PART 11

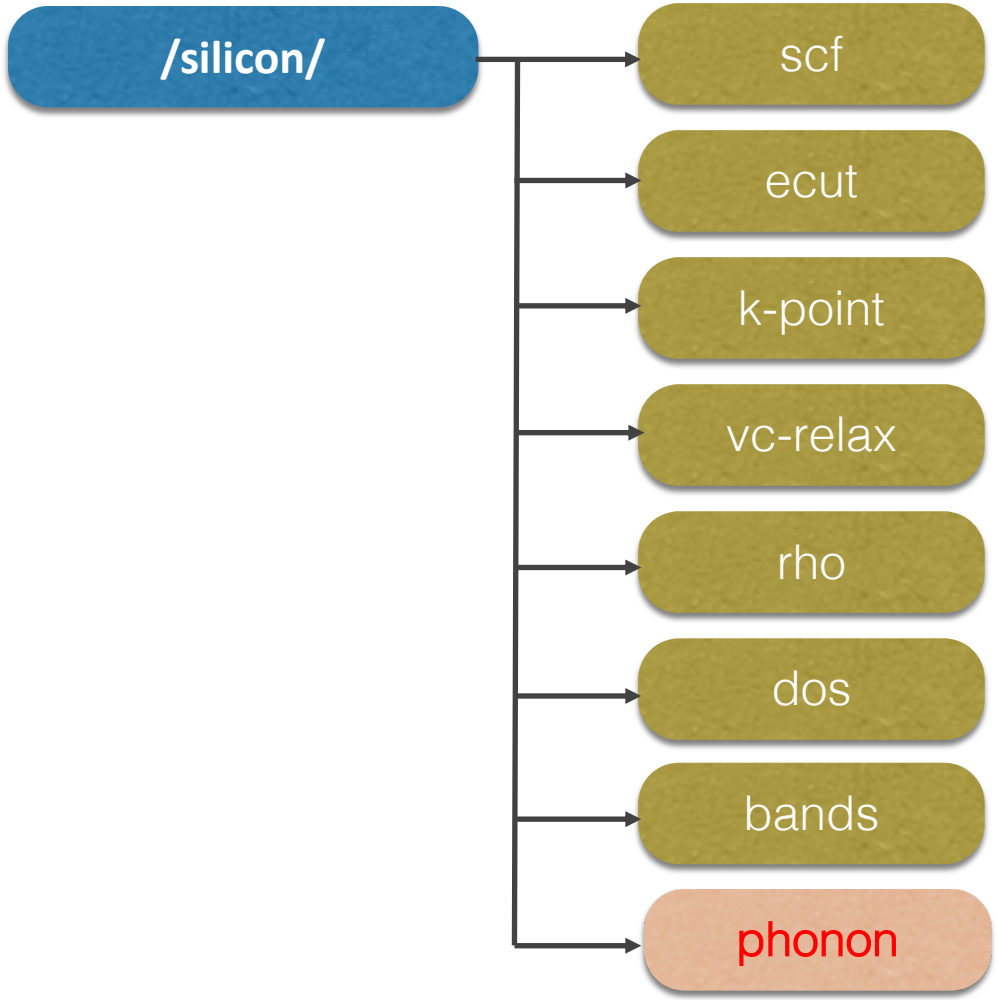
MATERIAL DESIGN

QUANTUM ESPRESSO PHONON

HANDS-ON #3

Hands-on #3 Phonon dispersion

Files for phonon



- Step 1: SCF calculation (Hands-on #1)
- Step 2: Calculation of dynamical matrices on q-vectors (**ph.x**)
- Step 3: Calculation of IFC's in real space (**q2r**)
- Step 4: A plot of the phonon DOS (**matdyn**)

Command:

```
$ pw.x < Si.scf.in > Si.scf.out
$ ph.x < Si.ph.in > Si.ph.out
$ q2r.x <Si.q2r.in > Si.q2r.out
$ matdyn.x <Si.matdyn.in > Si.matdyn.out
```

Phonon

Command:

```
$ pw.x < Si.scf.in > Si.scf.out
$ ph.x < Si.ph.in > Si.ph.out
$ q2r.x <Si.q2r.in > Si.q2r.out
$ matdyn.x <Si.matdyn.in > Si.matdyn.out
```

Step 1: SCF calculation (Hands-on #1)
Step 2: Calculation of dynamical matrices on q-vectors
Step 3: Calculation of IFC's in real space
Step 4: A plot of the phonon DOS

Si.ph.in

```
phonon calc.
&inputph
 outdir="../tmp/",
 prefix="si",
 tr2_ph = 1d-14,
 ldisp = .true.,
 nq1=4, nq2=4, nq3=4,
 amass(1)=28.0855,
 fildyn='si.dyn',
/
```

q-point

Interatomic Force Constants (IFC's) in real space

$$C_{st}^{ab}(\boldsymbol{R}) = \frac{\partial^2 E}{\partial u_s^a(\mathbf{0})\partial u_t^b(\boldsymbol{R})} = \frac{1}{N_c}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{R}}\ \tilde{C}_{st}^{ab}(\boldsymbol{q})$$

ph.x

- Calculation of $C_{st}^{ab}(\mathbf{q})$ on a suitable grid of $\mathbf{q}$-vectors

Density functional perturbation theory (DFPT): direct calculation of second-order derivatives of the energy

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Phonons and related crystal properties from density-functional perturbation theory

Stefano Baroni, Stefano de Gironcoli, Andrea Dal Corso, and Paolo Giannozzi
Rev. Mod. Phys. **73**, 515 – Published 6 July 2001

https://www.quantum-espresso.org/Doc/INPUT_PH.html

q2r

Command:

```
$ pw.x < Si.scf.in > Si.scf.out
$ ph.x < Si.ph.in > Si.ph.out
$ q2r.x <Si.q2r.in > Si.q2r.out
$ matdyn.x <Si.matdyn.in > Si.matdyn.out
```

Step 1: SCF calculation (Hands-on #1)
Step 2: Calculation of dynamical matrices on q-vectors
Step 3: Calculation of IFC's in real space
Step 4: A plot of the phonon DOS

Si.ph.in

```
phonon calc.
&inputph
 outdir="../tmp/",
 prefix="si",
 tr2_ph = 1d-14,
 ldisp = .true.,
 nq1=4, nq2=4, nq3=4,
 amass(1)=28.0855,
 fildyn='si.dyn',
/
```

Si.q2r.in

```
&input
 fildyn='si.dyn',
 zasr='simple',
 flfrc='si.fc',
/
```

Density functional perturbation theory (DFPT): direct calculation of second-order derivatives of the energy

Interatomic Force Constants (IFC's) in real space

$$C_{st}^{ab}(\boldsymbol{R}) = \frac{\partial^2 E}{\partial u_s^a(\mathbf{0})\partial u_t^b(\boldsymbol{R})} = \frac{1}{N_c}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{R}}\,\tilde{C}_{st}^{ab}(\boldsymbol{q})$$

q2r.x

ph.x

- Calculation of $C_{s\,t}^{a\,b}(\mathbf{q})$ on a suitable grid of $\mathbf{q}$-vectors
- Fourier transform to real space

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Phonons and related crystal properties from density-functional perturbation theory

Stefano Baroni, Stefano de Gironcoli, Andrea Dal Corso, and Paolo Giannozzi
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matdyn dos

Command:

```
$ pw.x < Si.scf.in > Si.scf.out
$ ph.x < Si.ph.in > Si.ph.out
$ q2r.x <Si.q2r.in > Si.q2r.out
$ matdyn.x <Si.matdyn.dos.in > Si.matdyn.dos.out
```

Step 1: SCF calculation (Hands-on #1)
Step 2: Calculation of dynamical matrices on q-vectors
Step 3: Calculation of IFC's in real space
Step 4: A plot of the phonon DOS

Si.matdyn.dos.in

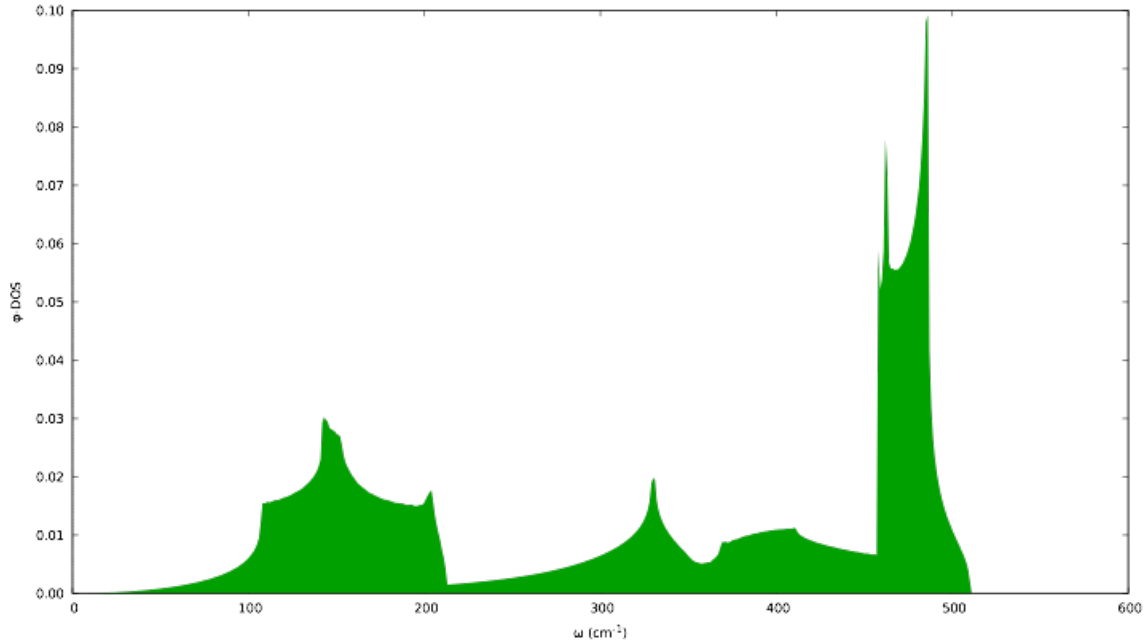
```
&input
 asr='simple',
 dos=.true.,
 amass(1)=28.0855,
 flfrc='si.fc',
 fldos='si.phdos',
 nk1=50,nk2=50,nk3=50,
/
```

→ Interatomic force constants (IFC's) in real space

→ Data file of phonon DOS

Command:

```
$ gnuplot < si_phdos.gnu
```



https://www.quantum-espresso.org/Doc/INPUT_DYNMAT.html

matdyn freq

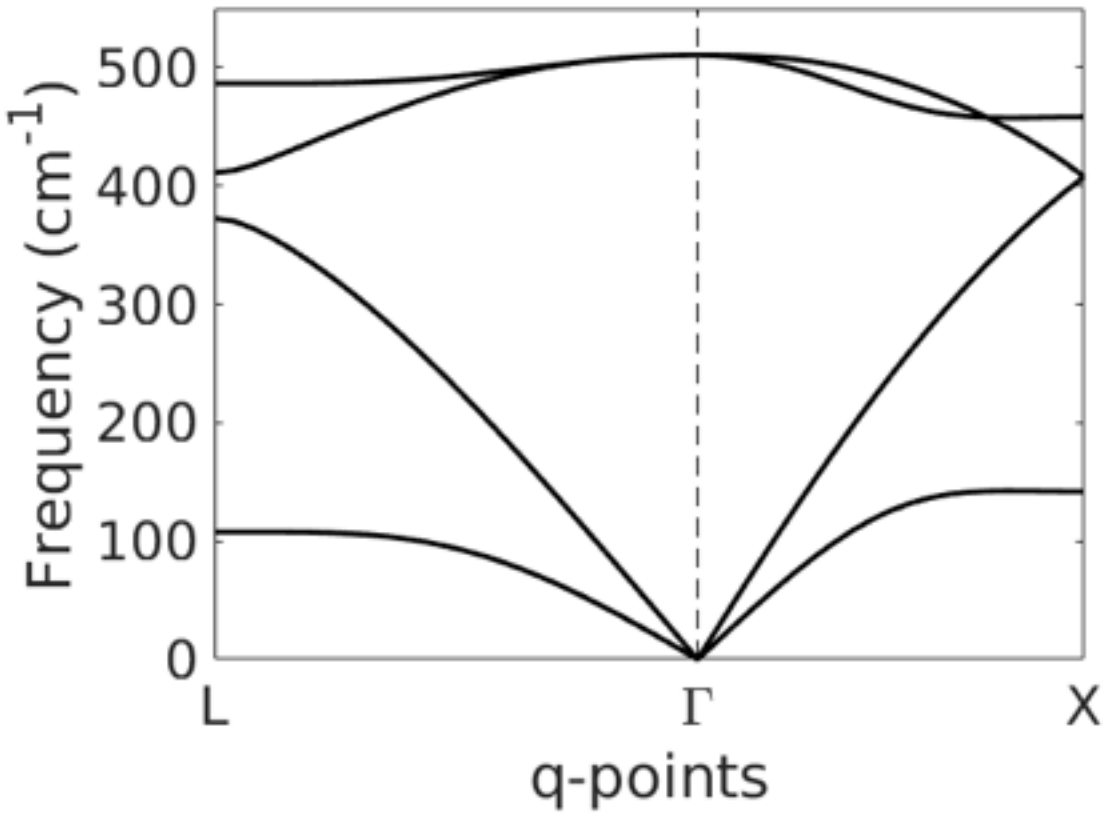
Command:

```
$ pw.x < Si.scf.in > Si.scf.out
$ ph.x < Si.ph.in > Si.ph.out
$ q2r.x <Si.q2r.in > Si.q2r.out
$ matdyn.x <Si.matdyn.freq.in > Si.matdyn.freq.out
```

Step 1: SCF calculation (Hands-on #1)
Step 2: Calculation of dynamical matrices on q-vectors
Step 3: Calculation of IFC's in real space
Step 4: A plot of the phonon frequencies

Si.matdyn.freq.in

```
&input
  asr = 'crystal'
  flfrc = 'si.fc'
  dos=.false.
/
46
0.50    0.50    0.50
0.48    0.48    0.48
0.46    0.46    0.46
0.44    0.44    0.44
0.42    0.42    0.42
0.40    0.40    0.40
0.38    0.38    0.38
0.36    0.36    0.36
0.34    0.34    0.34
0.32    0.32    0.32
0.30    0.30    0.30
0.28    0.28    0.28
0.26    0.26    0.26
0.24    0.24    0.24
0.22    0.22    0.22
0.20    0.20    0.20
.....
```



Γ-point Phonon

Command:

```
$ pw.x < Si.scf.in > Si.scf.out
$ ph.x < Si.ph0.in > Si.ph0.out
```

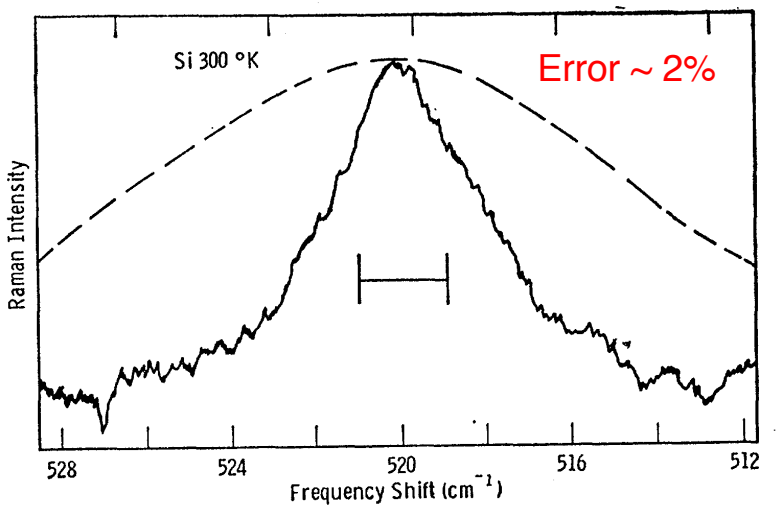
Step 1: SCF calculation (Hands-on #1)

Step 2: Calculation of dynamical matrices on q-vectors

Si.ph0.in

```
phonon calc.
&inputph
 outdir="../tmp/",
 prefix="si",
 tr2_ph = 1d-14,
 ldisp = .false.,
 epsil=.true.
 amass(1)=28.0855,
 fildyn='si.dyn',
/
0.0 0.0 0.0
```

→ Dielectric constant



Si.ph0.out

Si.ph_0.out

```
    Diagonalizing the dynamical matrix

    q = (    0.000000000   0.000000000   0.000000000 )

**************************************************************************
    freq (    1) =       0.373118 [THz] =      12.445876 [cm-1]
    freq (    2) =       0.373118 [THz] =      12.445876 [cm-1]
    freq (    3) =       0.373118 [THz] =      12.445876 [cm-1]
    freq (    4) =      15.307259 [THz] =     510.595193 [cm-1]
    freq (    5) =      15.307259 [THz] =     510.595193 [cm-1]
    freq (    6) =      15.307259 [THz] =     510.595193 [cm-1]
**************************************************************************

    Mode symmetry, O_h (m-3m)  point group:

    freq (  1 -  3) =         12.4  [cm-1]   --> T_1u G_15  G_4- I
    freq (  4 -  6) =        510.6  [cm-1]   --> T_2g G_25' G_5+ R

    PHONON       :     11.76s CPU     12.24s WALL

    INITIALIZATION:
    phq_setup    :      0.06s CPU      0.07s WALL (       1 calls)
    phq_init     :      0.12s CPU      0.12s WALL (       1 calls)

    phq_init     :      0.12s CPU      0.12s WALL (       1 calls)
    init_vloc    :      0.00s CPU      0.00s WALL (       1 calls)
    init_us_1    :      0.01s CPU      0.01s WALL (       1 calls)
```

Raman active