MDANSE Workshop 2018

Tutorial: CASTEP Phonon calculations for INS

SETTING UP THE STRUCTURE of NaH

Now you must create a crystal structure model of NaH. There are various options for doing this

- Create a crystal structure from lattice parameters and co-ordinates. We will not do this here.
- Import an existing crystal structure
- The structure of NaH is given with your data set.
- If you have a NaCl structure, you can change Cl by H to get NaH structure.

For calculation purposes it is best to work with the primitive cell. To view this structure you can open jmol.

We could simply edit the lattice parameters, but instead let CASTEP do the work.

Setting up a CASTEP Geometry Optimisation

For electronic structure calculations you need the .cell and .param files along with potentials.

The potentials are given within this block

%BLOCK SPECIES_POT
%ENDBLOCK SPECIES_POT

For geometry optimisation change the Task in the .param file as

Task: Geometry Optimization

The other important components will be:

Exchange-Correlation Functional "PPE-GGA"

Once you have in place the <seed>.cell and <seed>.param files, and the pseudopotentials, you are ready to submit the CASTEP job. The job can be submitted by putting:

castep NaH

When it has finished, you can examine the output file NaH.castep.

Near the end of the file you will find the "BFGS: Final Configuration" and a description of the final lattice parameters.

Setting up the phonon calcualation.

In the param file now change the

Task: Phonon

The NaH crystal structure which should contain the updated structure.

As before, start the CASTEP calculations.

To calculate phonon dispersion you have to put following information in the .cell file:

kpoint_mp_grid 7 7 4

and one to specify a gamma-point phonon wavevector

phonon_kpoint_mp_grid 1 1 1

*Theory note: The calculation does not compute the frequencies at each wavevector independently. Instead it computes the full force constant matrix of Lattice Dynamics theory using a regular grid of q-points, and uses Fourier methods to compute the DOS and dispersion. For this first run you should set the ""q-vector grid spacing for interpolation" to around 0.08. ** Warning - you can make the calculation arbitrarily expensive using this control!*

Analysing the phonon runs

You will see a list of possible analyses. Select "Phonon density of states"

To enable the reading in of the data you must first select the CASTEP output "NaH_PhonDOS" . and open "NaH_PhonDOS.castep"

To plot phonon DOS you can open Mantid and choose Indirect -> Simulations and -> Densities of States

You can download Mantid from http://download.mantidproject.org/ and install it in your desktop.

To visualize phonon vibrations we can use free software Jmol.

Load the .phonon file in the JMol File-> Load window. You will see the crystalline structure of NaH. To get the supercell form type:

load NaH.phonon {3 3 2}

You can then use the “Tools-Vibrate” menu to turn on mode animation, and navigate the modes.

You can also calculate some thermochemical properties by performing the "Thermodynamic Properties" analysis of the DOS results. To do that you have to put:

Task: Thermodynamics

The result will be zero point energy, heat capacity entropy and Debye temperature as a function of T.

N.B. You have been provided with the files from the NaH phonon calculation ready to analyse, in case of computer troubles.

Tutorial 2: Crystalline Benzene.

Crystalline benzene calculations is a bit more expensive than the crystalline NaH. Therefore the calculated files of crystalline benzene are supplied. With the file having extension .cell and .param files and potentials calculation can be proceed as for NaH,

Phonon calculation of molecular benzene

This is also the same as of NaH. The calculated DOS and dispersion files are supplied.

Phonon analysis of molecular benzene

This proceeds in a similar fashion to NaH.

I suggest you carefully read the main text output, and find the block containing the output frequencies and group-thory symmetry analysis, plus any ir and Raman intensities.

IR and Raman spectra

As in NaH to plot IR and Raman spectrum you can open Mantid and choose Indirect -> Simulations and -> Densities of States and choose IR or Raman.

Analyse crystalline benzene

A phonon calculation of crystalline benzene is supplied to you. Proceed as the same with NaH.

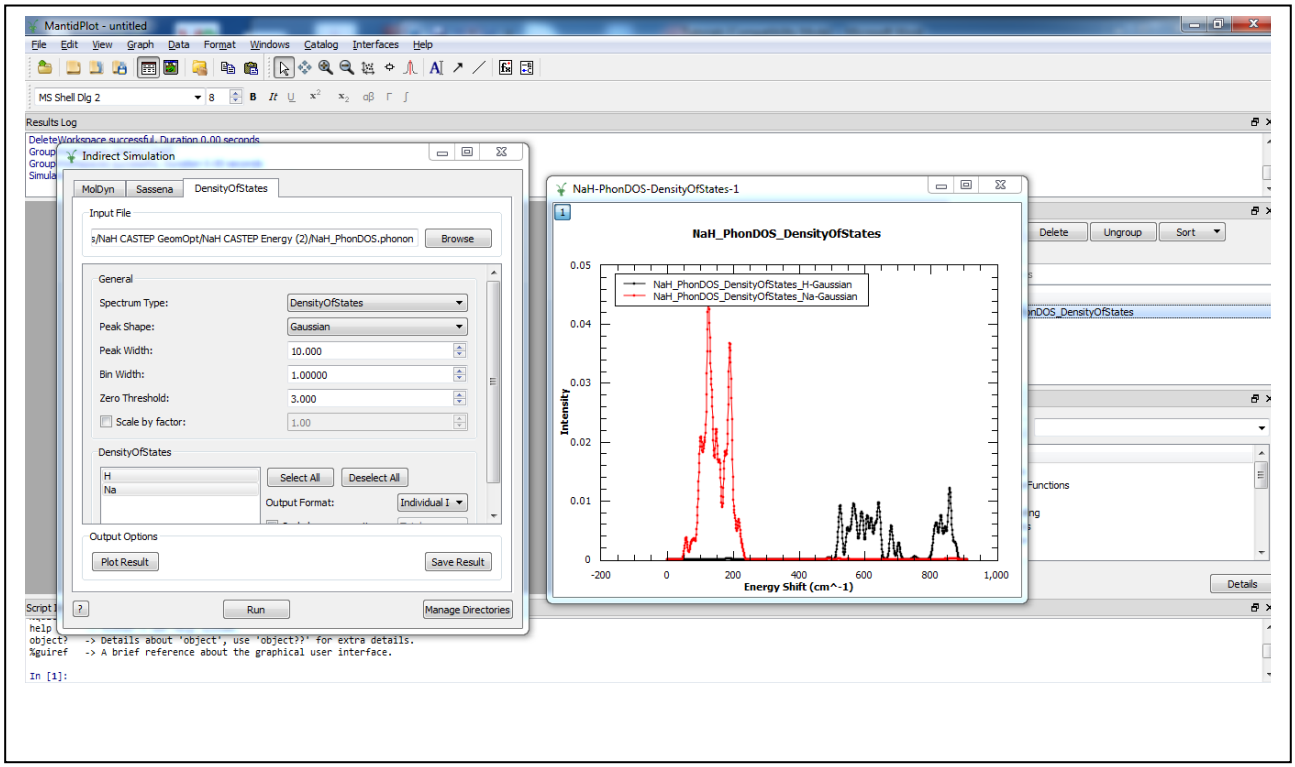
Use the same procedure to calculate INS for benzene and compare with experimental data.

Using Mantid to analyse phonon VDOS

Mantid is the data analysis tool for neutron spectroscopy.

Start Mantid. Set up directory to save data by browsing to the preferred directory through File -> Manage Users Save Directory -> Default Save Directory.

Load interface by clicking Interfaces -> Indirect -> Simulations and select the DensityOfStates option.



Load NaH_PhonDOS.phonon as input file. Keep all options as default and click on **Run**. The calculated file will appear on the workspace. Right click on the file. Select Plot spectrum option. In the appeared dialogue select spectrum number 0 to plot the VDOS. The VDOS of both Na and H will be plotted.

To get the position of the vibrational density as stick plot select spectrum 1.

The peak width can be changed to adjust the resolution of the instrument.

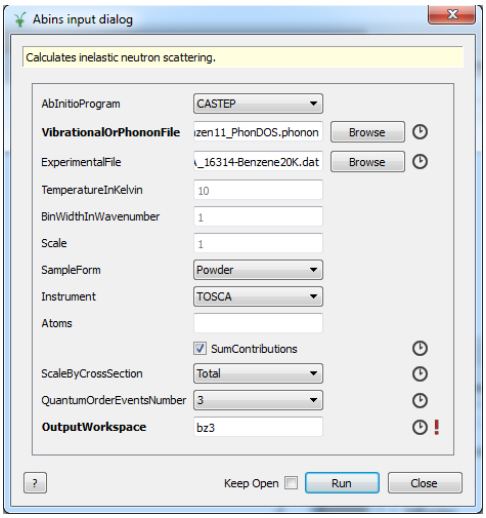
To weight the individual atomic peak with their neutron cross section click on scale by cross section on the original interface dialogue.

Results can be saved in Ascii format by clicking Save -> Ascii at the top bar menu at the top of the workspace window.

Calculations of INS spectrum using abINS

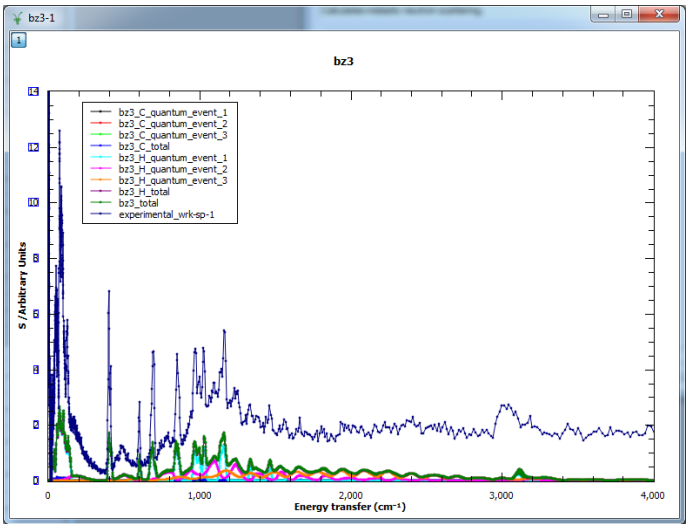
1. Run Mantid by clicking on the Mantid icon on your desktop. Set default directory where you would like to save the output data by clicking on **File -> Manage User Directories** available on the left most corner of the Mantidplot application GUI.
   In the **Manage user Directories** dialog go to the option **Default Save Directory** and brows to the directory where you would like to save output files.

2. Type **Abins** in the space of **Algorithm** at the right bottom space in the mantid plot and click the button **Execute**. A dialog like below will open.



3. Put following data in the Abins dialog:
   - Choose the option **AbInitioprogram** as **CASTEP**
   - Brows and load the phonon data file mentioned above in the space **VibrationalOrPhononFile**
   - Brows and load the data file from experiments (one is supplied with this tutorial) in the space **ExperimentalFile**. This step is optional.
   - Keep all other options as default as shown in the dialog box figure above.
   - Put **QuantumOrderEventsNumber** option as 2 for a quick calculations
   - Give a name for **OutputWorkspace** and click on **Run**.

4. After finishing the calculations the workspace will be saved in **WorkSpaces** space at the upper top space of the Mantidpot applications. Right click on that workspace and choose the option **Plot Spectrum**. A plot as given below will appear.



If you put the optional Experimental file in the Abins dialog, then you have to adjust the X-axis and Y-axis scales to get the above figure. This is because the TOSCA reduced file supplied here as an example of experimental file contains a huge elastic line at low energy transfer. At high energy transfer the difference between the experimental and calculated spectrum is due to the background of the instrument. The change of scale of these axes can be done by double clicking on axes of the plot.

5. The figure can be saved by right clicking on the plot and choosing **Export**.

6. The atom projected INS can be extracted by double clicking on the workspace file.

7. All workspace files will be saved automatically in the **Default Save Directory** in ASCII format to plot or analyse elsewhere.

Further source of experimental files: http://wwwisis2.isis.rl.ac.uk/INSdatabase/Theindex.asp
TOSCA instruments: https://www.isis.stfc.ac.uk/Pages/Tosca.aspx
Working principles of abINS: https://doi.org/10.1016/j.physb.2018.02.034