basic use of VNL+QE
on your own laptop or pc

The description in this document is deliberately limited. It tells you 'how to', not 'why'. The goal of this document is only to make you familiar with the practical procedure. Explanations about what every step really means, will follow gradually throughout the course.

The basics of running a DFT calculation with QE via VNL, is explained at http://docs.quantumwise.com/tutorials/espresso.html . It makes sense to spend four minutes first to watch the first video at that page, which gives a quick overview. The different steps are explained in written form in more detail further down on that page.

In the present document, some further explanations are given about issues that are dealt with more quickly on the QuantumWise website.

Let us go through the different steps needed to perform a DFT calculation for a perfect silicon crystal. The numbered headings hereunder hyperlink to the corresponding sections at the QuantumWise website. Click on the headers to keep the website tutorial next to this document.

1. setting up a configuration using VNL

Goal of this part: define the crystal you want to calculate (here plain silicon in the diamond structure).

Even on a fast computer, it might take 10 seconds or more to start VNL and/or to open a newly defined project. Don't be too impatient.

The provided example shows how to use a crystal that is predefined in the small database that is shipped with VNL. That's fine for now. But later on, you will probably want to access much larger databases. No need to do that now, but later you can select in that case 'Databases' from the icons at the left of the Lab Floor (same column where the 'Builder' icon sits), access the COD or MaterialsProject database, search your crystal of interest via the periodic table, select the crystal, and download its structure file in cif format to your computer. Then go to the Builder and import this file via Add/From Files.

2. exporting a Quantum ESPRESSO input file

In the previous step, you have defined the crystal in a format that VNL understands. Now you have to export it to a file in a format that QE understands.

If you do this on a Windows computer, then item 3 ('open a terminal') means that you should open the scf.in file in a simple text editor. It is a good strategy to use an editor that is sufficiently basic (MS Word risks to add lots of hidden characters that destroys the file). A good and free one is https://notepad-plus-plus.org/ .

3. adapting the input file

The scf.in file that you have created so far, is just a standard file. It knows about the crystal structure you defined, but all other input parameters for QE are just default values. Some values will need to be changed, some keyword will not be needed, other keyword will have to be added,… depending on the particular QE calculation you want to do. Simply follow the example described on the VNL website for the time being (except for the parameter nbnd, no need to specify that one). The meaning of some of the important keywords will be explained in the next weeks.

The instructions to "remove lines 20-22" and to "insert instead nbnd=10" can be omitted. It might result in a slightly slower calculation for this case, but will save you problems later. Without doing these two steps, your input is more universal (the procedure as described for silicon would result in problematic calculations for metals).

4. running the ground state calculations

Here the description on the Quantum Wise website is a little short, in particular for Windows computers. This is how you run QE in Windows:

use Start/Run cmd (=press the start button, and type 'cmd' in the field 'all programs', then press enter, or in Windows 10: click the start button, then type 'cmd' anywhere and enter). In the black terminal window, you can go to the folder where you have put your input file for QE (scf.in) by using the 'cd' command (followed by the name of the underlying folder(s), e.g. 'cd folderA/folderB' to go to folderB, which is a subfolder of folderA, the latter being a subfolder of your present folder). You can use 'dir' to know in which folder you currently are. Once you are in the folder that contains your silicon files, you start QE in the following way:

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pw –input scf.in > scf.out
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(note that under Linux you will need pw.x, while for Windows it's just pw). Don't copy-paste the above string from this pdf document, as some characters might not be recognized that way. Type it yourself, using a minus in front of 'input' (and not any other hyphen character).

Then proceed with item 2 on the QuantumWise webpage.

5. analyzing results

For this item, it is sufficient so far to be able to get the total energy (we'll see later what it means).