Guide to Research Meetings

- Individual (or sub-group) meetings with PI
- Internal discussions in the group
- External Collaborators

Meetings

Come prepared to meetings: You are/will be the person most familiar with your project, and thus the expert. Come to meetings with questions, results/progress, and where you are heading next. This can come in the form of a few slides, a few figures/plots, an outline or draft for something. The more specific and prepared you are for meetings, the more effective the meeting time can be used.

Take all individual/group/collaboration meetings seriously: This is good practice for presenting your results, for "thinking on your feet". Our goal is to be the most critical and supportive of the work coming out.

Take notes of what is discussed in meetings: This is true for individual, group, and collaboration meetings. Share with others if relevant. For example, you can make a shared folder and upload meeting minutes. These notes will provide valuable internal documentation for your research progress and gives you a way to reflect and think about how to proceed to next steps.

Procedure for preparing for meetings with PI:

We will have regular meetings, usually on the order of once per week. You are expected to come prepared with

1) any follow ups from previous discussions

2) what you worked on the previous week and new or updated data/analysis

3) questions/topics to discuss with PI or group

4) what next steps you will take

> A lab notebook is highly recommended. Having a permanent location where you jot ideas, work through concepts, or keep track of data is invaluable in your research. Documentation is a critical skill in scientific research and the more you write down and organize the better. Develop a system that works for you.

https://wang-materials-group.gitbook.io/group-handbook/group-policies/meeting-policies

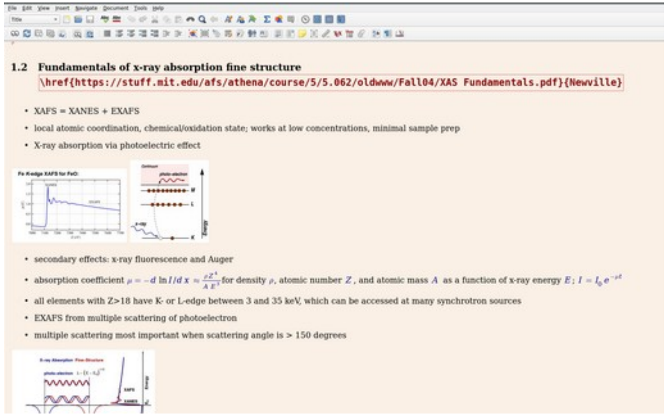
Remind people of what is happening.

Presentation-clear plots (not necessarily formal presentation polished)

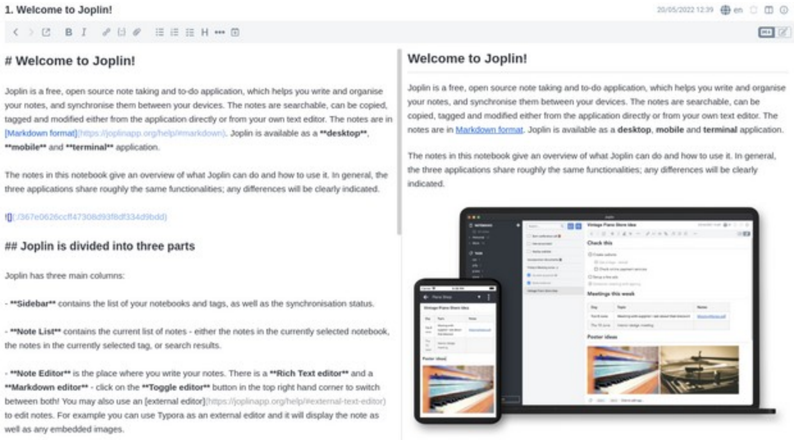
What is your interpretation of the data?
How does this compare with the literature?

Example open source note taking apps

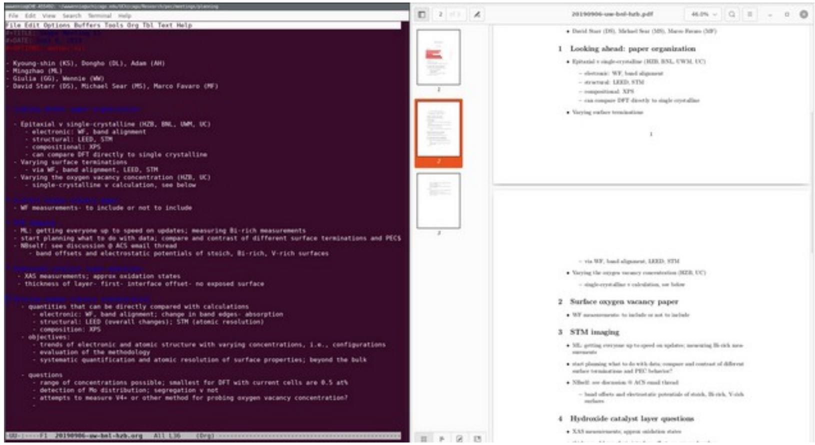
Lyx



Joplin: markdown, multimedia (audio, video, pdfs, html, latex)



Emacs



WW’s current system

- Written Notebook → seminar notes, free form thinking
- Emacs (org mode + evil vim bindings) → conference notes, meeting minutes
- Lyx → online seminar notes
- Joplin → projects, literature search
- Syncing files → Insync, Google Drive, UT Box
- Backup → daily on external hard drive

Expectations for research meeting discussions

- Rehash the last meeting:

  I do my best to keep track of everyone’s projects but you cannot and should not rely purely on my memory
- Data and plots + basic calculation parameters used
- Observations and interpretations from the data
  - What did you learn from the calculation? e.g., the appropriate running parameter, extracted a specific quantity
  - Are you convinced about the calculation? Do your results make physical sense?
- Minimal raw data- you need to have looked and thought through it
- Specific questions- research or technical
- Next steps- including next steps calculation plan
- Support qualitative descriptions with **quantitative data/plots**, e.g., a small band gap v a small band gap of 0.1 eV
- Bring up deadlines well in advance (add buffer time of about 2x what you think it will take to do)

- Make your meeting notes separate from your full documentation

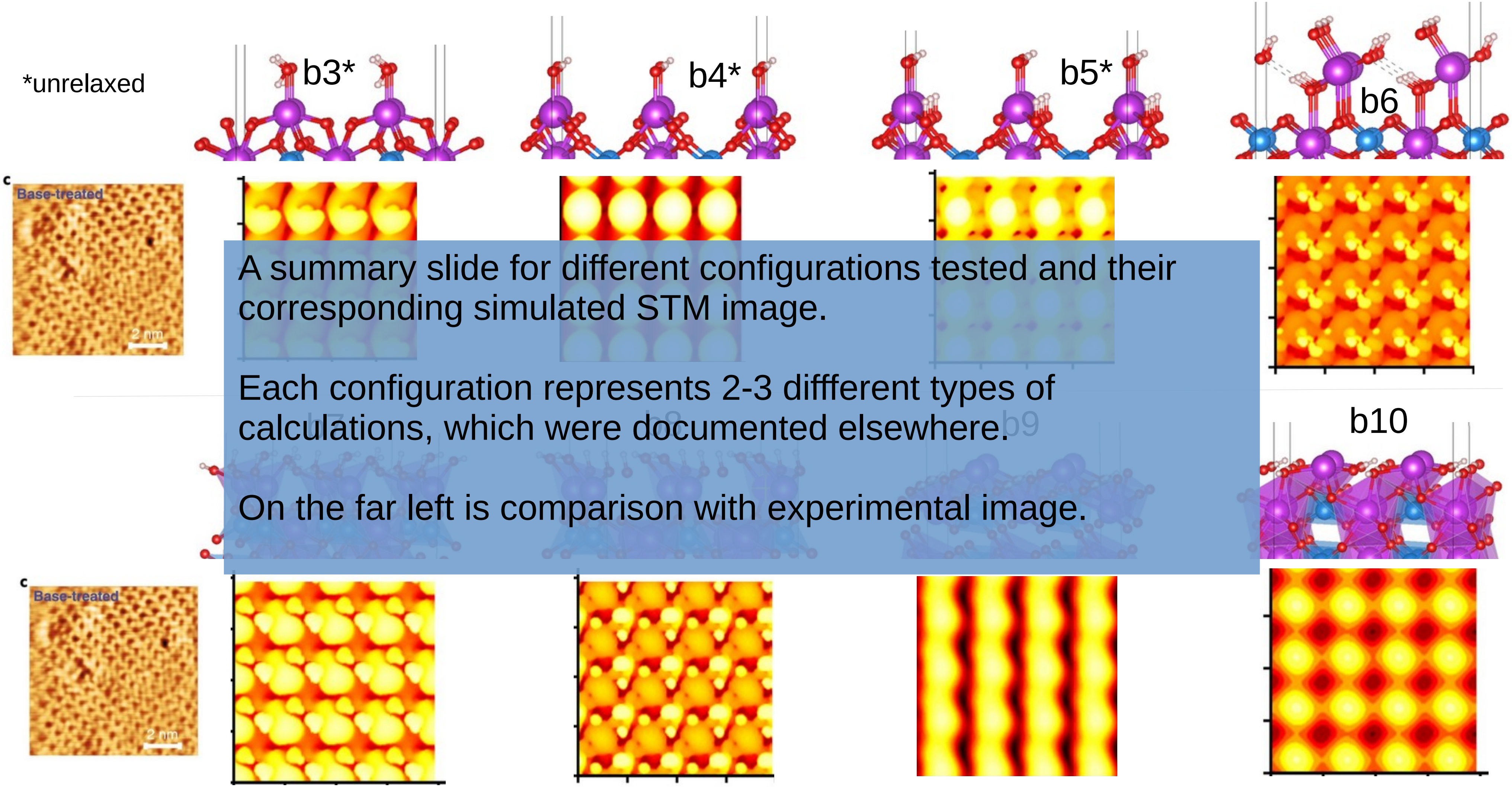
Strategies for working through research problems

- Did you go through the tutorial? Did you search through the forums? Could the literature help support or refute?
- Keep track of what you have tried- be as specific as possible
  - What is the error message?
  - What are your input parameters and calculation set up?
  - What clues can you find in <u>all</u> of the output files?
  - What version of the code are you using?
- Keep track of potential solutions- where did you find a solution
- Prioritize solutions that are more likely to work

An example of keeping track of data

Identifying the surface termination for the Bi-rich surface

*unrelaxed



A summary slide for different configurations tested and their corresponding simulated STM image.

Each configuration represents 2-3 diffferent types of calculations, which were documented elsewhere.

On the far left is comparison with experimental image.

Observations and comments

- There is some dependence on choice of isosurface and bias; this dependence is mostly which settings reveal finer details of certain features- some settings lead to certain features blurring out
- Relaxation makes a little bit of difference (some features are stronger compared to unrelaxed), but the differences are not significantly large (see b10), suggesting the orientation of the OH groups on the surface matter not too much
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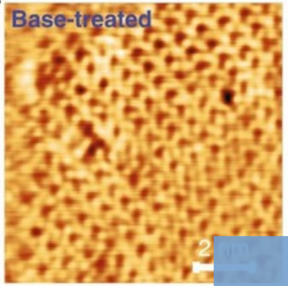
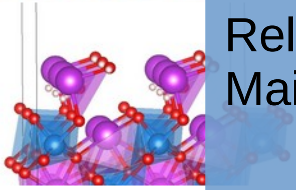
General observations from previous slide that might be important in future calculations

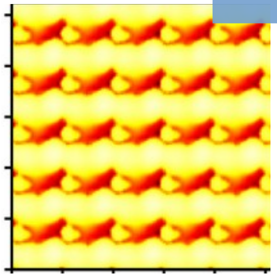
Hydroxylation of the Bi-rich surface: Initial calculations

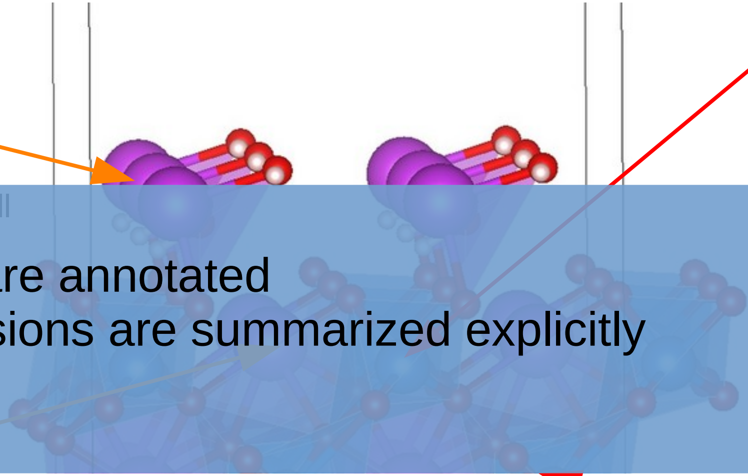
Using the b11 configuration, adopting a similar strategy as with stoichiometric surface

c









top electron
No converged scf
(~0.015 Ry fluctuations)

Top hole
Up to 1e-4 convergence
in total energies; but not all
iters converge

Relevant parts of data are annotated
Main points and conclusions are summarized explicitly

sub-top hole
Up to 1e-5 convergence

sub-top electron
No converged scf
(~0.3 Ry fluctuations)

possible calculation ideas:

- For understanding XPS peaks: simulation of XPS O1s – identification of the shoulder
- For understanding XPS shifts: Lowdin/Bader charge analysis