


Preparing figures for publications and presentations



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As researchers, we expend a great deal of thought, time, and money to generate data.

Surely it makes sense to treat data with respect, and to present data in the best possible manner, paying heed to verity, legibility, and æsthetics.

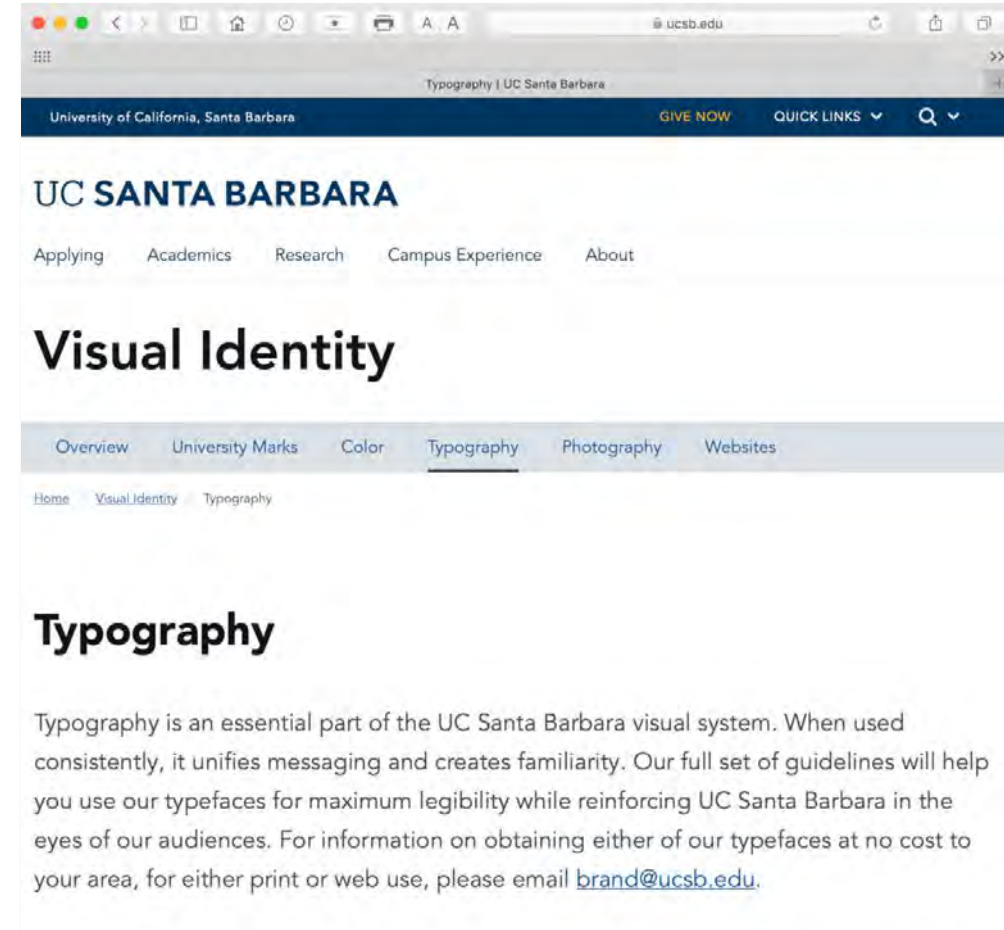
Thoughts on fonts typefaces



Good for labeling, and for short strings of text. NOT good with paragraphs. Projects well.



NOT good for labeling, or for short strings of text. Good with paragraphs. Prints well.



Thoughts on comic sans

A fun typeface to use in the invitation you send to your friends Heather and Pedro and Dylan and Kumar and Jazmyn and Fatima, to your 8th birthday party. Yay !



<http://www.bbc.co.uk/news/magazine-11582548>

Thanks to Jamie Neilson for the link.

ClearType: Microsoft's gift to the world

Calibri

Aa Ee Gg

Aa Ee Gg

a

Eiganes

abcdefghijklm

nopqrstuvwxyz

0123456789

Corbel

Aa Bb Cc

Aa Bb Cc

a

On-screen

abcdefghijklm

nopqrstuvwxyz

0123456789

Candara

Aa Ee Xx

Aa Gg Xx

N

Bildersturm

abcdefghijklm

nopqrstuvwxyz

0123456789

Consolas

Aa Kk Jj

Aa Kk Jj

a

Registration

abcdefghijklm

nopqrstuvwxyz

0123456789

Constantia

Aa Rr Gg

Aa Rr Gg

a

Jezyk

abcdefghijklm

nopqrstuvwxyz

0123456789

Cambria

Aa Ee Rr

Aa Ee Rr

a

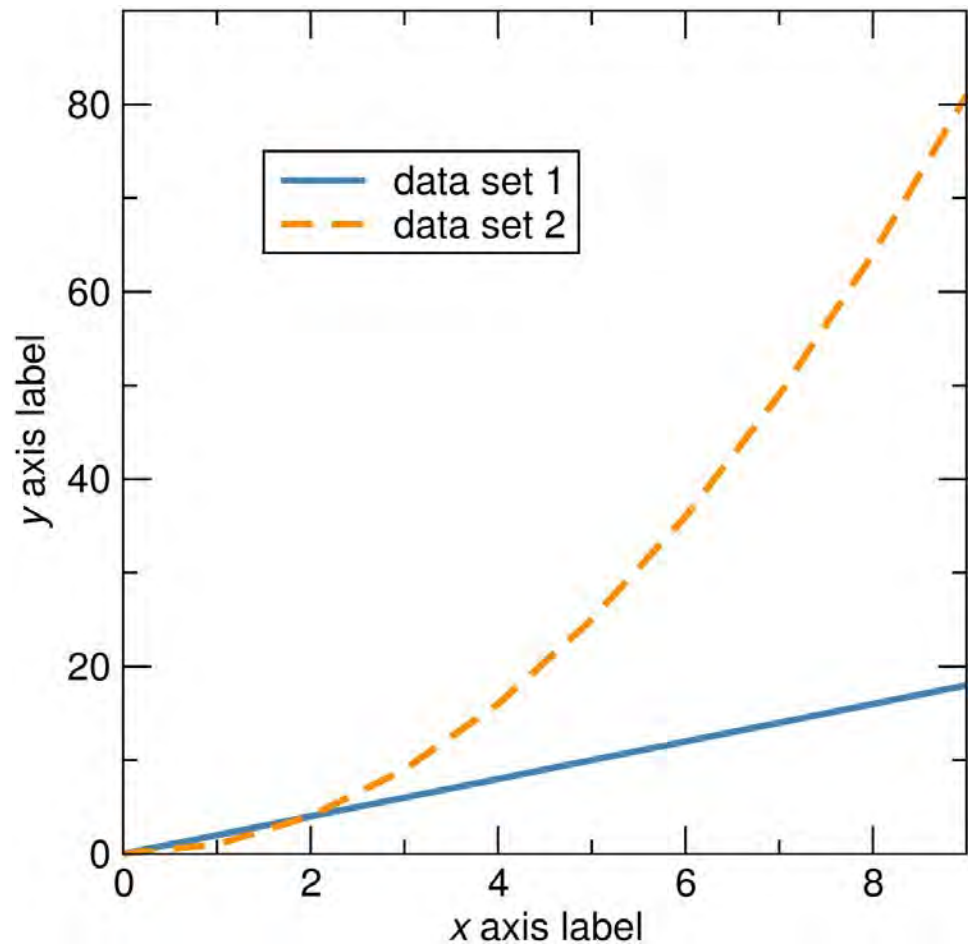
Doppelgänger

abcdefghijklm

nopqrstuvwxyz

0123456789

A good plot



Square plots are aesthetically appealing, convey information, and shrink gracefully. It is easy to use them in theses, single column journal articles, and talks.

Blue and orange are contrasting colors and have high visibility. They are usually visible to most color-blind people as well.

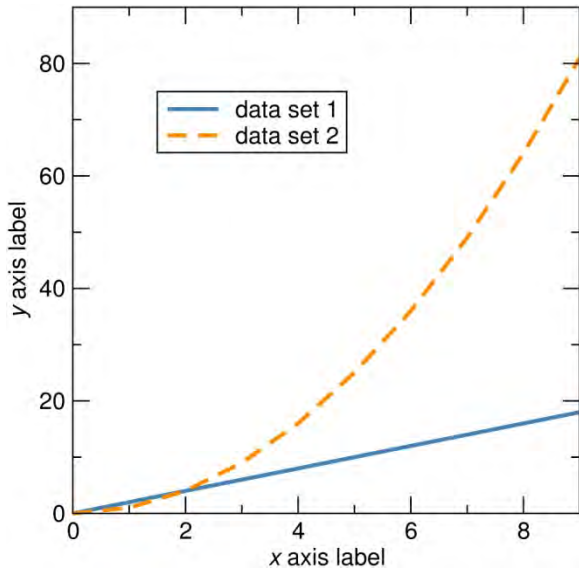
Using redundant coding is helpful. The plot shown here would be legible when reproduced in black and white as well, because one of the lines is dashed.

An appropriate frequency of tick labels should be used. Tick and axes labels should be the same size, preferably.

Serif-free fonts have higher legibility. Calibri, Gill Sans, and Helvetica look nicer than Arial. Times New Roman is a bad idea.

The important metric to control is the ratio of the size of text in the plot to the width of the plot.

A good plot



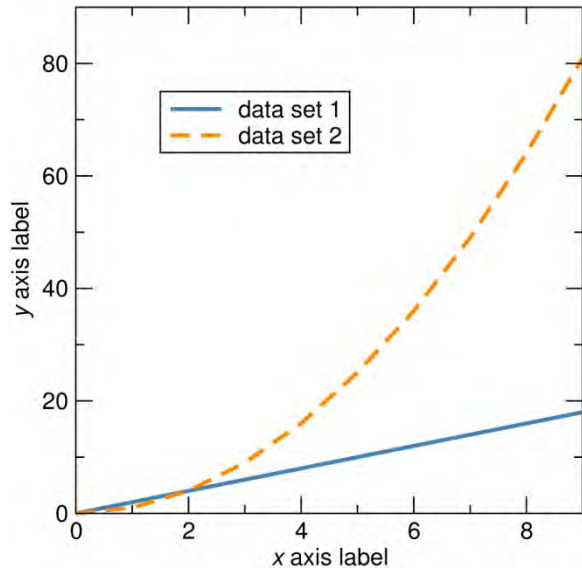
← 3 in →

The square plot reduces in size in a manner that retains legibility. It is important to create the original plot in a size that is close to what will appear in final use.

In particular, one should pay attention to the ratio of the size of the font used – in tick and axes labels, and in legends – to the height and width of the plot as it appears in the final document or presentation.

Place legends in the plot. Don't use terms like "dashed orange line" in the figure caption.

A good plot: The use of color

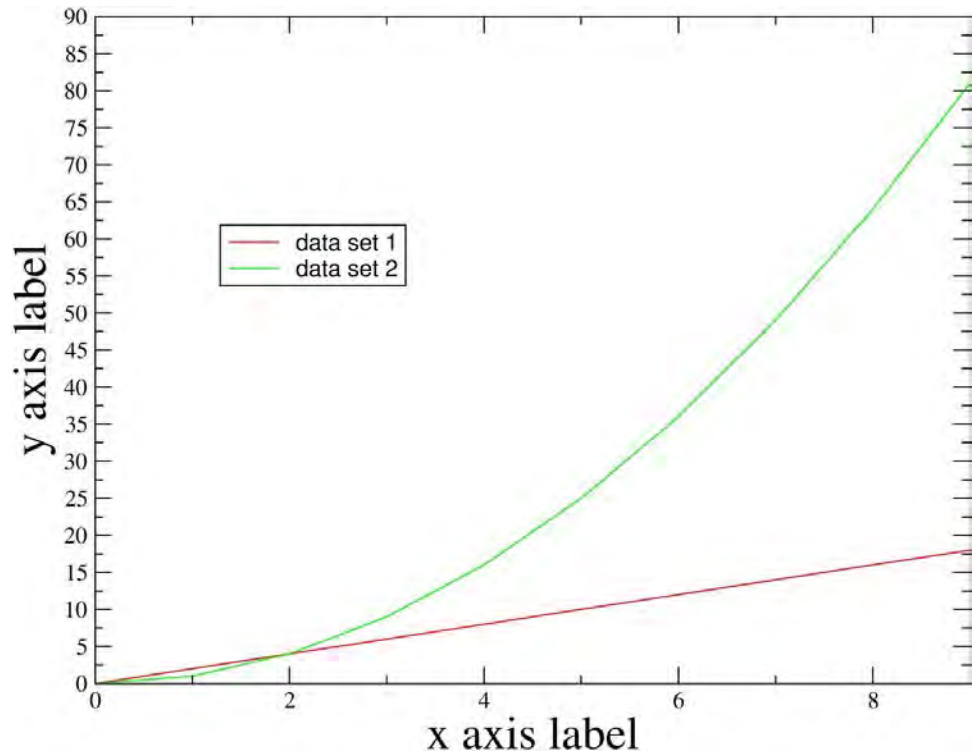


Use a few well-chosen colors: Not **green**, or **yellow**.

Not **exotic colors** that will destroy consistency.

←—————→
3 in

A bad plot



Rectangular plots (the default with some graphing programs) are less aesthetically pleasing, and the horizontal and vertical axes are imbalanced.

Such a plot may appear acceptable when printed out fully in landscape mode on a sheet of a4 or US letter paper, but does not shrink gracefully in publications.

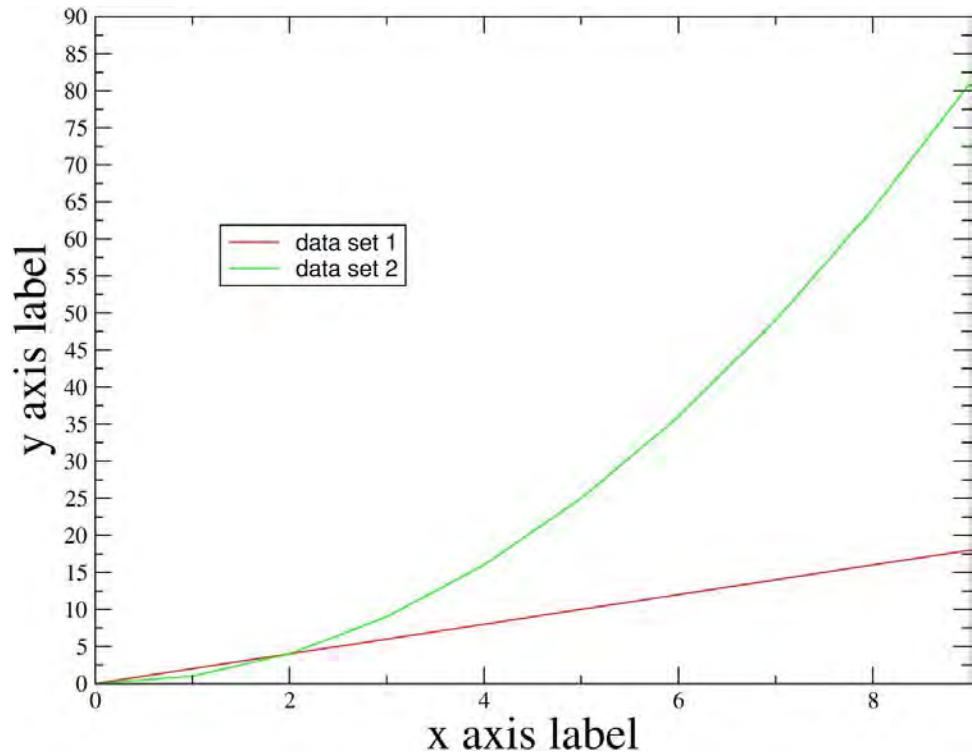
In this plot, there are many other problems:

Red and green are bad choices, with rather low visibility. A significant proportion of the population would not distinguish them. The lines in this plot are too thin as well.

Avoid primary red, blue, green, YELLOW

There is no redundant coding used. In a B&W printout, it would be hard to distinguish the lines.

A bad plot



Problems (contd.):

The lines are too thin (the plot thickens?)

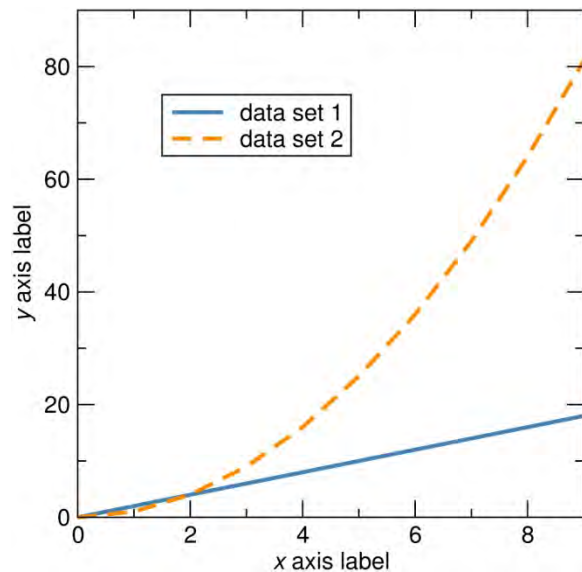
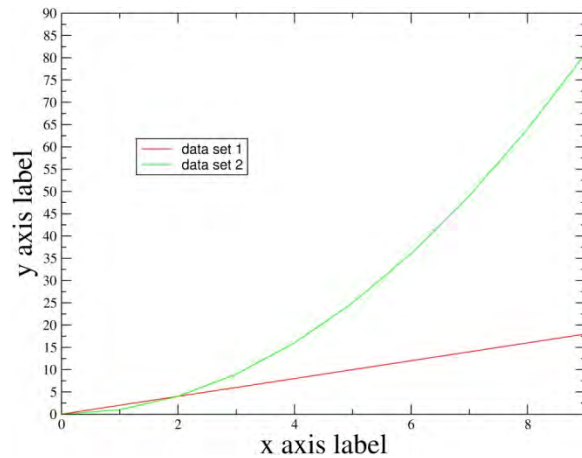
Fonts with serifs are used. These have reduced legibility, particularly when shrunk.

The tick labels are too small. **Why use different font sizes for the tick and axes labels ?**

The vertical axis has too many tick labels and tick marks. The vertical and horizontal axes are imbalanced in that sense.

The plot could be worse. At least it is not pixelated or badly aliased, and the resolution is acceptable.

A bad plot, compared



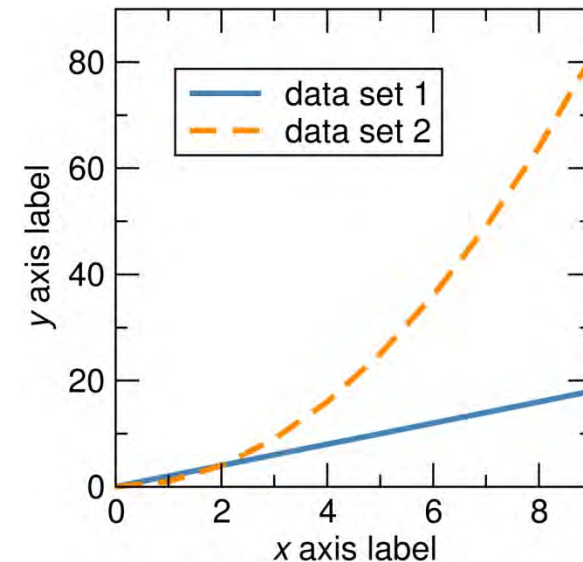
3 in

This plot absolutely does not shrink gracefully.

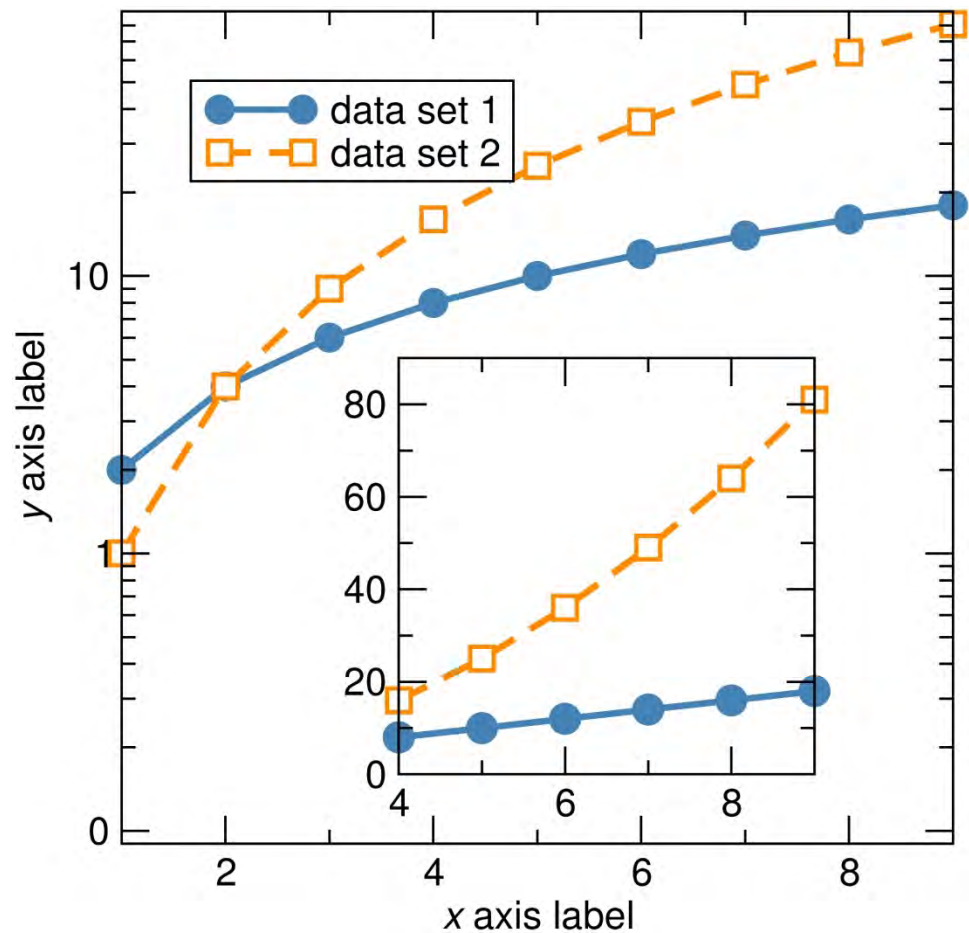
Compare it with our better example.

However, if this were the final size sought, both plots have labels that are too small.

The solution would have been to resize the plot in the original plotting software, as shown below in order to obtain an appropriate ratio between font size and plot size.



Insets (how to make them)



A common problem with insets is that they are frequently shrunk in every sense ... symbols, text etc.

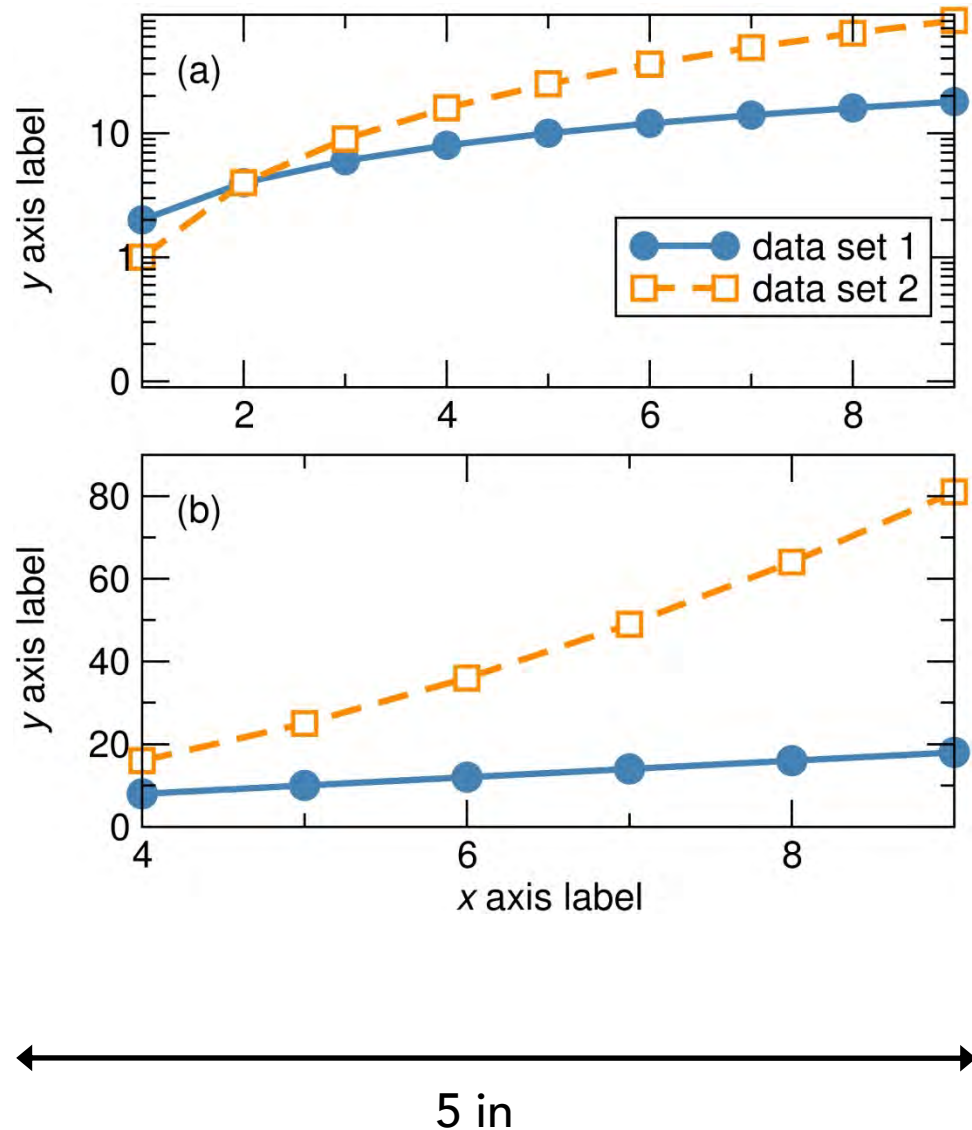
There is no need to shrink down the size of symbols, axes labels, tick labels etc.

Also, there is no need to provide axes labels for the inset if the inset only expands (or otherwise displays) the same data.

Note that in this and the next plot, we make use of symbols, with further redundant coding.

We use distinct symbols for the two datasets, in addition to using color-filled and white-filled (or unfilled) symbols.

Insets (alternatives to them)



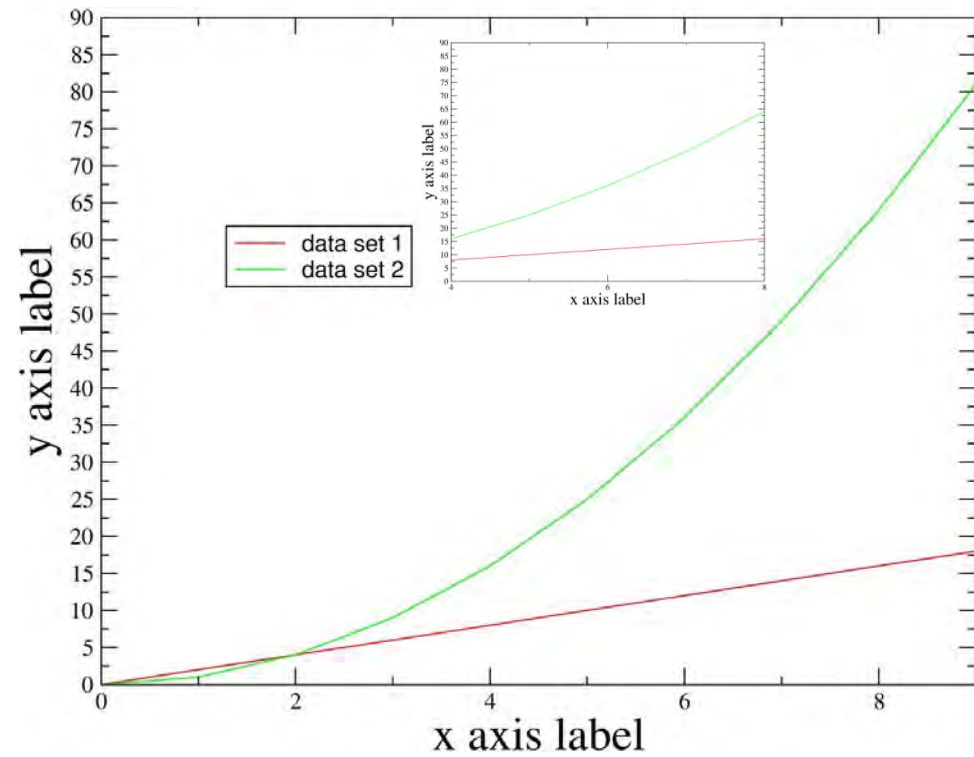
However, insets frequently do not do justice to data.

Consider multiple panels instead. Do note that in plotting the data as performed here, there is no more (screen/paper) real estate used than in the case when the inset was employed.

Note that the label on the horizontal axis is provided only once, since it is shared between panels (a) and (b).

Also note that the labels on the vertical axes are aligned, as are "(a)" and "(b)"

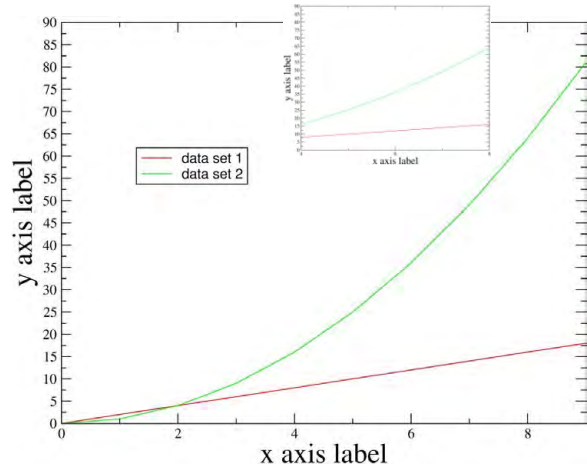
Insets (the example not to follow)



Perhaps an extreme example, but unfortunately not rare.

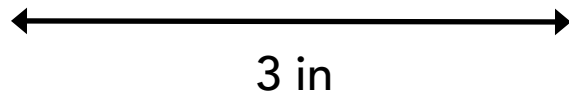
← 5 in →

Insets (the example not to follow)

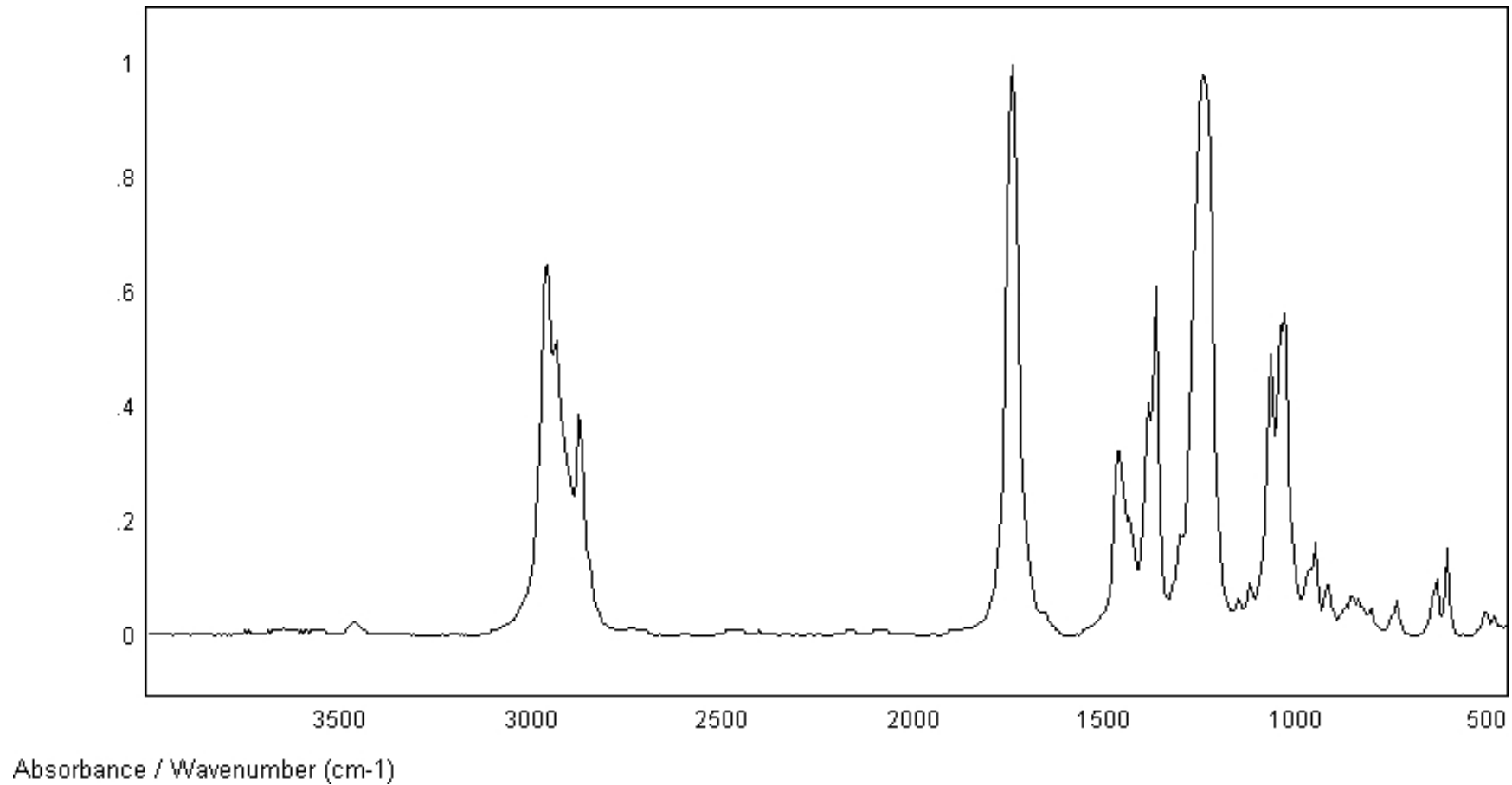


And just when you thought it couldn't get worse !

Remember that journals will reduce figures to the width of a single column.

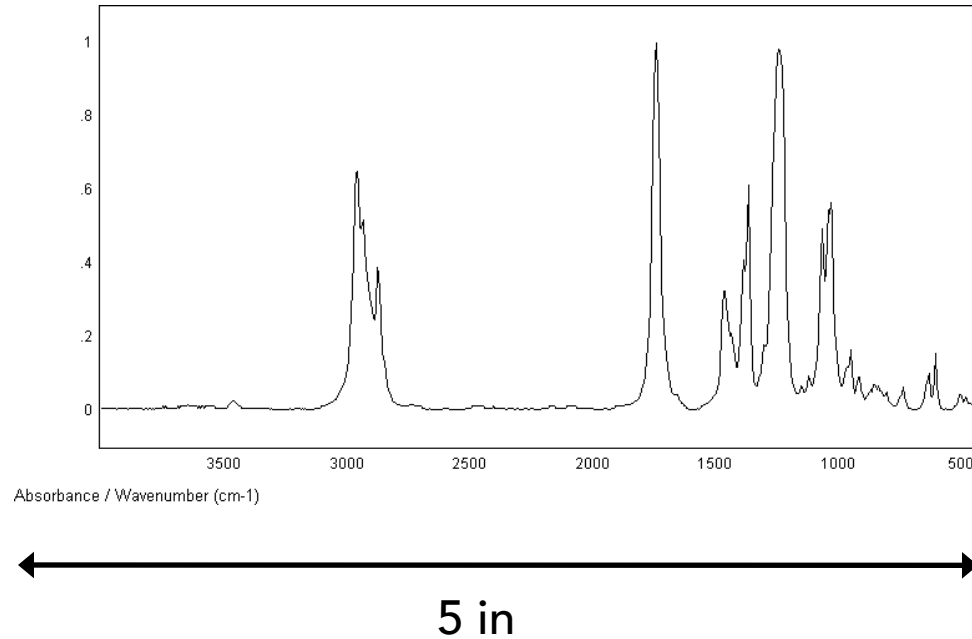


Plots from instruments



Vendors of commercial instruments (FTIR spectrum from a manufacturer's website shown here) are interested in presenting their data for A4/US letter landscape printouts ...

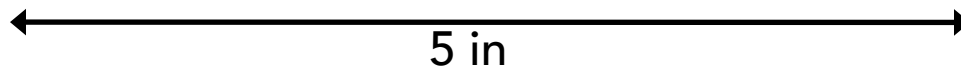
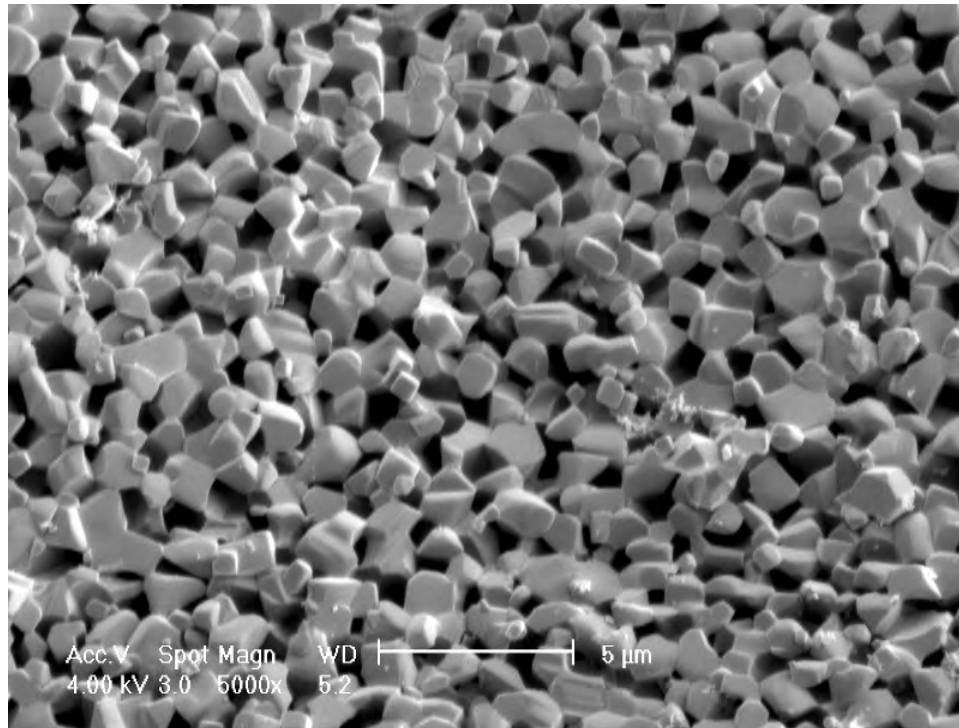
Plots from instruments



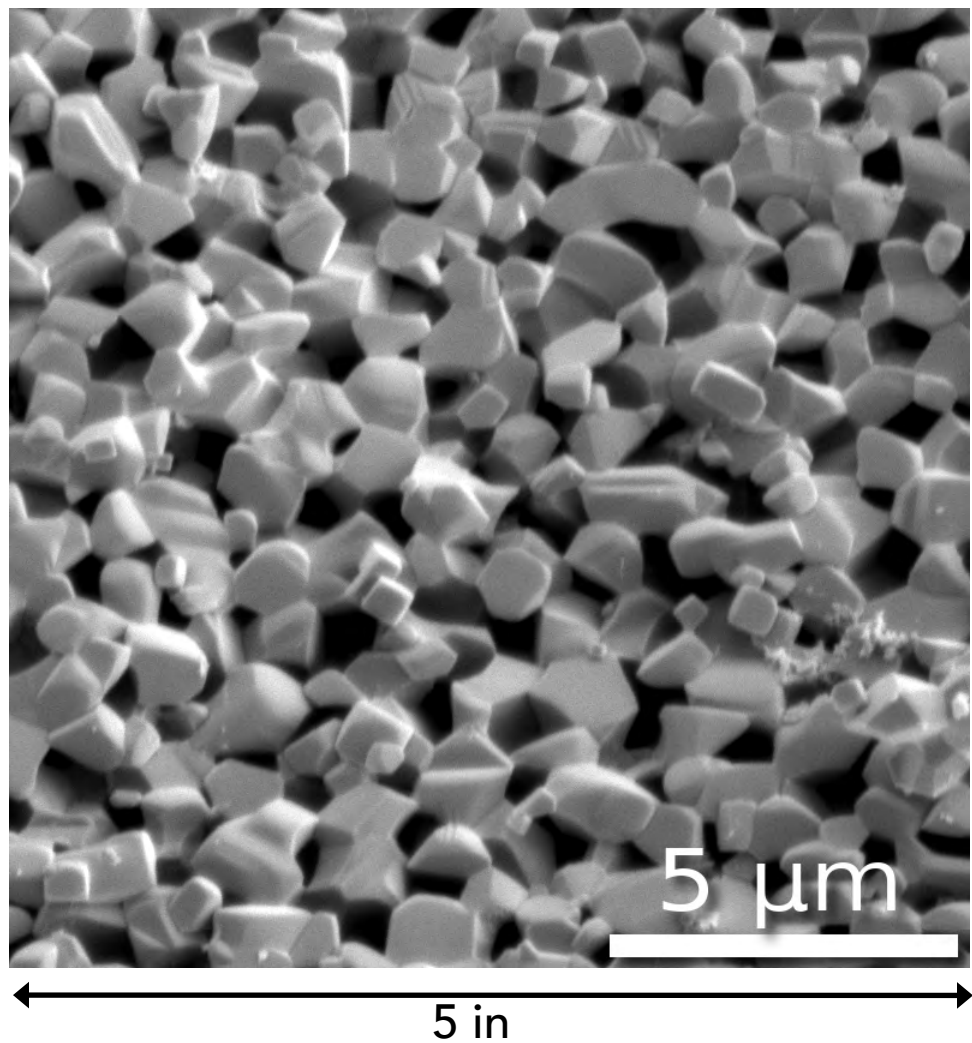
... not for reproduction in the scientific literature (or even in talks !) Also cm^{-1} is not a unit, cm^{-1} is. ".2" and ".4" etc. are preferred over ".2" and ".4"

The saving grace in this example is that the figure is not pixelated. Where are the tick marks ?

Do export ASCII (txt) files from the instrument and re-plot the data using appropriate graphing software.



The text on micrographs (SEM image from Eric Toberer) as obtained directly from the instrument, frequently carries useless information, and the scale bar is usually too small.



With a little effort using GIMP (www.gimp.org), a much more usable image can be created. The (personal) preference is for square images. Shadowing enhances text legibility here.

Exporting an annotated figure from PowerPoint

Ram Seshadri Group: Structure-Property Relations in Functional Inorganic Materials
Materials Department, and Department of Chemistry and Biochemistry
University of California, Santa Barbara CA 93106. <http://www.mrl.ucsb.edu/~seshadri>

The figure is a collage of scientific posters and slides from the Ram Seshadri Group. The posters include:

- Disordering SrTiO₃ and BaTiO₃**: Discusses the structural and electronic properties of these perovskites.
- Size effects in BaTiO₃**: Explores how the tetragonal distortion changes with particle size.
- The structure of Mg-doped ZnO**: Investigates the structural changes and electronic properties of ZnO with Mg substitution.
- Unraveling the local structure of Cu in Cu₂O**: Uses XRD and EXAFS to study the local environment of Cu ions.
- Magnetic properties of insulating oxides**: Discusses the magnetic ground states in various oxides.
- The structure of VO₂(B) in the rutile structure**: Examines the structural changes during the metal-insulator transition.
- Model compounds for catalysis by PGM ions**: Studies the catalytic activity of various transition metal ions.
- New Cu²⁺ phosphors for solid state lighting**: Develops new phosphors for LED lighting.
- Density functional theory visualization of lone pairs**: Visualizes lone pairs in various materials.

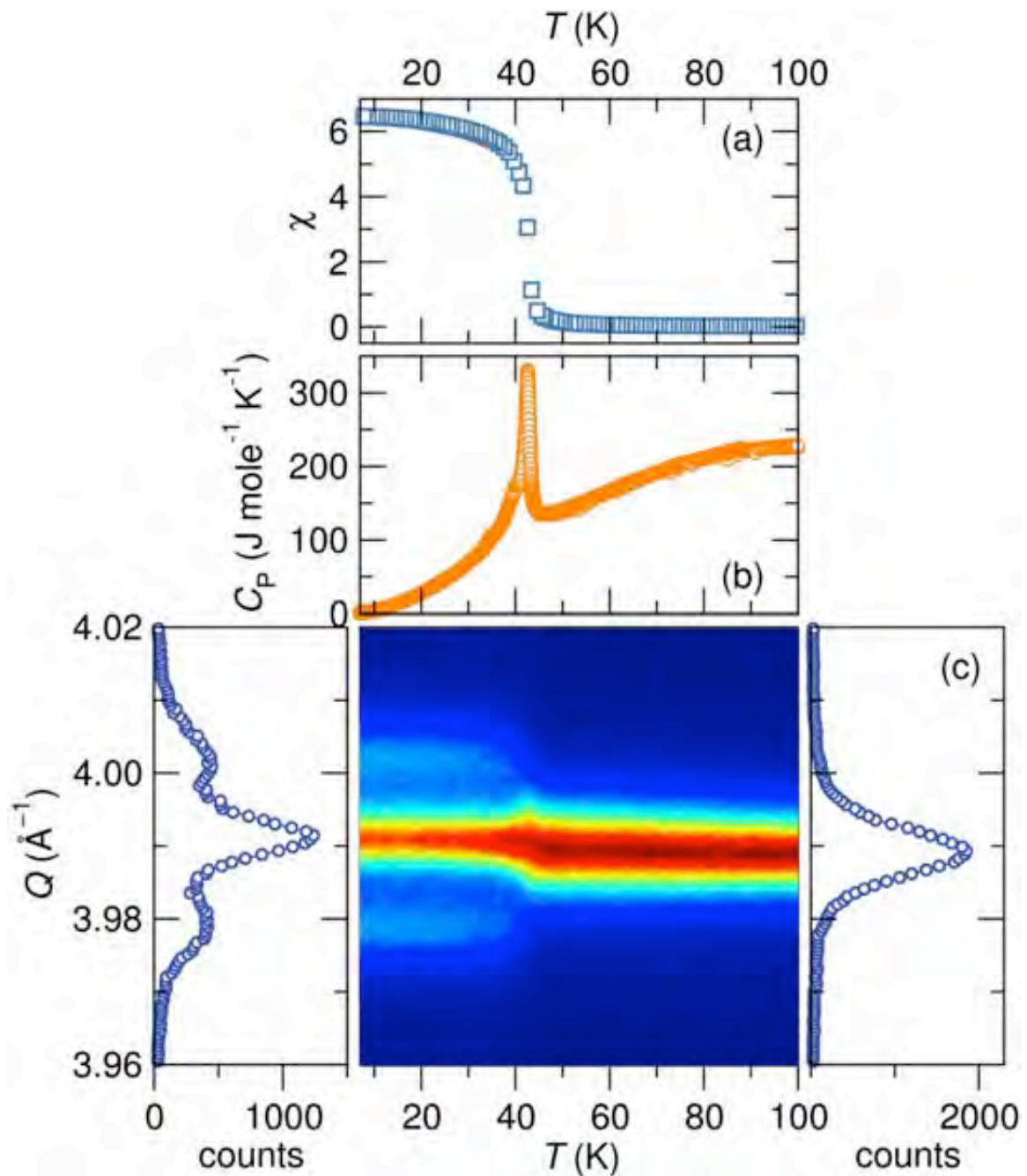
A large diagram in the foreground shows a phase diagram for Zn_{1-x}Co_xCr₂O₄. The diagram has a vertical axis for 'x' and a horizontal axis for 'T'. The regions are labeled 'paramagnetic', 'collim. FIM', and 'Electro...'. An inset image labeled '(a)' shows a scanning electron micrograph of a material.

Plots and images are annotated with ease, and the preparation of schematic images is convenient within PowerPoint.

How are these best exported? The resolution of jpg files (or other bitmap formats) saved from PowerPoint is rather low.

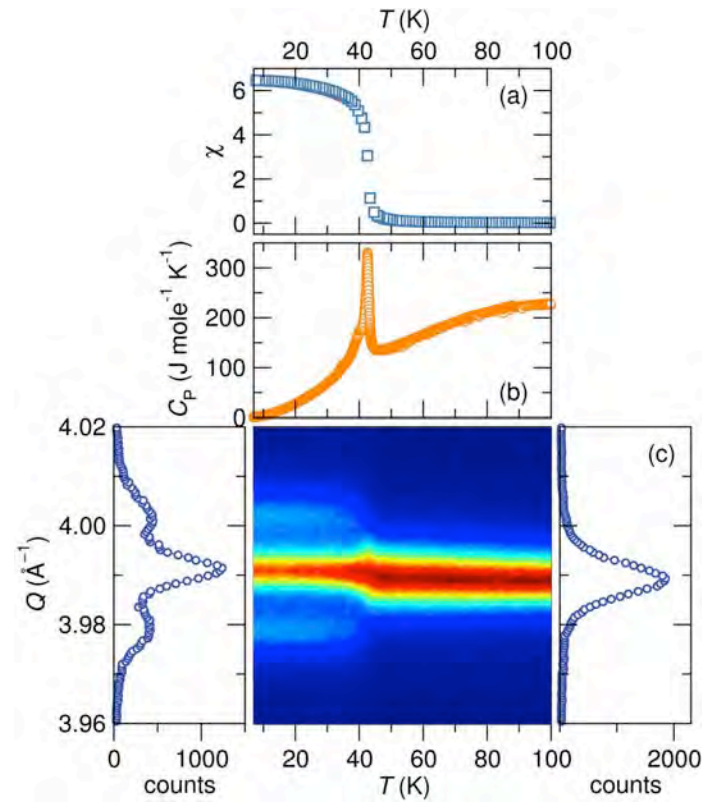
One solution is to export as a print quality PDF which can then be opened in GIMP with near arbitrary resolution, and then saved as a bitmap image. An example is displayed on the left, created from a PowerPoint poster. A portion of the jpg is shown as well, in order to show the resolution of the original image.

Examples of acceptable figures



Kemei, Harada, Seshadri, Suchomel,
Phys. Rev. B **90** (2014) 064418(1–8).

Examples of acceptable figures



Yes, it shrinks gracefully

Kemei, Harada, Seshadri, Suchomel,
Phys. Rev. B **90** (2014) 064418(1–8).

Examples of acceptable figures (also see TOC ROFL)

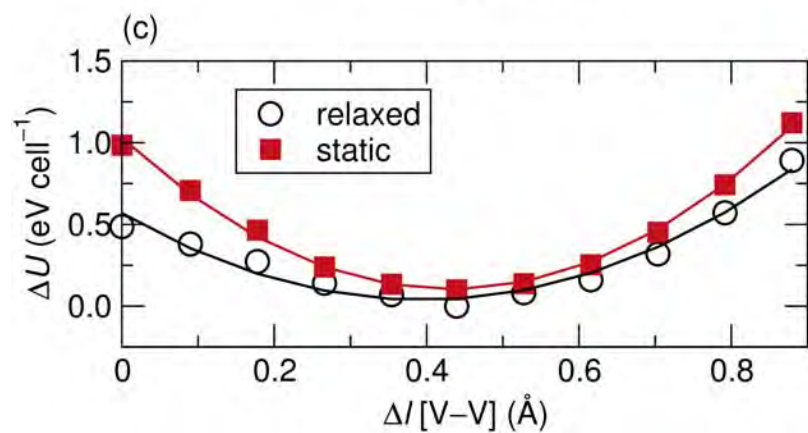
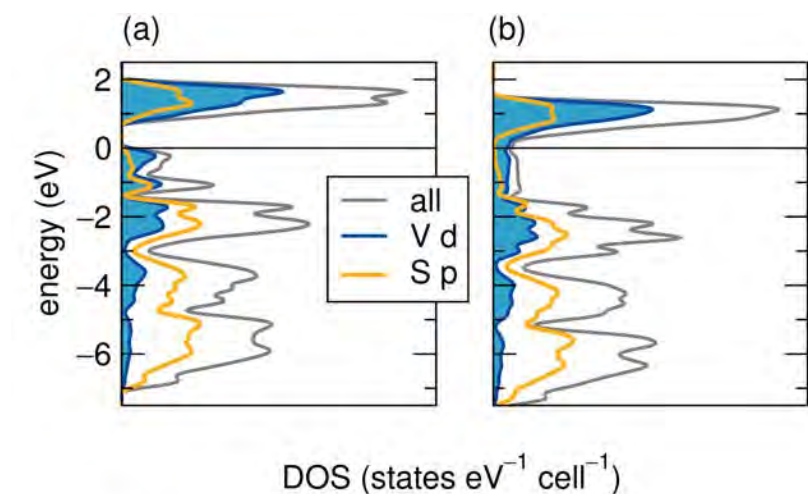
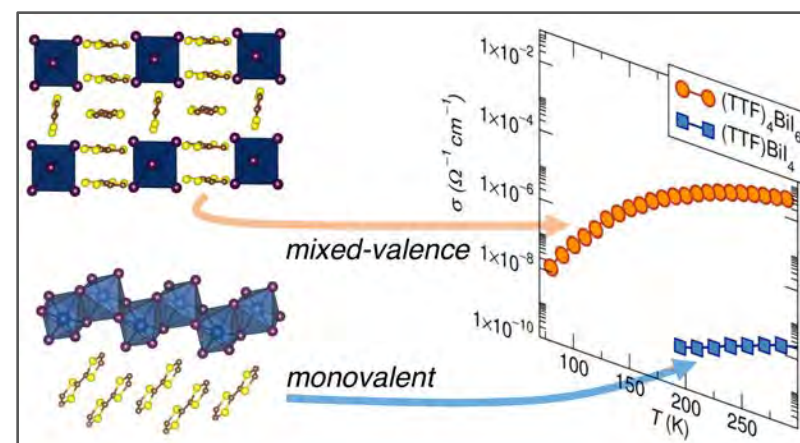
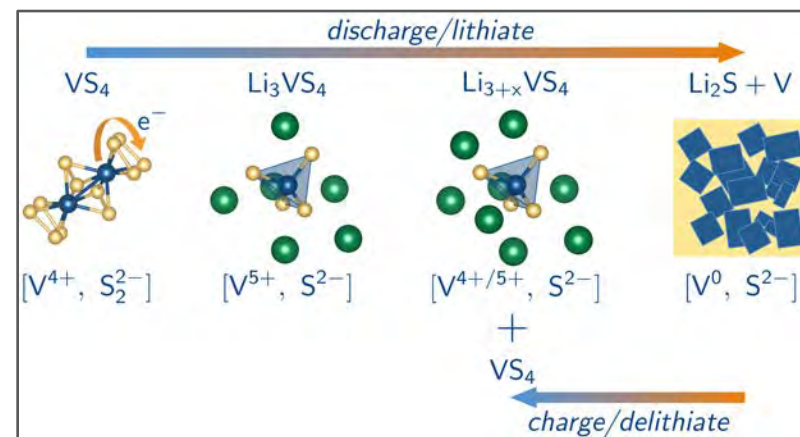


Table of contents graphic



Britto, Leskes, Hua, Hébert, Shin, Clarke, Borkiewicz, Chapman, Seshadri, Cho, Grey, *J. Am. Chem. Soc.* **137** (2015) 8499–8508 (above, above right).

Evans, Labram, Smock, Wu, Chabiny, Seshadri, Wudl, *Inorg. Chem.* **56** (2017) 395–401.

Titles and Table of Contents Images: The Candy Store Analogy



Everyone is familiar with the scenario of the indecisive kid in the candy store—the vast array of choices can be overwhelming to anyone, since the final choice of what to buy is predicated upon many sources of information that are convoluted to become a train of thought, and ultimately a decision. Possible variables that influence the decision include the name of the candy (its title), one's past experience with candy (was it good/interesting?), one's learned preferences (I like chocolate/graphene, but I do not like mints/oligonucleic acids), and a host of intangibles. It is similar for readers who may be shopping in a scientific "candy store", or journal, for potential papers—each reader must make a decision regarding which paper to click on, download, and read, all of which are actual separate and not entirely connected actions. The types of scientific candy stores frequented by readers may be quite varied, as some will skim tables of contents on journal web sites, and others will rely on social media or RSS feeds, search engine results, and/or a mix of any or all of these. So the question for all authors is this:

How does one maximize the chances that one's paper will be downloaded?

Both the title and the table of contents (ToC) image are important tools for authors to give potential interested readers insight into what a paper is about. As has been summarized in an earlier editorial, a reader may make a decision to click on a paper within 100 ms.¹ A clear title and compelling ToC image will play a significant role during this short time, and we cannot emphasize enough the importance of these two parts of a paper. As scientists, we spend months or years working toward submission of a manuscript, and it would be a shame to present this new scientific insight to the world with an overly complicated title and/or a poorly executed ToC image. Scientists are humans, and so like dining at a high-end gourmet restaurant, the esthetics of presentation of the meal (or in our case, the paper) is an important part of the enjoyment and, ultimately, consumption of the meal (the scientific results). Time taken to develop an interesting and nicely presented ToC

image and title reflects pride in one's research, and since it is typically the first encounter of a potential reader with this particular piece of work, a good first impression is critical, the impact of which cannot be underestimated.

■ TITLE

A good title is one that is succinct, makes the focus obvious, and is free of acronyms and excessive jargon. The title may be difficult to write if one has not developed a clear emphasis for the paper and, thus, should serve as a red flag for authors that their manuscript requires more thought. A title that states that the material described within has promise for a laundry list of applications sounds unappealing, as does a title that places too much emphasis on the results being the highest, biggest, smallest, grandest, most novel, brightest, most efficient, best, etc.; the latter "superlative" papers suggest that the work contained within is merely a series of incremental improvements, which may not be creative or interesting. As an author, you are telling a story, so be honest with your readers and portray the theme and subject matter of your story as lucidly as possible. Do not mislead, and hence frustrate, your readers; since your first readers are almost always the editors and reviewers, annoyance that the title does not accurately reflect the content of your paper could lead to negative consequences.

■ TABLE OF CONTENTS (ToC) IMAGES

The *Chemistry of Materials* Author Guidelines tries to provide the very basic premises of how to conceive of a good ToC image:

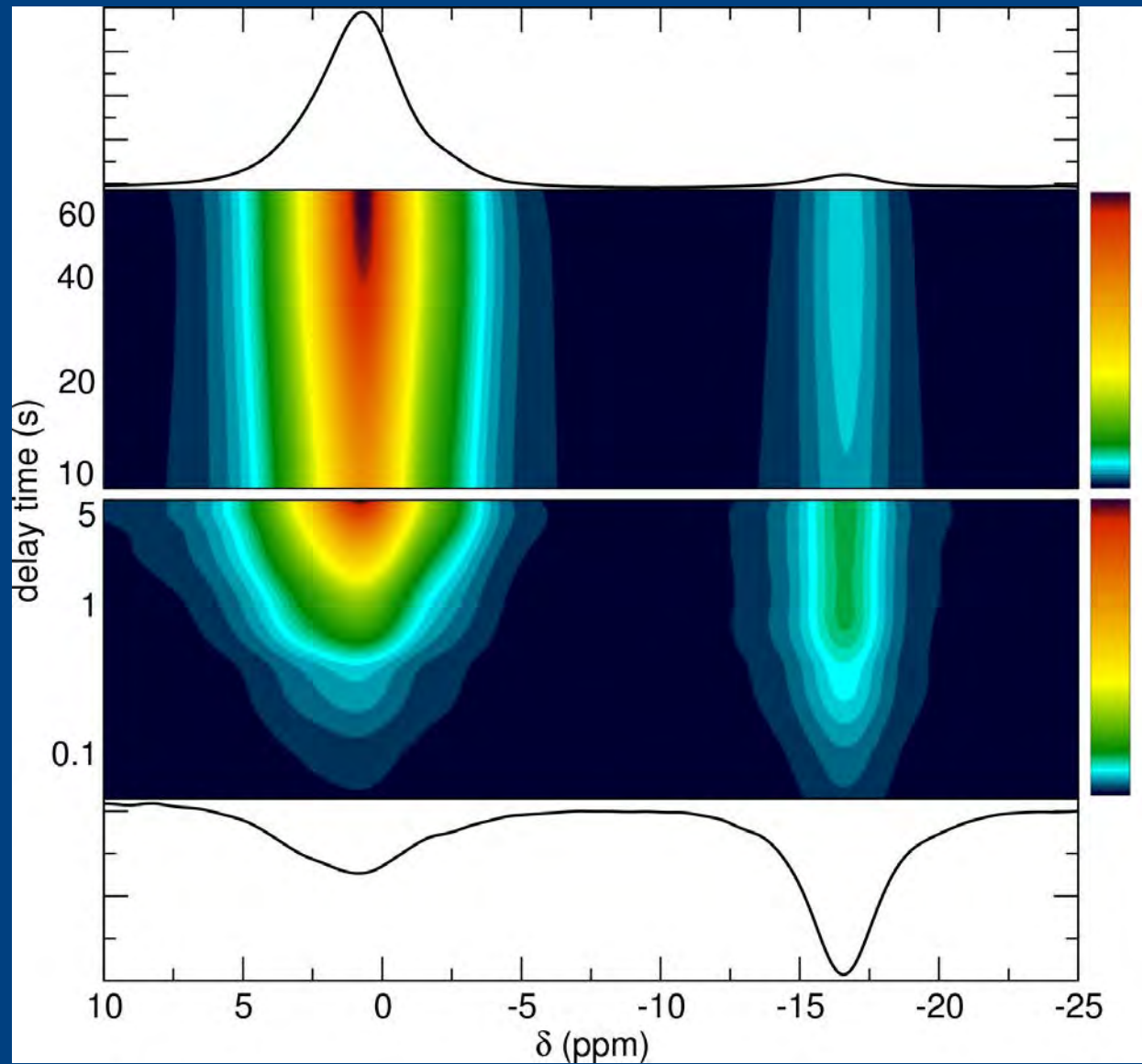
"The TOC/abstract graphic should capture the reader's attention and, in conjunction with the manuscript title, should give the reader a quick visual impression of the essence of the paper without providing specific results.... Some of the best images are simple, relatively free of text and technical characters, and make use of color for visual impact. It is best to stay away from complex structure schemes and small-sized details."

Do not simply cut and paste a figure from your manuscript to use as the ToC image, as they typically are ill-suited due to a high level of scientific detail, and they lack in the context to make them rapidly understood. One very useful article on how to design scientific figures, "A Brief Guide to Designing Effective Figures for the Scientific Paper," is a helpful place to look for pointers on graphical design, layout, and many "do not do this, and why" examples.² While it may seem obvious, make sure that your font or other details are not too small to discern when shrunk down to the size they will appear on a screen or on the printed PDF page. Ensure that the ToC image resonates with your title so that it enthralls your (potential) readers to want to look further. This is a scientific candy store, with many other exciting papers within easy reach, so think about why authors will want to choose to spend time out of their busy day downloading and reading your paper.

Published: February 11, 2014

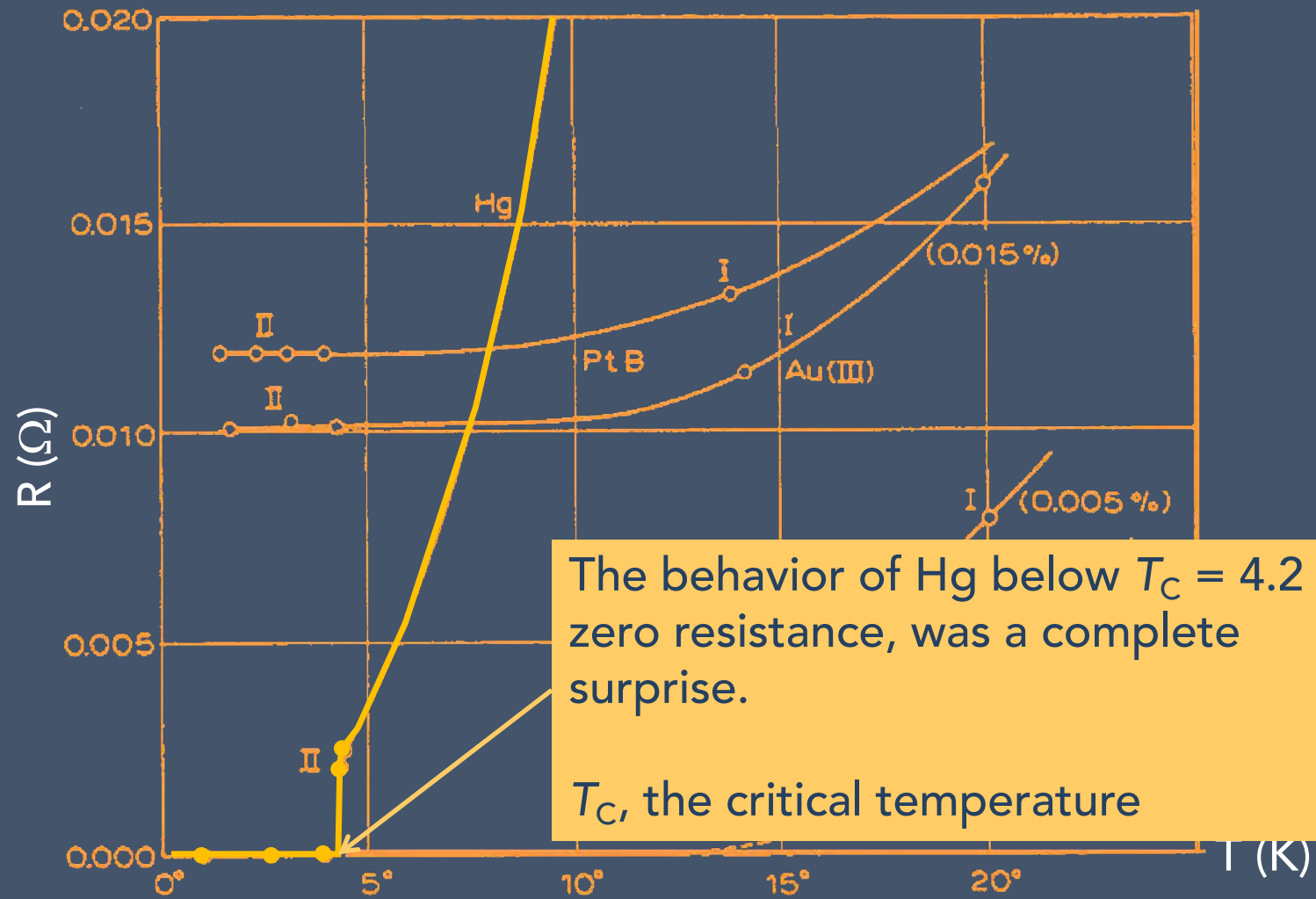
Buriak, *Chem. Mater.* **26** (2014) 1289–1290. DOI:
10.1021/cm500170v

Dark backgrounds (yuk !)



Nathan George

The discovery of superconductivity in Hg (1911)

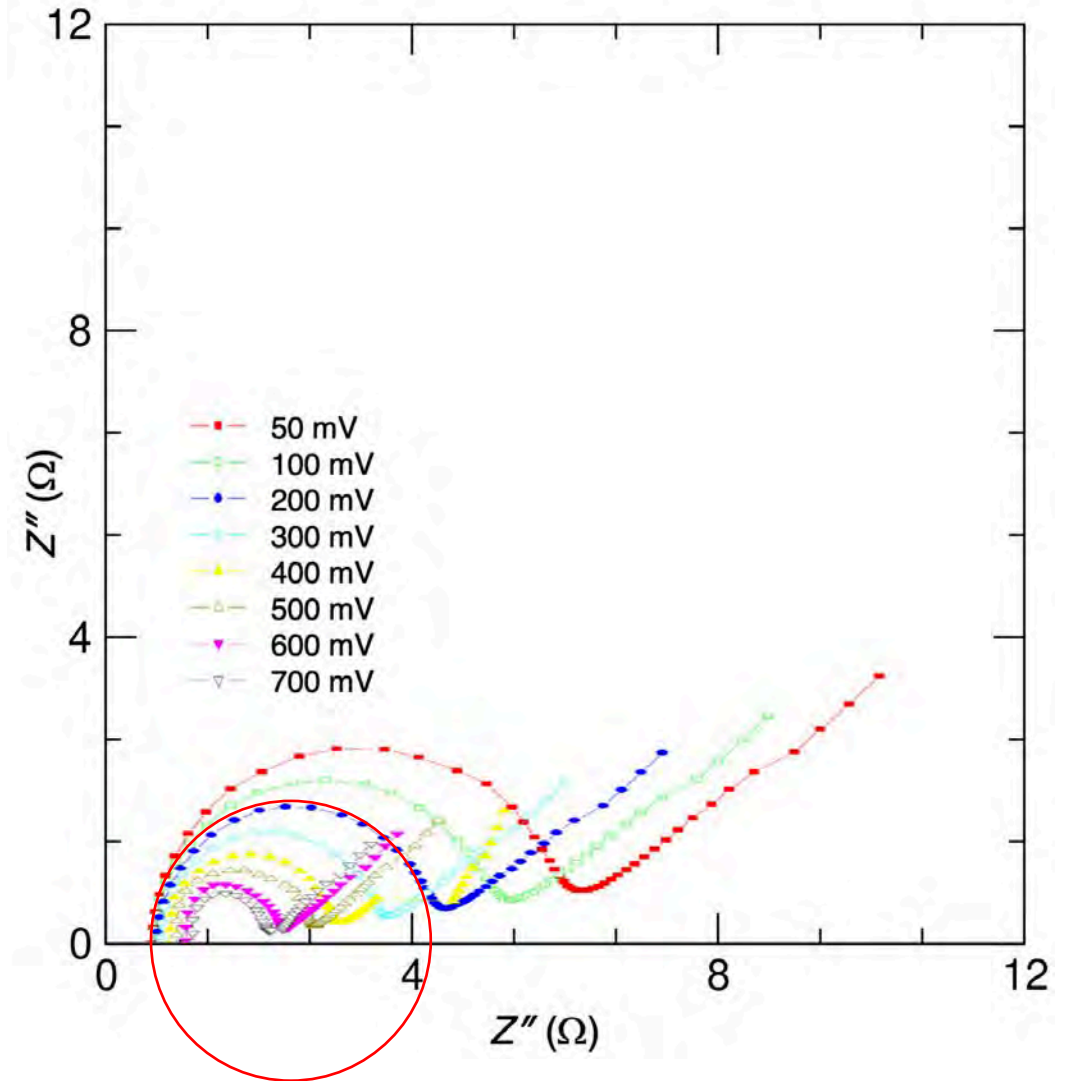
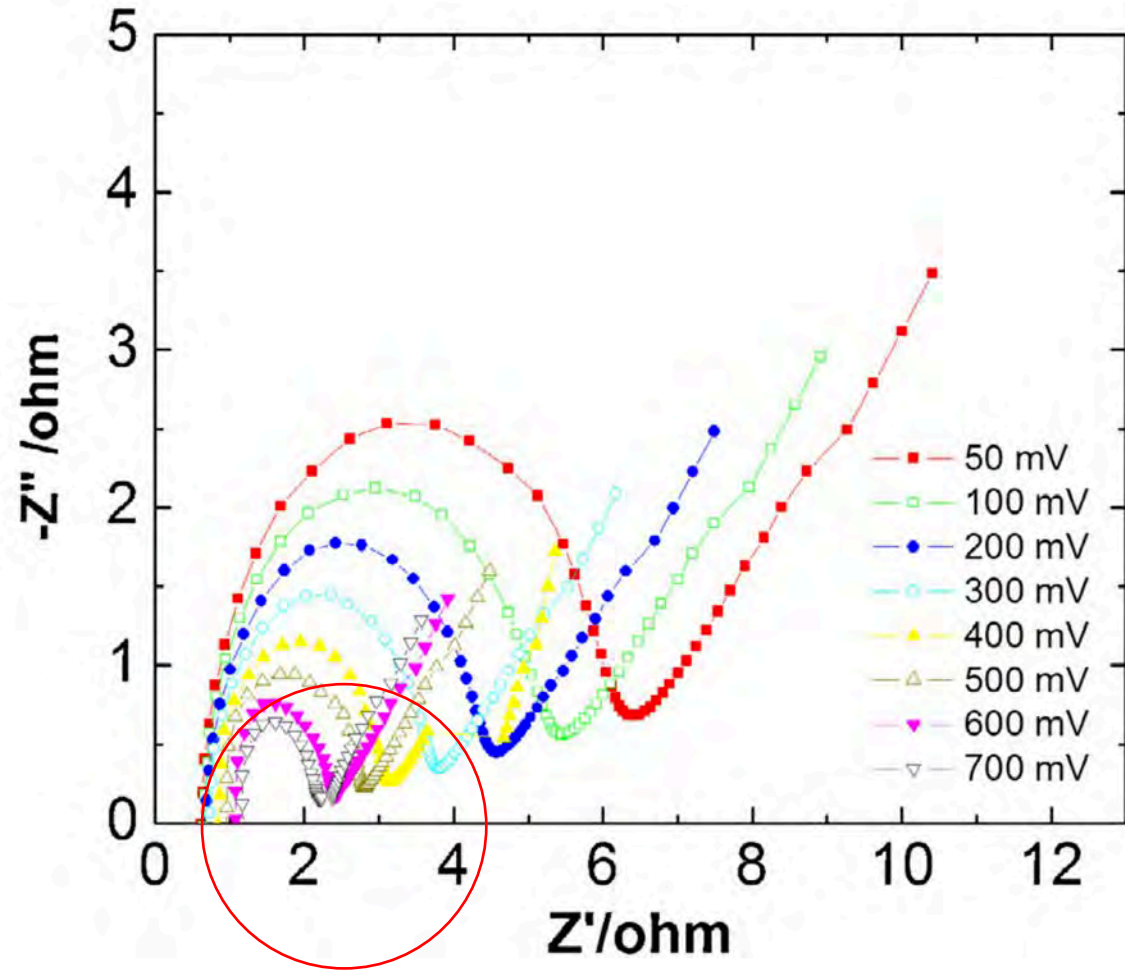


The behavior of Hg below $T_C = 4.2$ K; zero resistance, was a complete surprise.

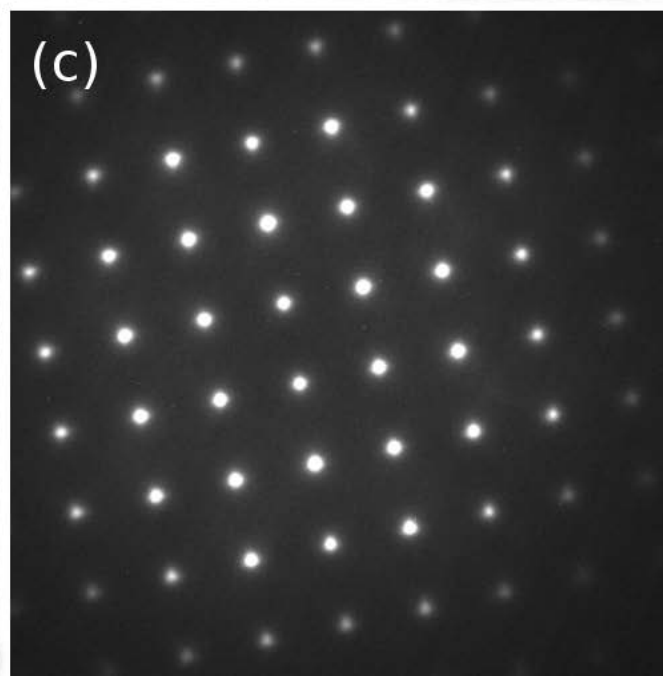
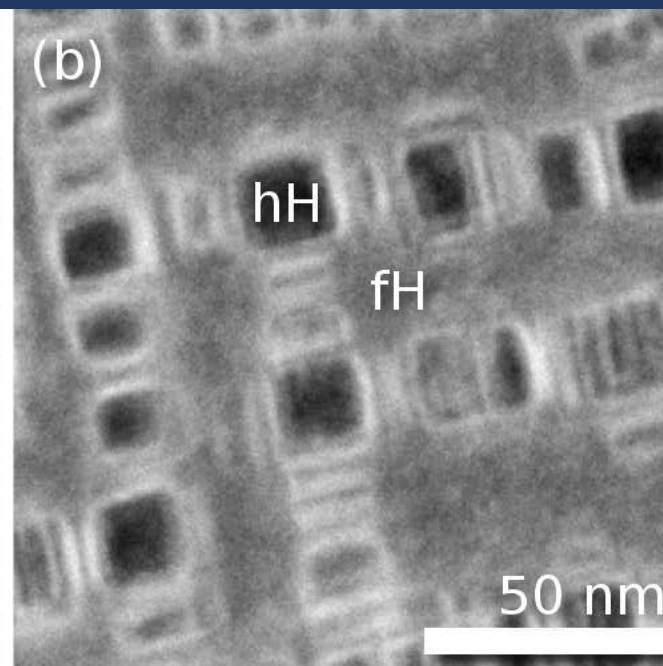
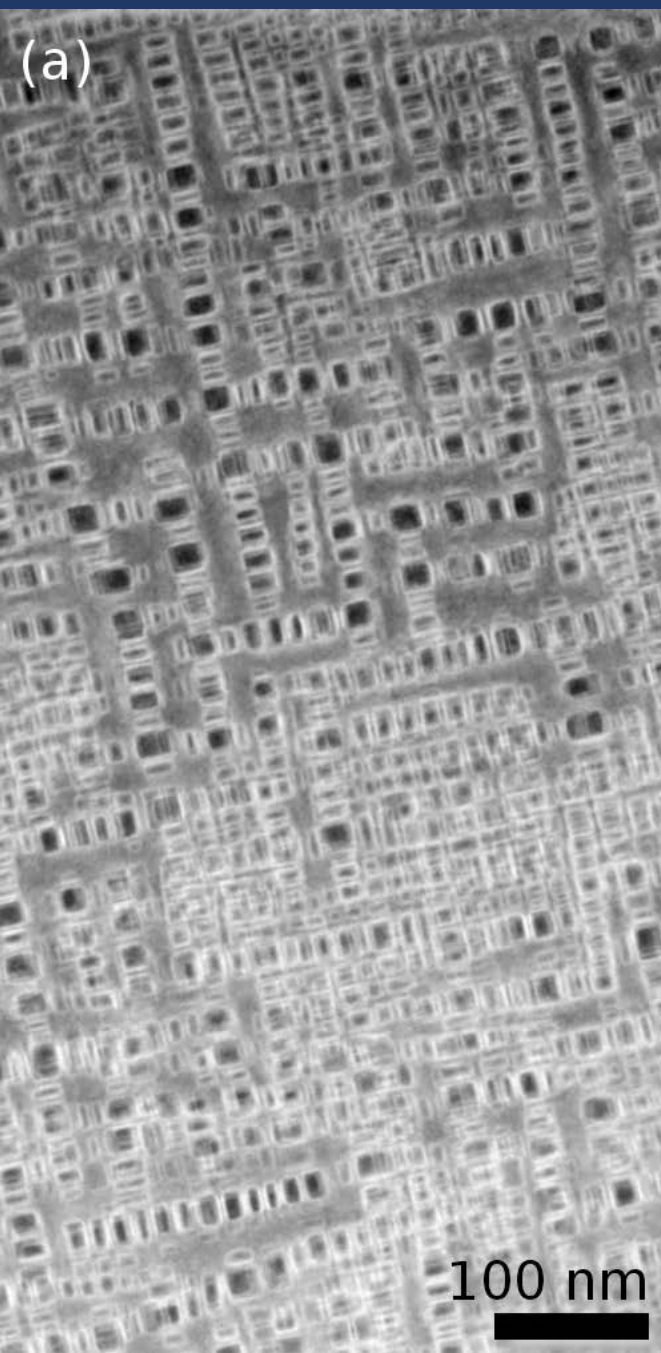
T_C , the critical temperature

H. Kamerlingh Onnes, Nobel Lecture, December 11, 1913.

Hacking figures to make them acceptable: Impedance analysis MUST be equiaxed!



Examples of acceptable figures

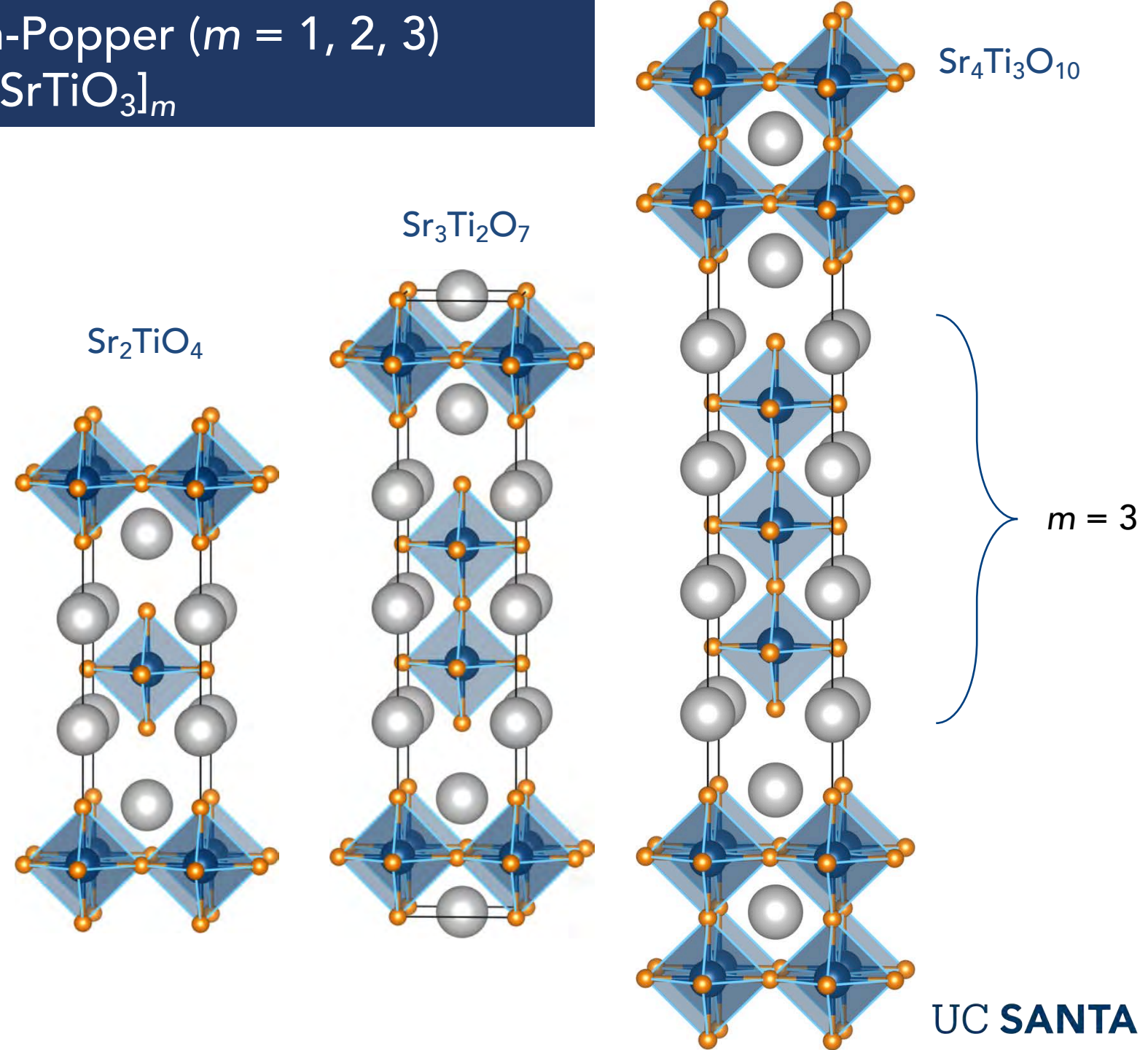


Samples and image assembly by Jason Douglas.

Microscopy by Dr. Nisha Verma

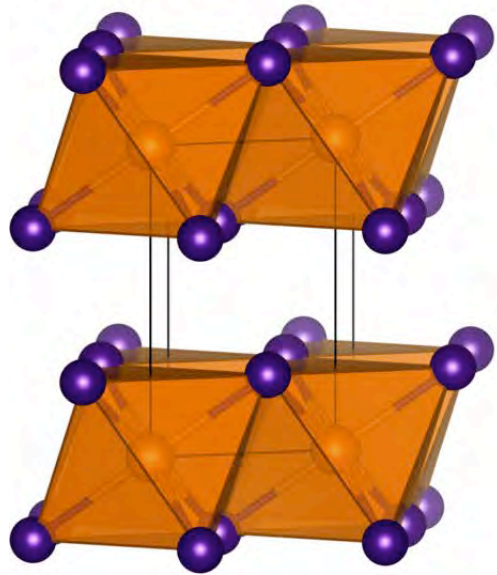
K_2NiF_4 and Ruddlesden-Popper ($m = 1, 2, 3$)
General formula: $[SrO][SrTiO_3]_m$

Please don't use the horrible compass directions output by VESTA.

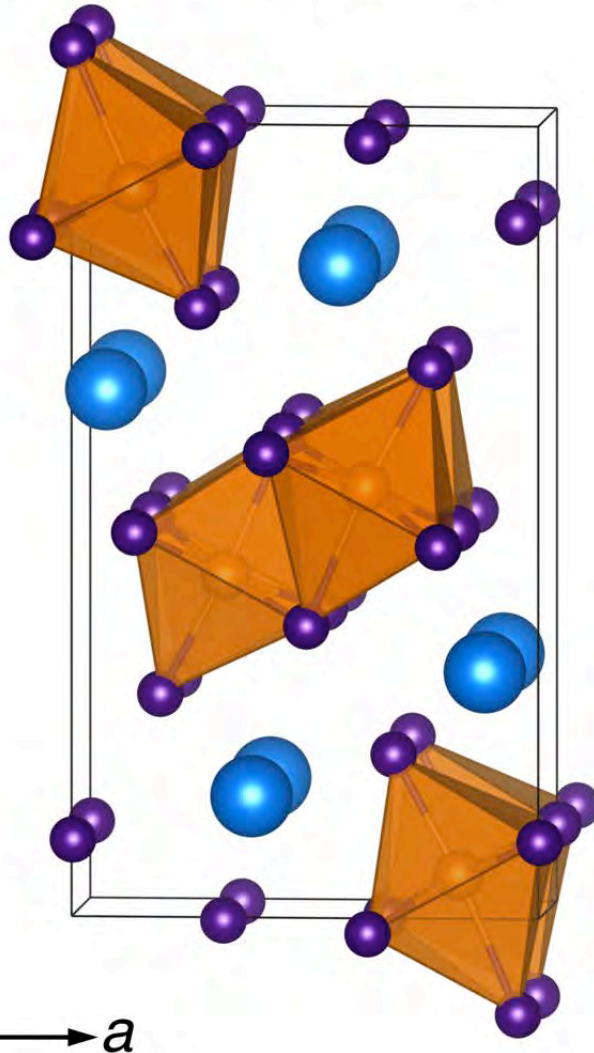


Examples of acceptable figures (care with labeling)

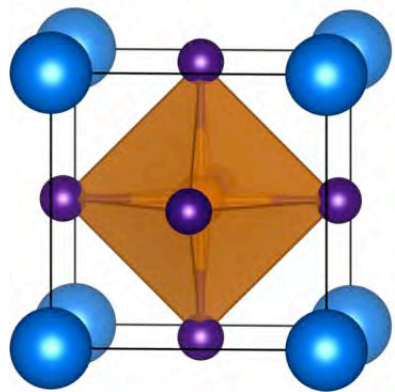
(a) PbI_2 $P\bar{3}m1$



(b) $\delta\text{-APbI}_3$ $Pnma$



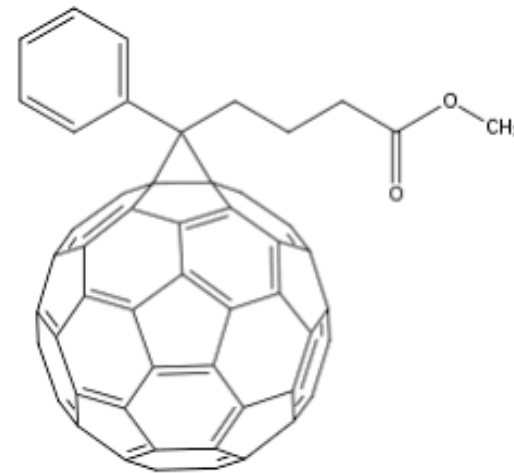
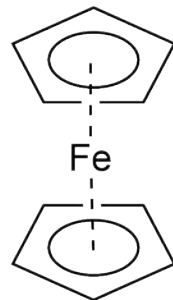
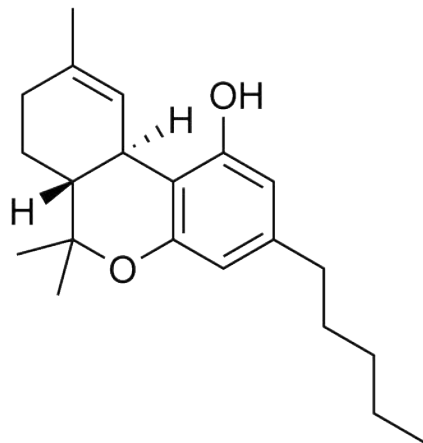
(c) $\alpha\text{-APbI}_3$ $Pm\bar{3}m$



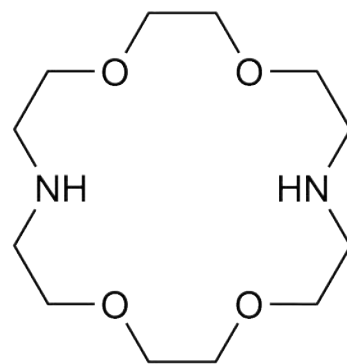
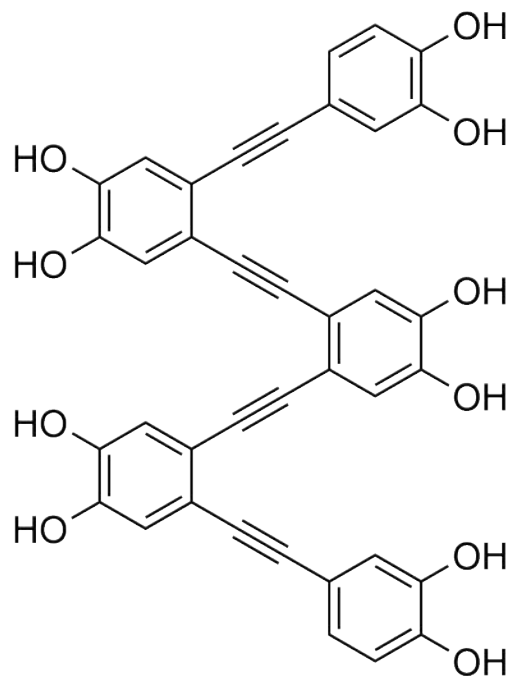
All structures to scale.

Labeling using LaTeXiT and PowerPoint.

Brgoch, Lehner, Chabynec, Seshadri,
J. Phys. Chem. C 118 (2014) 27721–27727.

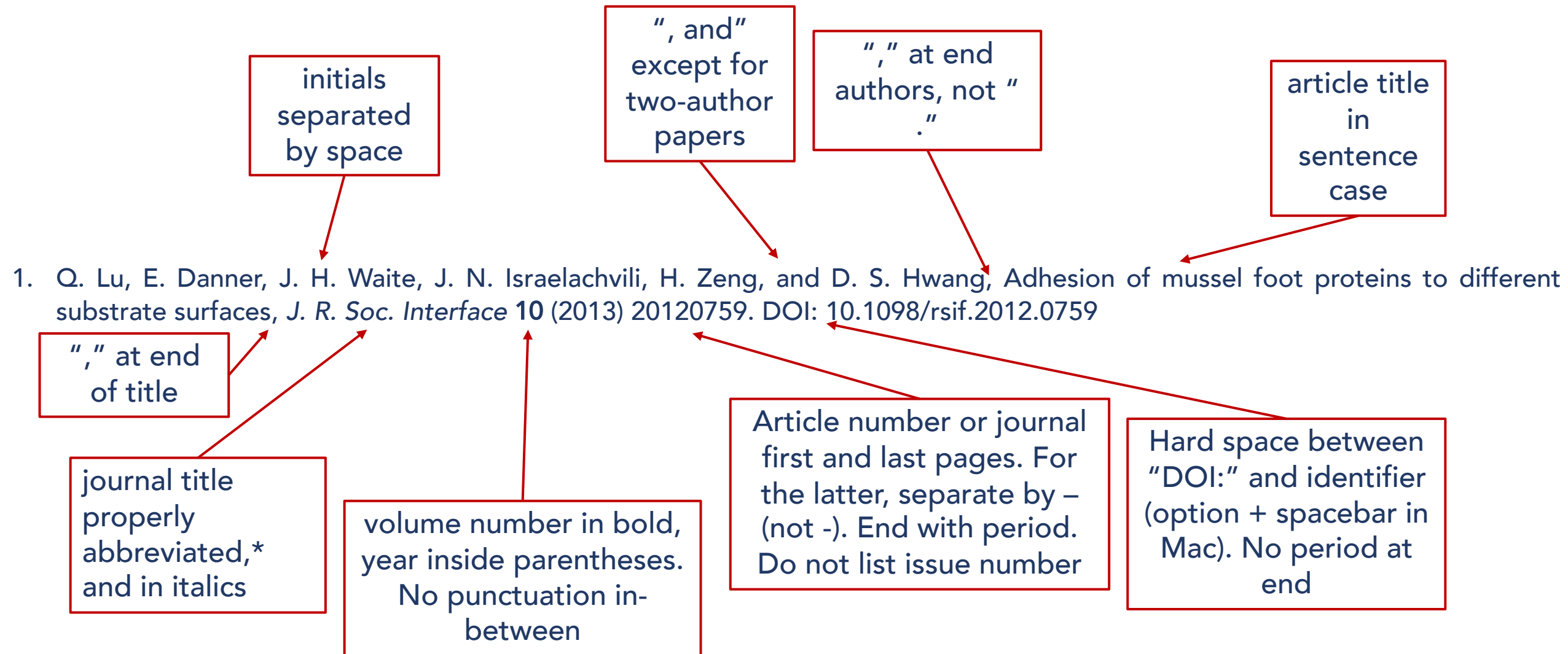


A not-so-nice PCBM from *wikipedia*



Thanks to Molleigh Preefer

Anatomy of a reference: The goal is to be complete and consistent !



*Journal abbreviations, see: <http://cassi.cas.org/search.jsp>

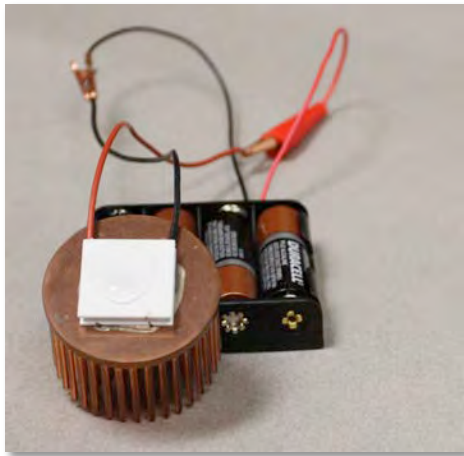
Some typesetting etiquette for Word and PowerPoint

- The minus sign: – not -
- Multiply: × not x
- Approximately: ≈, not ~ and certainly not ~
- Proper chemical nomenclature: never H2O
- Spaces after units: 300 K, never 300K.
- Ranges written 300 K to 2 K, never 300 - 2 K
- Variables are always in *italics*: $T = 300\text{ K}$
- $A_{1-x}B_x$
- CsBBr₃ vs. Cs*B*Br₃

Still and video photography



Dr. Jason Grebenkemper and Dr. Joya Cooley



- Use a real camera, with a fixed focal-length lens allowing a wide aperture
- Keep the camera still: In the case of videos, the camera does not need to move; allow the action to.
- Remove any clutter in the background
- Learn about depth of field, and even possibly, *bokeh*
- Aim for even lighting

Resources:



For example, books by:

- Jean-Luc Doumont
- Felice Frankel
- Edward Tufte

This document

Production notes:

Most graphs were produced using XMGRACE (<http://plasma-gate.weizmann.ac.il/Grace/>; free software that runs under Linux and Mac).

Vector graphics (eps files) were exported from XMGRACE and opened with GIMP (<http://www.gimp.org/>; also freely available for all platforms) at 600 dpi with strong text antialiasing, and converted into jpg or png images of appropriate quality.

QtGrace is free and works on Mac, Linux, Win

VESTA for the crystal structure depictions: <http://jp-minerals.org/vesta/en/>

These were imported into PowerPoint.

As a general rule, directly copying and pasting from graphing software into Word or PowerPoint is ill-advised, and creates problems associated with cross-OS (in)compatibility and missing fonts. It is always preferred to export high resolution image files.

All image widths and positions have been specified using the size and position commands in PowerPoint.