

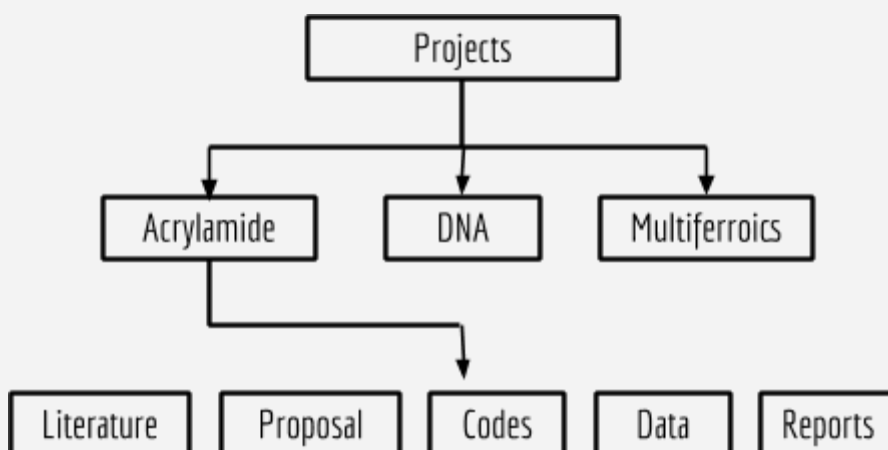
# INSTRUCTIONS FOR THE MEMBERS OF AITG

## DATA ORGANISATION

### 1. Directories

- On all the machines you use, be it clusters or workstations or NAS, try to use the same directory structure for all your work files. This will allow for easy backups and easy data retrieval.

Example: Directory structure below



- In the project folders, all the raw work files (ongoing calculations) go in the Work directory.
- The output files and coordinates, go in the Data directory under appropriate folders.
- The reports you will generate (short reports, updates, presentations, paper drafts, etc.) will go under Reports.
- Codes generated for the project will go under Codes (or Scripts).

### 2. Data

- In the data directories above, you can follow the structure below to ensure easy retrieval and reproducibility.
- Make subfolders for each system you handled within the project and, within that, for each case (bulk, slab, molecule, ground state, excited state, etc.) you considered.

- Divide each of these directories into four major sub-folders - Input, Output, Run scripts (job scripts, if relevant, or python scripts, if used), and Results.
- The Output could only have the text output on running the job as well as coordinates, trajectories, forces, stresses, etc. generated as a result of running the job.
- The processed data in the form of plots and tables could be saved in the Results folders.
- There should be one script, if possible, that takes an input file, runs the appropriate code on it, and generates the output files as well as the plots and tables. This will require some work from your end but it is a one-time effort.

### 3. The naming convention of files

- Name all files related to the same calculation with the same prefix for easy identification. Also, use names that allow anyone to understand what the calculation is about.
- Do not name files after the date on which the calculation was done or any other such key which would only be known to you.
- Remember that the organization that we are proposing here is not only for your benefit for anyone else reading through your files.
- Typical names can tag the system, the case considered, the code used, and another serial number indexing the trial number. As a suffix or as the extension of the file you can then tag it as an input, output, script, or result file.

### 4. Backup from clusters

- Take a backup of your cluster data **EVERY DAY**.
- The clusters are not meant as permanent file storage. On many machines, you are sharing space with others in the group. Please be considerate.
- Also, it is very important to backup as clusters can often shut down and you can lose access to your data.
- You are responsible to retrieve your data. I will not accept any excuse in this regard if the data is needed urgently and you have not backed it up.

# REPORTS

## 1. Lab journal

- Every member **MUST** have a lab journal (we can pay for it or you can use copies available in the lab) where all details of daily work are entered.
- This should include the purpose of any calculation in brief (aim), the assumptions being made, the code (versions and variants) used, the parameters used for the calculation, a copy (handwritten or printout) of the input file, input geometry, output geometry, energy and force thresholds used for optimizations, etc.
- The lab journal will be a property of the lab, to be left behind when leaving the lab.

## 2. Weekly reports

- Everyone, regardless of the source of funding, **MUST** generate and provide weekly reports.
- These can be in the form of slides and/or pdf documents. Please do not send me doc or tex files.
- There is a common group dropbox folder where you can upload these reports for me to see.
- Please archive older reports of finished projects and keep only current projects in the Dropbox.

## 3. Final reporting on projects

- Every finished project is expected to have a final report and/or a paper draft along with all necessary tables, plots, graphics, etc.
- Additionally, have the habit of making one presentation summarizing all the findings (including back up slides to highlight additional data).
- This presentation can also be used as a guide through your data and calculations for the project for others.

## 4. Making presentations

Whether you are making a group meeting presentation or a more formal one, please follow the best practices. Some of these are noted below:

- Each slide should convey 1 idea/concept and should take no more than a minute to present.
- Every point on the slide should stem from your understanding or an attempt to understand. If there are potential confusions/errors/lack of understanding, this should be clearly pointed out.

- Divide every (non-title) slide into three parts : premise/claim, result/observation, inference/punchline.
- Image qualities should be good. Plots should be well labeled, their axes and labels visible, use bold fonts where possible, use thick lines to plot, distinguishable colour scheme for multiple plots plotted on one panel, etc.
- You are responsible for your presentation. Do not try to dump the responsibility of mistakes and lack of understanding on others.
- Group meeting presentations are about your understanding of whatever you are presenting. Make sure that you know whatever you are presenting and that your presentation is complete.