Instructions for writing a good report

General aspects

1. Answer every question with your own words using lectures and given literature as a source, and try to explain underlying physics and connect it with the results that you obtained. Answers need to be concise, but not superficial and vague. Stick to the main point. **(No copycats allowed!)**
2. Every table and graph need to have a concise but complete caption, allowing readers to understand the plot even without reading the rest of the report. You need to label both the x and y axes and remember to always put units for all quantities that you display. In case of multi-series plots, a legend is also needed.
3. For tables, remember to add a detailed caption, as well as report all units. Pay attention to using the appropriate number of significant digits, as better explained in the examples below.
4. There is no need to put your python/bash scripts in the report, only the final results and fits with explanation are enough.
5. If you are using external sources, papers, books, etc remember to always properly cite them.

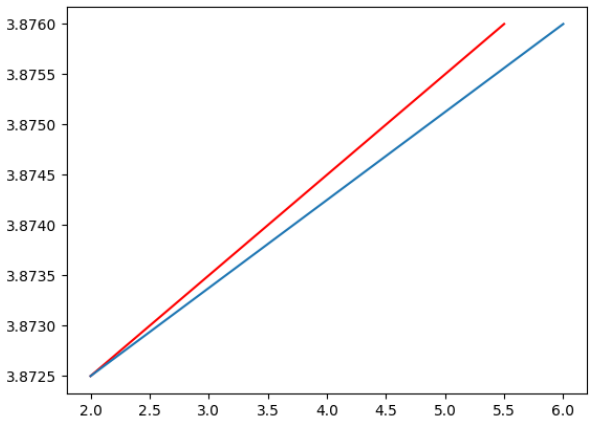
A few examples

In the text below you can find some examples of how graphs and tables should (or should not) look like, as well as a simple example of how you should answer a question.

How to organise your graphs and plots

A bad example

The following example has a number of issues: there are no x and y labels (and, in particular, no specification of units), there is no legend even if more than one line is present, and the caption is too short to really explain what the plot is about.



Surface energy convergence

A better example

In this example, x and y-axis labels are present and indicate clearly the quantity being plotted and the units. A legend clearly explains the meaning of each curve. Finally, a concise but complete caption is provided that allows a reader to fully grasp the content of the figure, without being too verbose (for good examples, you can check most of the captions of figures in published scientific papers).

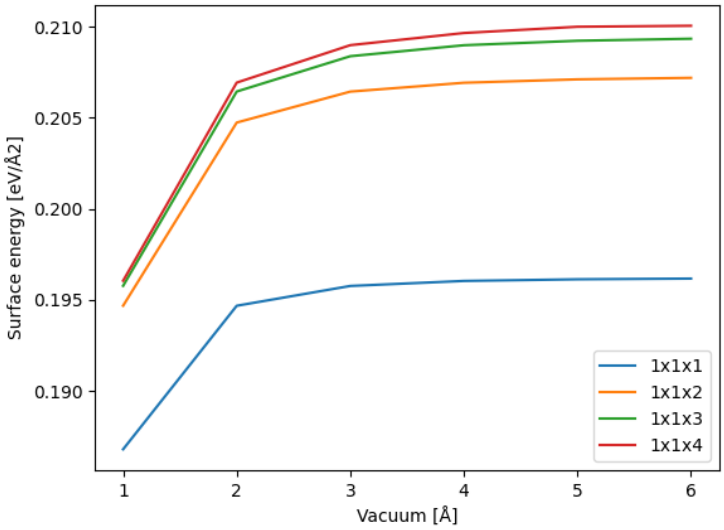


Fig. 1: Convergence of the surface energy as a function of the thickness of the vacuum region. Each curve represents the results for a different slab thickness (from 1 to 4 unit cells).

How to organise your tables

How to organise your tables: here you can find some of the examples for how a table should look like, starting again from a bad example **a)** and giving a good example **b).**

A bad example

The following example does not present the units for the energy (that is just labelled with a generic E letter) and does not provide any table caption explaining the goal of the table or the meaning of the symbols (E, in this case). In addition, too many significant digits are reported (see also the note on the number of significant digits below).

Supercell size	E
2x2x2	3.924856892
3x3x3	3.929826548
4x4x4	3.930

A better example

This table has a sufficiently detailed caption that explains the goal of the table and which data is reported (e.g. specifying the potential used, and if relaxation was performed), making it unambiguous which data is being displayed. Moreover, the caption explains the meaning of any symbol used in the table header. Units are reported, and a balanced number of significant digits has been chosen to report the results.

Supercell size	$E_{f,v}$ [eV]
2x2x2	3.9249
3x3x3	3.9298
4x4x4	3.9305

Table 1. Vacancy formation energy $E_{f,v}$ as a function of the supercell size for fcc Au, using a LJ potential (without subsequent relaxation).

Note about significant digits

Usually, in each exercise you will know to which precision you are calculating a given quantity, so you can make an appropriate decision on the number of significant digits to show. For instance, if the convergence threshold is 0.001 eV, you want to take into consideration enough digits to display if the value is converged, but not too many more. For example: if the energy values are those of the examples above, showing only 3.92, 3.93 and 3.93 as values would not be enough. You want enough digits to see the change in the values, but not many more that make the results confusing and harder to read.

How to answer your questions

Example of a possible question

In your GULP input file with a Lennard-Jones potential, you have a line of this kind:

> *Lennard 12 6*
>
> *Au core Au core 214180.2000 625.482 0.0000 40.000 0 0*

What are the parameters 0.0000 and 40.000? Why do you need a cutoff in your potential? How is that performed in practice? Which issues can the procedure generate?

A bad example

The following answer is too short, and does not allow the teachers to assess if the student has really understood the problem and/or how the quantities being discussed have an effect on results and on the accuracy of the simulations.

> They are parameters of the potential. I need a cutoff because I am simulating an infinite cell. There are different mathematical ways to do it.

A better example

This example answers in detail to the various questions, showing that the student has fully understood the problem, the numerical aspects associated with the simulation, and the consequences of the numerical approximations.
Note: a much longer answer is *not* needed (for instance, one does not need to explain from the very beginning how the LJ potential is written and re-explain the full theory: this is not required, it will take much more time both for you to write and for us to correct, and you also risk to write something incorrect, risking to lose points!)

By using periodic boundary conditions, we can simulate an extended infinite system. The LJ potential contains a sum over all pairs of atoms in a system, which is infinite in our case, thus for computational reasons such sum needs to be truncated.
The first type of truncation that can be performed is of a radial type. This is achieved by specifying a spherical cut-off radius. It is also possible to use two radii, a maximum and a minimum one, so that one can have overlapping potentials.
An obvious disadvantage of this method is the introduction of a discontinuity at the boundaries of the cut-offs, which may lead to numerical issues during the energy minimization, in particular because the derivative of the energy (that is proportional to the forces in the system) is infinite at this discontinuity point. As a consequence, an atom whose distance from another one is close to the discontinuity will be subject to a very strong artificial force that will make the numerical algorithm unstable.
This issue can be partially circumvented by rigidly shifting part of the potential so that it becomes continuous.