Practical 6 – Phonons

Example - Si

Use the DFPT method to generate a straightforward phonon calculation for silicon (in the diamond structure). Examine the `Si_DFPT` input files, make sure you understand the structure and all the settings. Run the calculation and examine the `.castep` output file.

Now use the interpolation method to evaluate the dynamical matrices at a finer set of q-points. For the runs `Si_DoS` and `Si_Dispersion`, first copy the `.check` file from the `Si_DFPT` run to `Si_DoS.check` and `Si_Dispersion.check` so we can restart from the previous run. Examine and understand the input files and plot the output data using `dos.pl` and `dispersion.pl`. Use the `-w` flag in `dos.pl` to smooth the plot a little.

Visualization

You can use the "Tools/Vibrate" option in jmol to visualize the phonon modes in real space from a `.phonon` file. Click the forward & back arrows to move between modes at a single q-point. You can use these jmol console commands:

`vibration scale 10` to change the scale of the vibration motion

`load "" {1 2 3 } filter "q=3"` to visualize all the modes at the 3rd q-point, or "`q=all`" etc otherwise only see modes at first q-point

Example - NaCl

Examine and understand the `NaCl` input files. Run the calculation and examine the output. Particularly note the Born effective charges. Using a similar method to Si, take the NaCl output and interpolate a DoS and Dispersion curve.

Example - Quartz

Run the `Quartz` calculation. This will take some time ... Generate the dispersion plot given in lectures. Vary the q tends to zero flag (**`phonon_gamma_directions`**) to see the effect on the LO/TO splitting. The IR intensities will also be calculated here. Plot the IR spectrum (`dos.pl -ir`)

Extension Activity

On any run you choose (some of the above or an example of your own), edit the `.param` file to add the flag "**`calculate_raman : true`**". This now calculates the 3rd derivatives of energy to obtain the Raman spectrum. WARNING – this is an expensive calculation! Plot the results (`dos.pl -raman`) and compare to experimental values.