# A Realistic Research Example of EELS

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# 1 Objective

This is an advanced practical, for those who have already got to grips with CASTEP and would like experience performing a computational research-style mini-project. As such, there's not a *right* answer. You should come to a conclusion, and have evidence that your conclusion is robust: enough to convince two referees.

The outline of the project is vague: some experimentalists are interested in understanding whether there is nitrogen present in amorphous carbon. Since they have newly had an EELS detector fitted to their (Scanning) Transmission Electron Microscopes ((S)TEMs), they are keen to use it. You supervisor has told them that you are familiar with CASTEP and that CASTEP can "do EELS" – away you go...[1]

# 2 Modelling

The experimentalists are probably most interested in seeing whether there is a difference in the EELS spectra between nitrogenatied amorphous carbon and non-nitorgenatied carbon. It would be even better if you could show which types of N defects (if any) are present. They are probably not going to be interested in SCF total energies or other quantities that their spectrometer cannot see. However, knowing that your structures are stable is probably a good sanity check – unless the experimentalists are specifically looking at *high-explosive amorphous carbon!*. CASTEP generates machine-readable `<seed>.elnes_bin` files: in order to do something that the experimentalists will want to see, there is a post-processing code called OPTADOS.

Your first problem is making a suitable model of the system. An amorphous model might be too difficult under the circumstances: developing a tetrahedrally bonded random network is almost a Ph.D. project in itself. But it seems unlikely that you need to go this far: if we had answers for $sp^2$ and $sp^3$ bonded crystalline carbon, we'd probably be making good progress. Showing that both types of bonding environments give (roughly) the same answer would be a good start – so maybe we should have two or more approximate models rather than one perfect one?

# 3 Initial Thoughts

- **Read everything you have, before doing anything.**
- You need a copy of OPTADOS an experience using it – (www.optados.org) – maybe a system administrator has installed it already?
- You need a literature review of DFT EELS. Who is doing calculations like this? Maybe an OPTADOS developer? (hint)
- You also need a literature review of common nitrogen defects in carbon-based materials.

[1] The same thing happened to me with time-dependent density-functional theory.

- How will you model amorphous carbon – graphite and diamond? Perhaps from the ICSD?

# 4 OptaDOS

Someone has helpfully provided an OptaDOS manual. So it would be a good idea to have a go at the examples within it.

There is also an OptaDOS mailing list for help. In this example you should not need to post to it, although you should be aware of its existence. The quickest ways to get ignored on a mailing list are to:

- Ask questions that have already been answered. (Look at the archive before posting).
- Not give enough information to reproduce the problem. (Which versions of OptaDOS and CASTEP are you running?)
- Give an example of your system that is so large that someone would require a supercomputer to see your problem.

Hence the best way to get an answer is to have done the examples. If your problem exists in the examples set – then everyone on the mailing list with a copy of OptaDOS already has the system to test, and they can all help you using only their laptop. If OptaDOS gives errors in the examples, then there is probably something wrong with the way your versions of OptaDOS, CASTEP and/or computer is set up – this greatly narrows down the search space for solutions.

# 5 Convergence

What level of accuracy do you need to convince the experimentalists of your findings?

- Plane wave cutoffs.
- Brillouin Zone sampling of the SCF calculations **and** the spectral calculation
- OptaDOS's integration grids.
- Different bonding environments, different N defects? What about vacancies?
- Should the cells be relaxed?
- Which functional is *best*? Does it matter?
- Are you using a core-hole? Is it necessary? Is the answer robust to your choice?

# 6 Presentation and Interpretation

To successfully complete the project you must provide a labelled graph/ graphs and suitable figure captions to explain what your findings are to the experimentalists. Of course, you should also provide a supplementary information section showing how your results are robust to you calculation's parameters.

Answers may be e-mailed to `ajm255@cam.ac.uk`.

# 7 Appendix

## 7.1 Final thought

Now you're finished carefully reading everything before you start, you should find that the footers of these pages contain DOIs to the literature review that your hasty colleagues have started in earnest.