

Investigation of Bond Strain Effects on XANES Structure Spectra by Supervised Machine Learning

by
Jeremy K. Thaller

Professor Anatoly Frenkel, Advisor

A thesis submitted in partial fulfillment
of the requirements for the
Erasmus Mundus Joint Masters Degree:
Masters in Materials Science Exploring Large Scale Facilities

Brookhaven National Labs
Brookhaven, New York
December 8, 2020

Abstract

Your abstract will summarize your thesis in one or two paragraphs. This brief summary should emphasize methods and results, not introductory material.

Executive Summary

Your executive summary will give a detailed summary of your thesis, hitting the high points and perhaps including a figure or two. This should have all of the important take-home messages; though details will of course be left for the thesis itself, here you should give enough detail for a reader to have a good idea of the content of the full document. Importantly, this summary should be able to stand alone, separate from the rest of the document, so although you will be emphasizing the key results of your work, you will probably also want to include a sentence or two of introduction and context for the work you have done.

Acknowledgments

The acknowledgment section is optional, but most theses will include one. Feel free to thank anyone who contributed to your effort if the mood strikes you. Inside jokes and small pieces of humor are fairly common here . . .

Contents

Abstract	i
Executive Summary	ii
Acknowledgments	iii
1 Introduction	1
1.1 A section	1
1.2 Another section	1
1.2.1 A subsection	1
1.3 Some figures	2
2 A second chapter	4
A An appendix	5

List of Figures

1.1	Short-form caption	2
1.2	Another short-form caption	3

Chapter 1

Introduction

The introduction is one of the most important pieces of your thesis. Here is a place for you to introduce the problem(s) on which you have worked and place them in the larger context of your field. You should aim to ensure that this section is completely understandable to virtually anyone - and certainly anyone with a sophomore-level grasp of physics. Presumably this will include references to the literature.

In addition to setting your work into context, a second good idea for your introduction is to give a short outline for what the rest of your thesis will discuss. This is often done in the closing paragraph(s) of the introduction with sentences like “In the following chapters ...” and “Chapter 2 discusses ...” Tremendous detail is not required in this outline, but rather just a brief road map for the rest of the document.

1.1 A section

The `\section` tag will create a new section within a chapter. Sections will be sequenced with digits following a decimal point in the table of contents, i.e. this is section 1.1.

1.2 Another section

This second section is, obviously, 1.2.

1.2.1 A subsection

Subsections are created using the `\subsection` delineate smaller pieces of your document, and will appear after a second decimal point; this is subsection 1 of section 2 of chapter 1, i.e. 1.2.1.

A subsubsection

Subsubsections are still smaller sections. By default, this is the finest subdivision of a chapter in \LaTeX , and they will *not* appear in the table of contents.

1.3 Some figures

You will surely want to add figures to your thesis to help explain your ideas. There are a number of different ways to include such things, but the most typical way would be to generate the figure in another piece of software (MATLAB, Mathematica, Adobe Illustrator, ... and simply include it in your \LaTeX code. This will require use of the *figure* environment.¹ See this document's \LaTeX code for details . . .

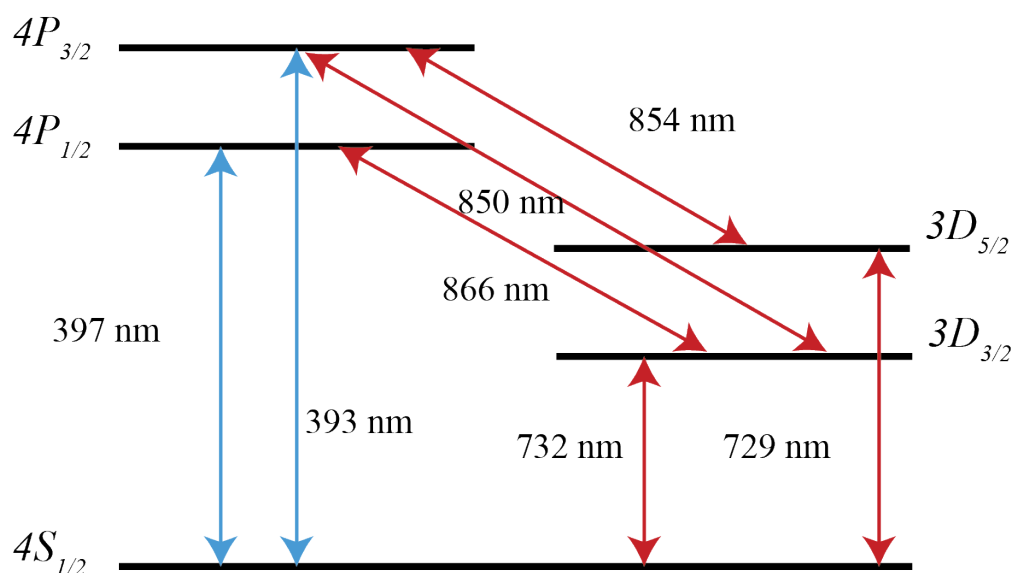


Figure 1.1: Long-form caption that appears in main body of the document

Here, back in the main body of the text, we can create a reference to figure 1.1. This is automatic; the actual numbers are not typed into the code, but rather the `\ref` tag has been used.

¹there are many other possible environments to include figures, such as `wrapfigure`, but these will require including additional packages . . .

As an alternative to the ordinary figure environment, you might deem it desirable to tuck a figure in more closely amongst the text. This has a separate environment known as *wrapfig*. Here we will include the same figure as above a second time, but this time using the *wrapfig* environment. This will insert the figure into your document with the text wrapping around the perimeter, rather than offsetting it into its own separate chunk of page, as above. As before, we can use an automated reference to the figure using the `\ref` tag; here we have figure 1.2. Working with the *wrapfigure* environment sometimes requires a little bit of massaging to ensure that everything lines up properly in your document, but with a small amount of work you will find that you can get the text to box the figure quite nicely.

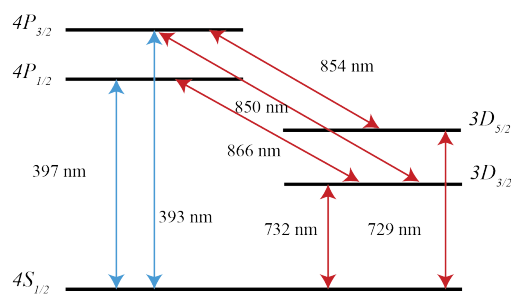


Figure 1.2: A figure included using the *wrapfig* environment

Chapter 2

A second chapter

Here is a second mock chapter. As far as the \LaTeX is concerned, it is in no way different from the introduction excepting that it appears after it in the main .tex file. As before, it can be populated with sections, subsections, figures, etc. as you see fit.

In fact, you will probably write perhaps three to six chapters for your thesis depending on how your work is most effectively organized. Most theses will contain an introduction, at least one ‘body’ chapter, and some sort of conclusions/future directions chapter. Most theses will also include an appendix or two ...

Appendix A

An appendix

Appendices are a good idea for almost any thesis. Your main thesis body will likely contain perhaps 40-60 pages of text and figures. You may well write a larger document than this, but chances are that some of the information contained therein, while important, does *not* merit a place in the main body of the document. This sort of content - peripheral clarifying details, computer code, information of use to future students but not critical to understanding your work ... - should be allocated to one or several appendices.

Bibliography