' ! or 'cg' iterative solver for KS eigenstates
  mixing_mode= 'plain' ! how n(r) is mixed: n_new = (1-a) n_old + a n_out
  mixing_beta = 0.70 ! defines a parameter, typically 0.3-0.7
  conv_thr = 0.1D-08 ! Convergence threshold for SCF in n(r)
/
&ions
  ion_dynamics = 'bfgs' ! if calculation = 'relax' or 'vc-relax', relax ions
/
&cell
  cell_dynamics = 'bfgs' ! if calculation = 'vc-relax' to relax cell param.
ATOMIC_SPECIES
  Si 28.086 Si.upf ! species, mass in a.u., and pseudofile name
                ! numb. of entries = ntyp
...
```

Input structure for pw.x - III, [link](#)

```
K_POINTS automatic
  6   6   6   0   0   0 ! uniform grid with no offset
! OR
! K_POINTS tpiba ! read k-points in Cartes. Coords, in units of 2 pi/a
! 100 ! number of k-points
! k_x(1) k_y(1) k_z(1) wk(1) ! Coords of 1st k-point and weight
! ...
! k_x(100) k_y(100) k_z(100) wk(100) ! Coords of 100th k-point and weight
CELL_PARAMETERS (angstrom) ! if ibrav=0
-2.69880    0.00000    2.69880
  0.00000    2.69880    2.69880
-2.69880    2.69880    0.00000
ATOMIC_POSITIONS (crystal) ! can be angstroms (i.e. Cartes. Coords.)
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
```

k -points in Practice



Square: 1st BZ with Monkhorst-Pack k -mesh and a band path $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$

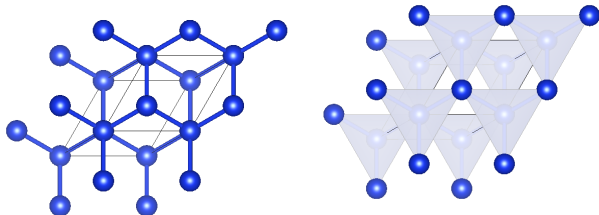
- Finer k -meshes \Rightarrow Check for convergence of:
 - ▶ Total energies and forces
 - ▶ Band structures for the path, Density of states
 - ▶ Optical spectra
- For large simulations cells (supercells) \Rightarrow only the Γ -point may be sufficient.

Structure Visualization with VESTA I

- [VESTA](#): Visualization for Electronic and STructural Analysis
- Prepare the file `geometry.in` for Si (FHI-aims format):

```
lattice_vector  -2.69880    0.00000    2.69880 # in Å
lattice_vector   0.00000    2.69880    2.69880
lattice_vector  -2.69880    2.69880    0.00000
atom_frac  0.00 0.00 0.00  Si # use "atom" for Cart. Coords. in Å
atom_frac  0.25 0.25 0.25  Si
```

- Then: `vesta geometry.in`
- Other formats: [POSCAR](#), [.xsf](#),
[.xyz](#), [.cif](#), and many others

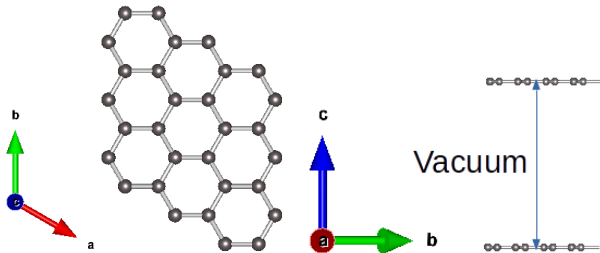


Structure Visualization with VESTA II

- Prepare the file `geometry.in` for graphene:

```
lattice_vector    2.46708    0.00000    0.00000
lattice_vector   -1.23354    2.13655    0.00000
lattice_vector    0.00000    0.00000   30.00000
atom      0.00000    0.00000    0.00000  C
atom      0.00000    1.42437    0.00000  C
```

- Then: `vesta geometry.in`
- We add **vacuum** to avoid interaction of periodic images in 2D materials
- Set $k_z = 1$, i.e. grid to:
6 6 1 0 0 0

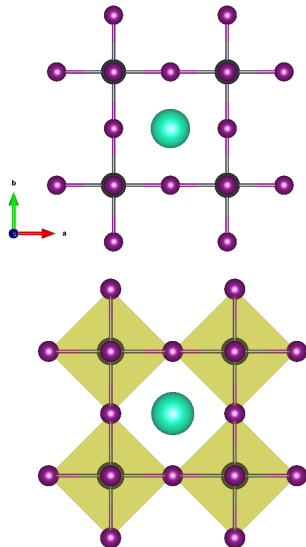


Structure Visualization with VESTA III

- Prepare the file `geometry.in` for cubic CsPbI_3 :

```
lattice_vector  6.2509 0.0000 0.00000
lattice_vector  0.0000 6.2509 0.00000
lattice_vector  0.0000 0.0000 6.2509
atom_frac  0.500000 0.500000 0.500000  Cs
atom_frac  0.000000 0.000000 0.000000  Pb
atom_frac  0.000000 0.000000 0.500000  I
atom_frac  0.000000 0.500000 0.000000  I
atom_frac  0.500000 0.000000 0.000000  I
```

- Then: `vesta geometry.in`
- Octahedra coordination



Symmetries in QE: graphene

```

atomic species  valence  mass  pseudopotential
C               4.00    12.01070  C ( 1.00)

24 Sym. Ops., with inversion, found (12 have fractional translation)
Space Group: P6/mmm (#191)
s                                frac. trans.

ism = 1  identity
cryst.  s( 1) = (   1   0   0 )
           (   0   1   0 )
           (   0   0   1 )
cart.    s( 1) = ( 1.0000000  0.0000000  0.0000000 )
           ( 0.0000000  1.0000000  0.0000000 )
           ( 0.0000000  0.0000000  1.0000000 )

ism = 2  180 deg rotation - cart. axis [0,0,1]  Fractional Translation
cryst.  s( 2) = (  -1   0   0 )  f = ( -0.3333330 )
           (   0  -1   0 )  (  0.3333340 )
           (   0   0   1 )  (  0.0000000 )
cart.    s( 2) = ( -1.0000000  0.0000000  0.0000000 )  f = ( -0.5000000 )
           (  0.0000000 -1.0000000  0.0000000 )  (  0.2886757 )
           (  0.0000000  0.0000000  1.0000000 )  (  0.0000000 )

ism = 3  180 deg rotation - cart. axis [0,1,0]
cryst.  s( 3) = (  -1   0   0 )
           (   1   1   0 )
           (   0   0  -1 )  Symmetry Operations
cart.    s( 3) = ( -1.0000000  0.0000000  0.0000000 ) (lower comp. cost)
           (  0.0000000  1.0000000  0.0000000 )
           (  0.0000000  0.0000000 -1.0000000 )
    
```

- In &control add verbosity = 'high' to print symmetries

- Graphene is semi-metal (Dirac-cone):

```

occupations = 'smearing'
smearing='gaussian',
degauss=0.005d0
assume_isolated = '2D'
    
```

- QE searches for Syms. of the input structure and prints them: reduces computat. burden, reducing number of **k**-points
- Space group: $P \rightarrow$ Primitive lattice, $6 \rightarrow$ 6fold rot. axis, $mmm \rightarrow$ mirror planes

Symmetries in QE: Silicon

```
atomic species  valence  mass  pseudopotential
Si              4.00    28.08600  Si( 1.00)

48 Sym. Ops., with inversion, found (24 have fractional translation)
    Space group: Fd-3m (# 227)
              s              frac. trans.

    isym = 1      identity

cryst.  s( 1) = (   1       0       0       )
           (   0       1       0       )
           (   0       0       1       )

cart.   s( 1) = (  1.0000000  0.0000000  0.0000000 )
           (  0.0000000  1.0000000  0.0000000 )
           (  0.0000000  0.0000000  1.0000000 )

    isym = 2      180 deg rotation - cart. axis [0,0,1]

cryst.  s( 2) = (   0       1      -1       )
           (   1       0      -1       )
           (   0       0      -1       )

cart.   s( 2) = ( -1.0000000  0.0000000  0.0000000 )
           (  0.0000000 -1.0000000  0.0000000 )
           (  0.0000000  0.0000000  1.0000000 )

    isym = 3      180 deg rotation - cart. axis [0,1,0]

cryst.  s( 3) = (   -1       0       0       )
           (   -1       0       1       )
           (   -1       1       0       )

cart.   s( 3) = ( -1.0000000  0.0000000  0.0000000 )
           (  0.0000000  1.0000000  0.0000000 )
           (  0.0000000  0.0000000 -1.0000000 )
```

- In &control add verbosity = 'high' to print symmetries
- Silicon is semiconductor, occupations fixed: 0 (CB) or 1 (VB)
- QE searches for Syms. of the input structure and prints them: reduces computat. burden, reducing number of **k**-points
- Space group: $F \rightarrow$ Face-centered cubic, $d \rightarrow$ Diamond glide plane, $-3 \rightarrow$ inversion with a 3fold rotation, $m \rightarrow$ mirror plane
- Other Fd-3m materials: Ge, Diamond

Symmetries in QE: CsPbI₃

```
atomic species  valence  mass  pseudopotential
Cs              9.00    132.90545  Cs( 1.00)
Pb             14.00    207.20000  Pb( 1.00)
I               7.00    126.90447  I ( 1.00)

48 Sym. Ops., with inversion, found
    Space group: Pm-3m (# 221)
              s          frac. trans.

isym = 1      identity

cryst.  s( 1) = (      1      0      0      )
          (      0      1      0      )
          (      0      0      1      )

cart.    s( 1) = ( 1.0000000  0.0000000  0.0000000 )
          ( 0.0000000  1.0000000  0.0000000 )
          ( 0.0000000  0.0000000  1.0000000 )

isym = 2      180 deg rotation - cart. axis [0,0,1]

cryst.  s( 2) = (     -1      0      0      )
          (      0     -1      0      )
          (      0      0      1      )

cart.    s( 2) = ( -1.0000000  0.0000000  0.0000000 )
          ( 0.0000000 -1.0000000  0.0000000 )
          ( 0.0000000  0.0000000  1.0000000 )

isym = 3      180 deg rotation - cart. axis [0,1,0]

cryst.  s( 3) = (     -1      0      0      )
          (      0      1      0      )
          (      0      0     -1      )

cart.    s( 3) = ( -1.0000000  0.0000000  0.0000000 )
          ( 0.0000000  1.0000000  0.0000000 )
          ( 0.0000000  0.0000000 -1.0000000 )
```

- In `&control` add `verbosity = 'high'` to print symmetries
- CsPbI₃ is semiconductor, occupations fixed: 0 (CB) or 1 (VB)
- Pb is a heavy atom → large relativistic effects, add in `&system`:

```
lspinorb = .true.
noncolin = .true.
```

- We need to account for spin-orbit coupling (SOC) on the electronic structure
- Space group: $P \rightarrow$ Primitive cubic, $m \rightarrow$ mirror plane,

Spin–Orbit Coupling (SOC)

Physical meaning:

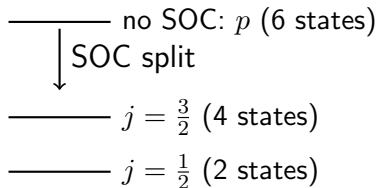
- Interaction between an electron's **spin magnetic moment** and the **magnetic field** produced by its orbital motion
- Originates from relativistic effects (*Dirac equation correction*).
- Couples spin (**S**) and orbital (**L**) angular momenta.

Hamiltonian term:

$$\hat{H}_{SO} = \frac{1}{2m^2c^2r} \frac{dV}{dr} \hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$$

- $V(r)$: potential due to nucleus
- Energy splitting of states with $j = l \pm \frac{1}{2}$

Example: *p*-level splitting



In DFT:

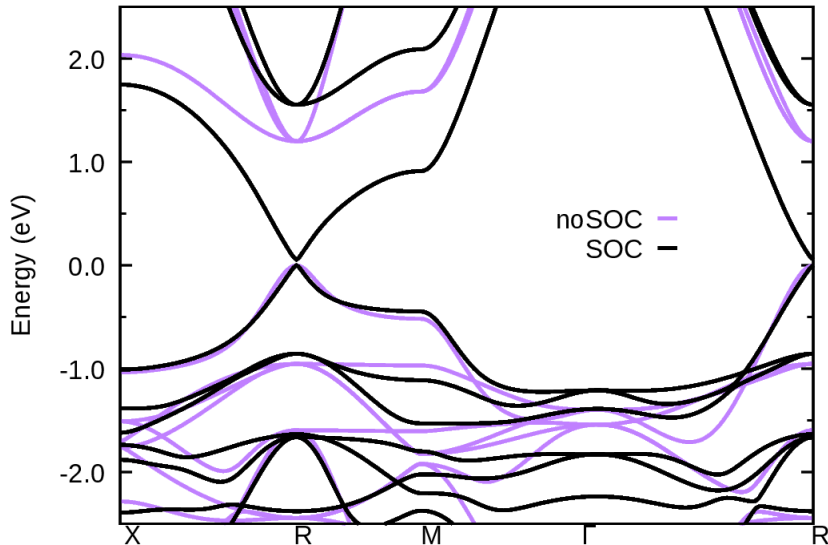
- Use fully relativistic pseudopotentials
- QE: `noncolin=.true.`, `lspinorb=.true.`
- Important for: Pb, Bi, Pt, W, topological insulators

Band structure calculation

```
&control
  calculation='bands', restart_mode='from_scratch', prefix = 'scf',  outdir='./',
  pseudo_dir='~/path_to_fully_relativistic_pseudos/'
/
&system
  ibrav=1, nat=5, ntyp=3, ecutwfc= 120, A = 6.2456, nbnd = 60, ! important to add empty bands
  lspinorb = .true., noncolin = .true.
/
&electrons
  diagonalization='david', mixing_mode='plain', mixing_beta=0.7, conv_thr=1e-9
/
ATOMIC_SPECIES
Cs 132.90545 Cs.upf
Pb 207.2      Pb.upf
I  126.90447 I.upf
ATOMIC_POSITIONS (crystal)
Cs  0.500000 0.500000 0.500000
Pb  0.000000 0.000000 0.000000
I   0.000000 0.000000 0.500000
I   0.000000 0.500000 0.000000
I   0.500000 0.000000 0.000000
... continue to K_POINTS --->
```

	K_POINTS	{crystal_b}			
	5				
	0.5000	0.0000	0.000000	106	! X
	0.5000	0.5000	0.500000	75	! R
	0.5000	0.5000	0.000000	106	! M
	0.0000	0.0000	0.000000	130	! Gamma
	0.5000	0.5000	0.500000	1	! R

Band structure calculation



- $E_g^{\text{noSOC}} = 1.2 \text{ eV}$
- $E_g^{\text{SOC}} = 0.06 \text{ eV}$
- $E_g^{\text{expt}} = 1.78 \text{ eV}$
- SOC leads to a band gap reduction of $\sim 1 \text{ eV}$
- Far from experiment
- Need to account for **local disorder** in supercells
- Need to account for better **treatment to xc effects**

Hybrid functional calculation: PBE0 $\Delta E_g^{\text{PBE0}} = 1 \text{ eV}$ for CsPbI_3

```
&control
  calculation='nscf', restart_mode='from_scratch', prefix = 'scf',  outdir='./',
  pseudo_dir='~/path_to_fully_relativistic_pseudos/'
/
&system
  ibrav=1, nat=5, ntyp=3, ecutwfc= 80, A = 6.2456, nbnd = 60, ! important to add empty bands
  lspinorb = .true., noncolin = .true.
  input_dft = 'pbe0',           ! Specifies the PBE0 hybrid functional, or 'HSE'
  exx_fraction = 0.25,          ! PBE0 uses 25% exact exchange
  screening_parameter = 0.0,    ! Set to 0 for full-range hybrid functional
/
&electrons
  diagonalization='david', mixing_mode='plain', mixing_beta=0.7, conv_thr=1e-9
/
ATOMIC_SPECIES
Cs 132.905 Cs.upf
Pb 207.2 Pb.upf
I 126.904 I.upf
K_POINTS {automatic}
2 2 2 0 0 0
... continue to ATOMIC_POSITIONS --->
ATOMIC_POSITIONS (crystal)
Cs  0.500000 0.500000 0.500000
Pb  0.000000 0.000000 0.000000
I   0.000000 0.000000 0.500000
I   0.000000 0.500000 0.000000
I   0.500000 0.000000 0.000000
```

Phonon Calculation: `ph.x` - [link](#)

Phonons of Silicon

`&inputph`

```
amass(1)= 28.0855,  
prefix = 'si' ! where charge density is saved from scf  
outdir = './' ! output directory  
fildyn = 'si.dyn' ! File where the dynamical matrix  
tr2_ph = 1.0d-14 ! Threshold for self-consistency > 1.0d-12  
ldisp = .true. ! run calculates phonons for a grid nq1xnq2xnq3  
nq1 = 4 ! Monkhorst-Pack grid for phonons  
nq2 = 4  
nq3 = 4
```

Calculation within Density Functional Perturbation Theory ([DFPT](#))

Phonon Calculation: q2r.x - [link](#), matdyn.x - [link](#)

```
&input                                q2r.in
  fildyn='si.dyn',
  flfrc = 'si.444.fc' ! output file for Interatomic Force Constants in real space
/
```

```
&input                                matdyn.in
  asr='crystal', ! the type of Acoustic Sum Rule imposed
  amass(1)=28.0855, flfrc='si.444.fc', flfrq='si.freq', ! output file for frequencies
  q_in_cryst_coord = .false., q_in_band_form = .true. ! q-points in band form as for k-points
/
```

```
9
0      0      0      100
0.75   0.75   0.0      1
0.2500 1.0000 0.2500 100
0.000  1      0.000 100
0      0      0      100
0.5000 0.5000 0.5000 100
0      1      0      100
0.5000 1.0000 0      100
0.5000 0.5000 0.5000 100
```

