WARNING

GRAPHIC CONTENT

baptiste auguié

PG | Post-Grad supervision advised


40%
30%
0%
40%
THE GOOD THE BAD AND THE UGLY
DVD video

GRAPHICS 101

USE NAVY BLUE & MAGENTA

and your favourite font

MY GOAL: challenge us

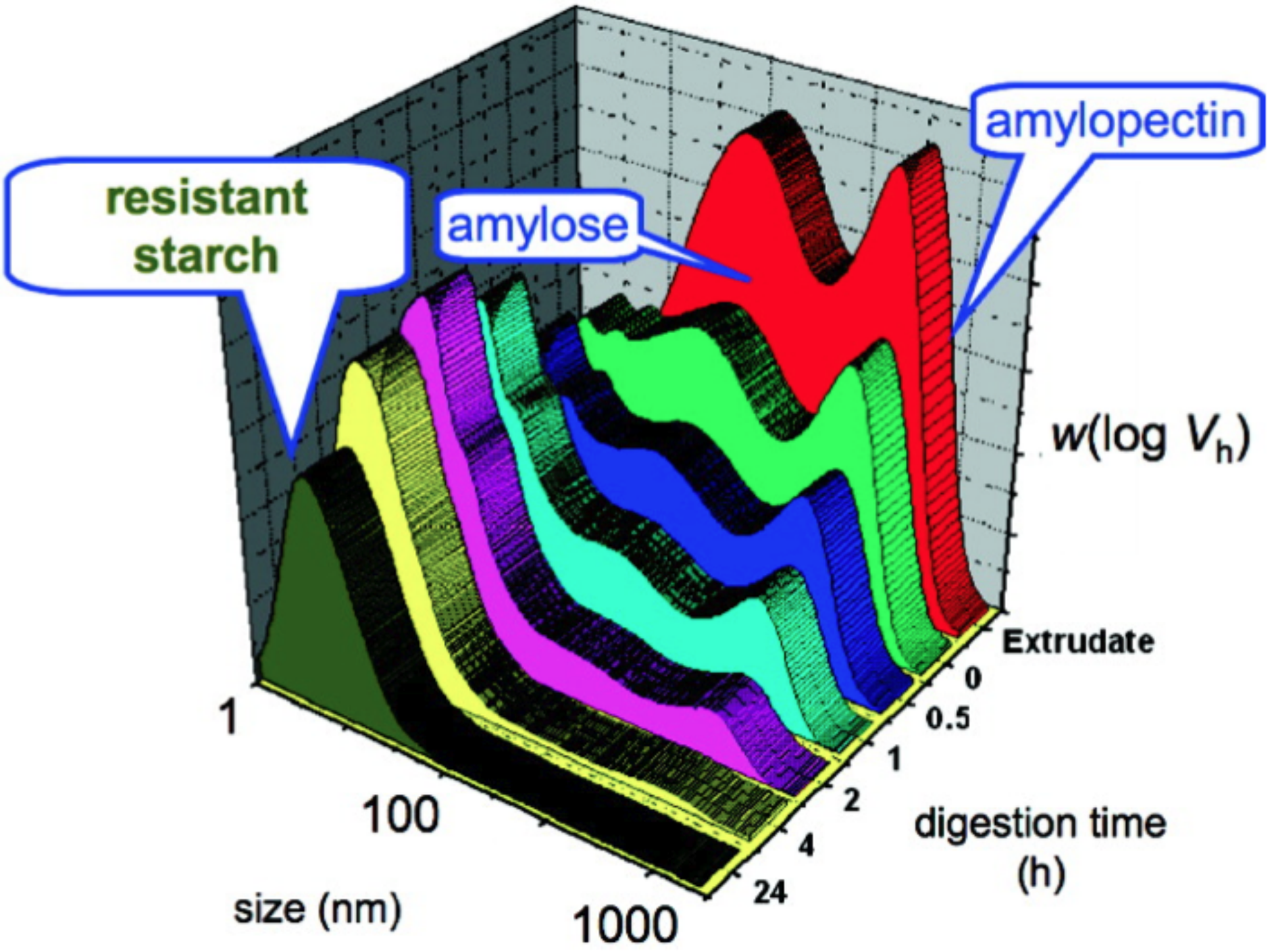
to think differently

about graphics

OUTLINE

- **MOTIVATION: A PHILOSOPHY OF GRAPHICS**
  - *The good*
  - *The bad, and the ugly*
- **FRAMEWORK: A GRAMMAR OF GRAPHICS**
  - *What's in a plot?*
  - *Tips and guidelines*
- **ILLUSTRATION: A VISION FOR GRAPHICS**
  - *Aesthetics and impact*
  - *TOC figures, slides, posters*

1 MOTIVATION


resistant starch
amylose
amylopectin
w(log V_h)
Extrudate
0
0.5
1
2
4
24
digestion time (h)
1
100
1000
size (nm)

Tatsuo Horiuchi

Excel artist

TOOLS DON'T MATTER

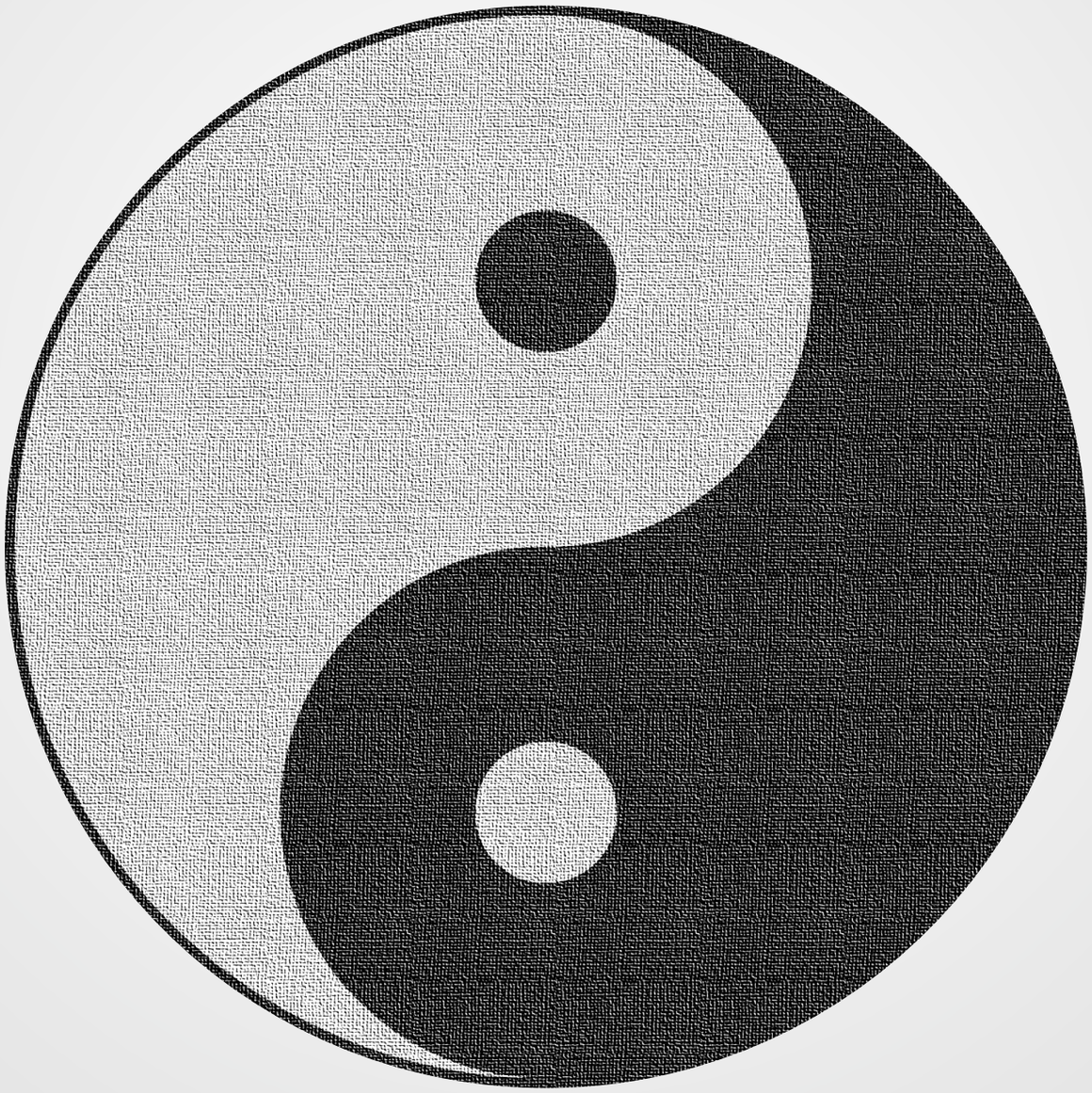
(but they do)

1 MOTIVATION

(SOME ILLUSTRATIONS)

- worrydream.com/TenBrighterIdeas/
- jasondavies.com/maps/transition/
- mbostock.github.io/d3/talk/20111116/#17
- https://observablehq.com
- https://www.visualcinnamon.com/

A PHILOSOPHY OF GRAPHICS



ANALYTIC

Esthetic

key message

DATA-TO-INK RATIO

be deliberate with
your pixels

1 MOTIVATION

LETTERS NATURE PHOTONICS DOI: 10.1038/NPHOTON.2012.300

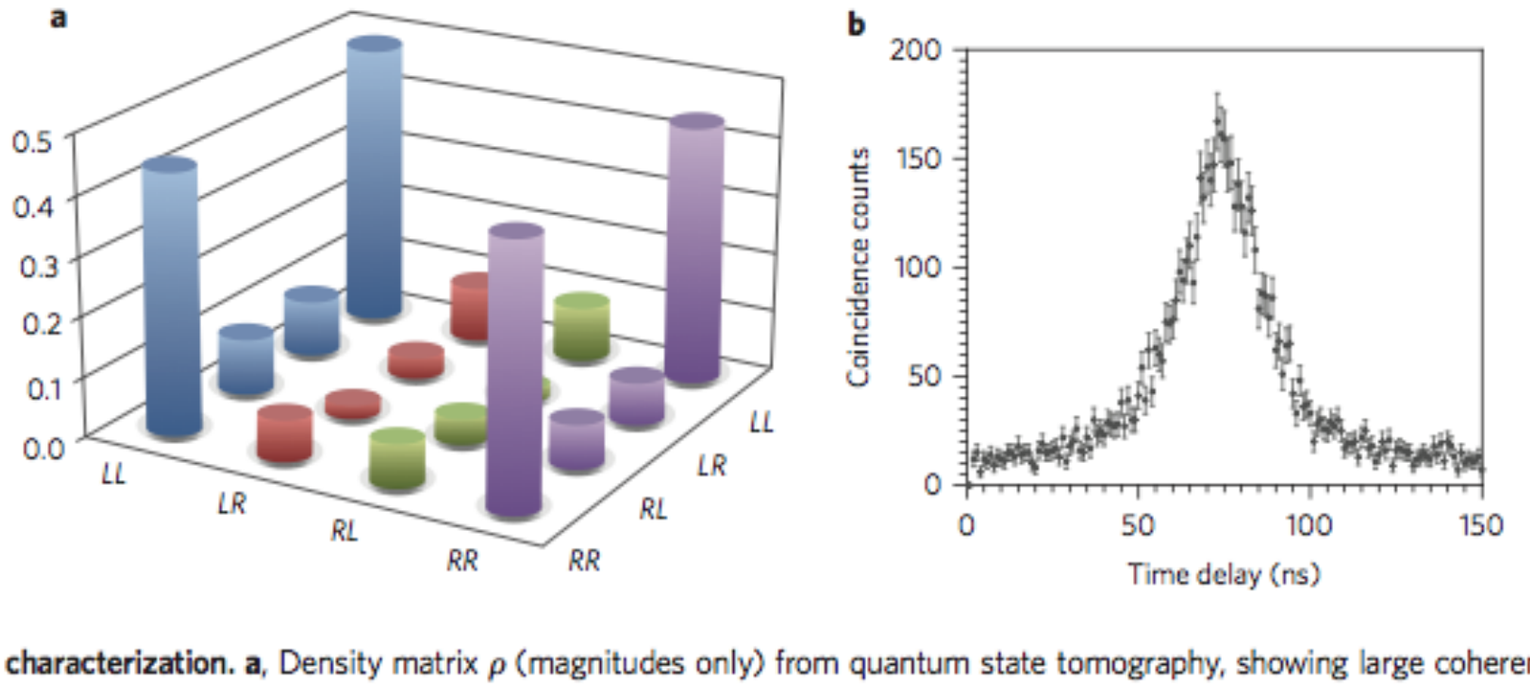
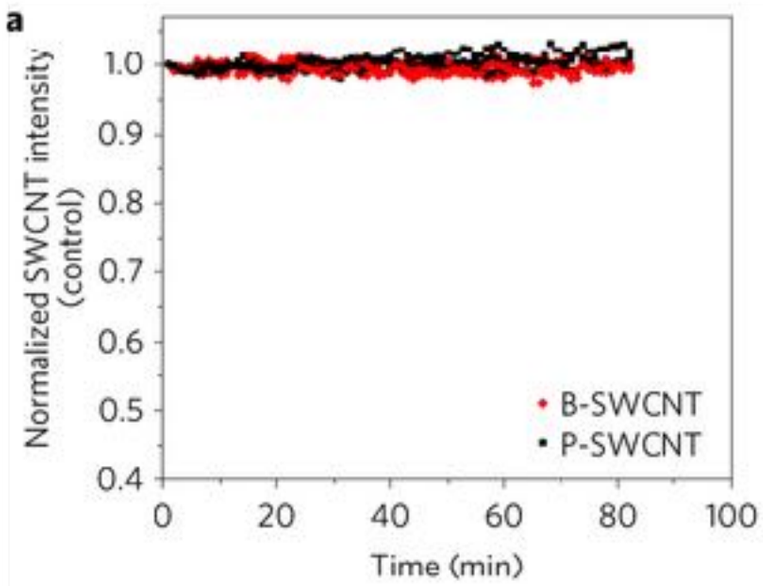
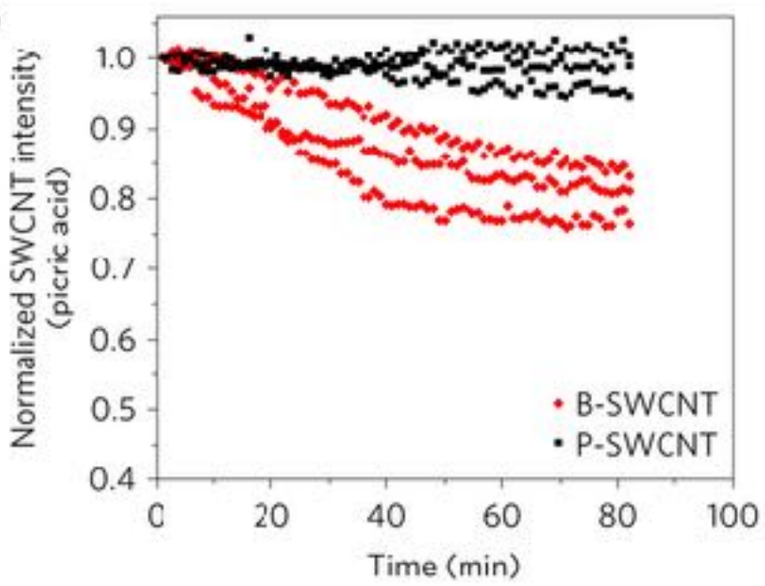
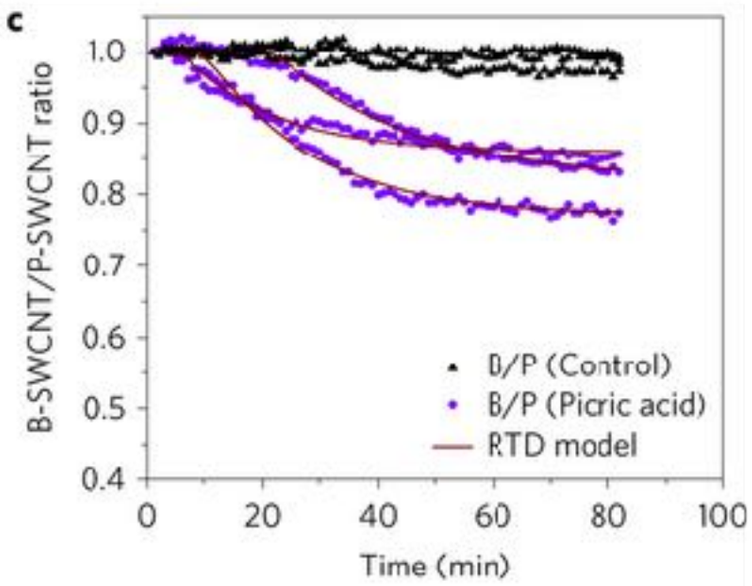
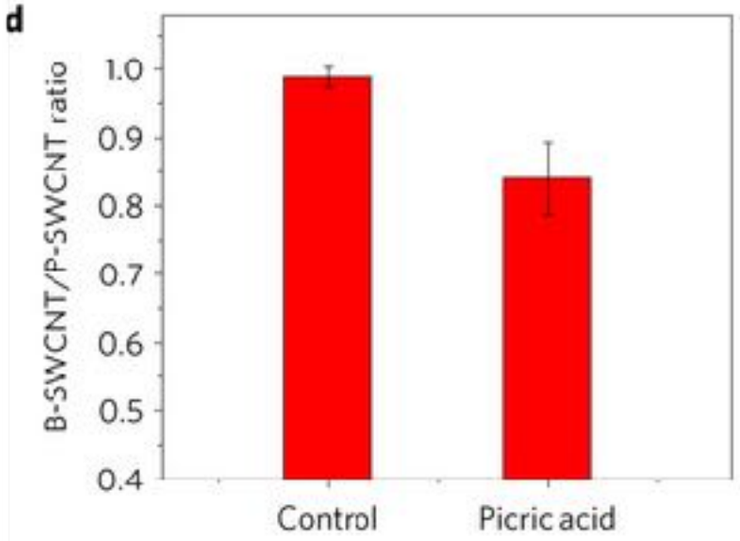


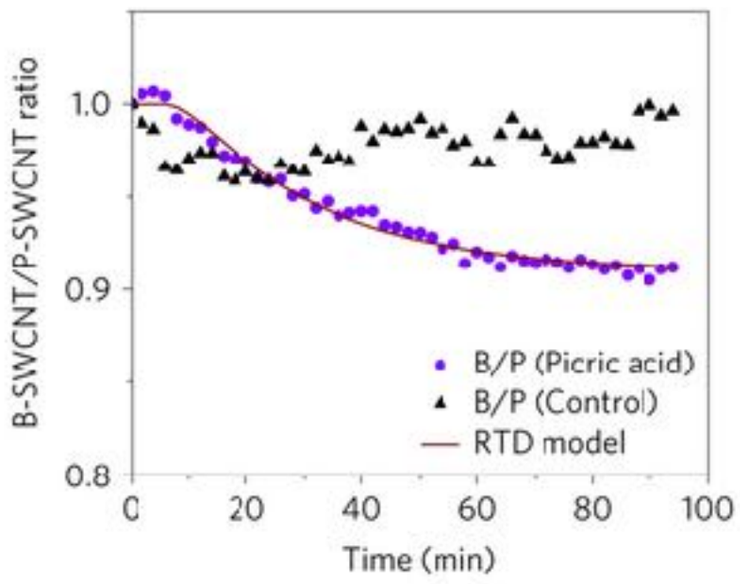
Figure 3 | NOON state characterization. a, Density matrix ρ (magnitudes only) from quantum state tomography, showing large coherence between $|LL\rangle$ and $|RR\rangle$ components. **b**, Measured correlation of the filtered CESPDC pairs (no background subtracted). The absence of modulation at the 2 ns cavity roundtrip time indicates the presence of a single cavity mode.

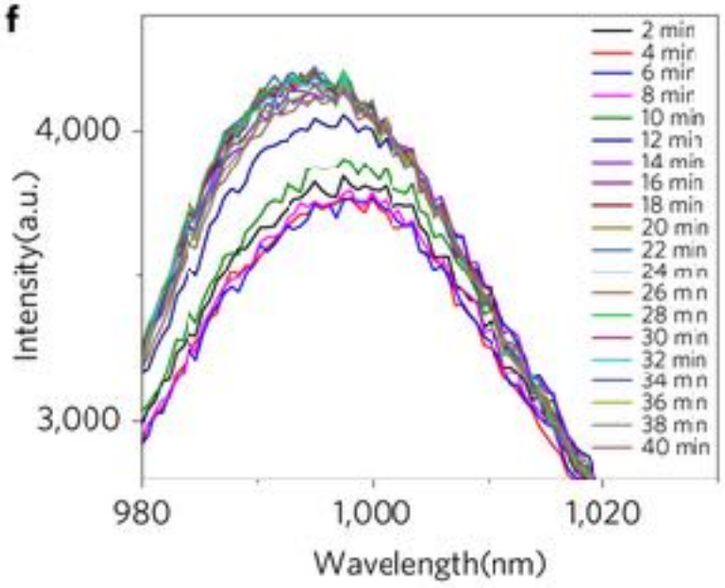

a
Normalized SWCNT intensity (control)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0
20
40
60
80
100
Time (min)
B-SWCNT
P-SWCNT

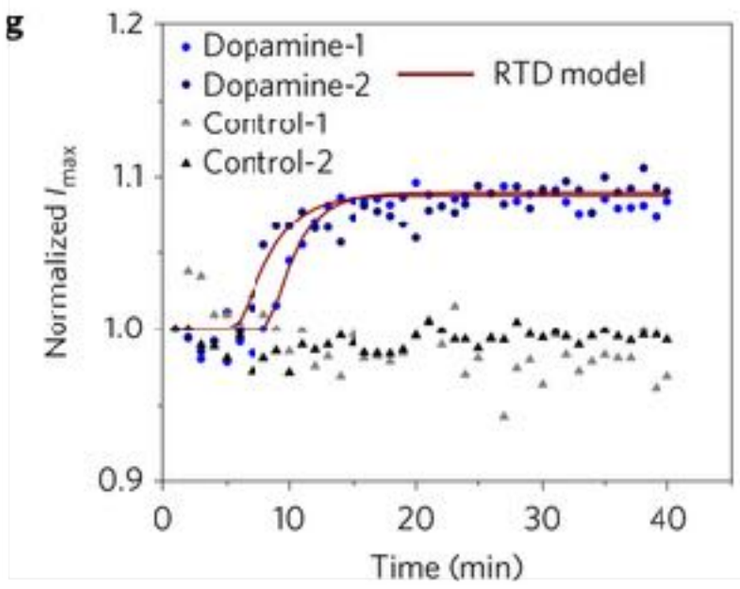

b
Normalized SWCNT intensity (picric acid)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0
20
40
60
80
100
Time (min)
B-SWCNT
P-SWCNT

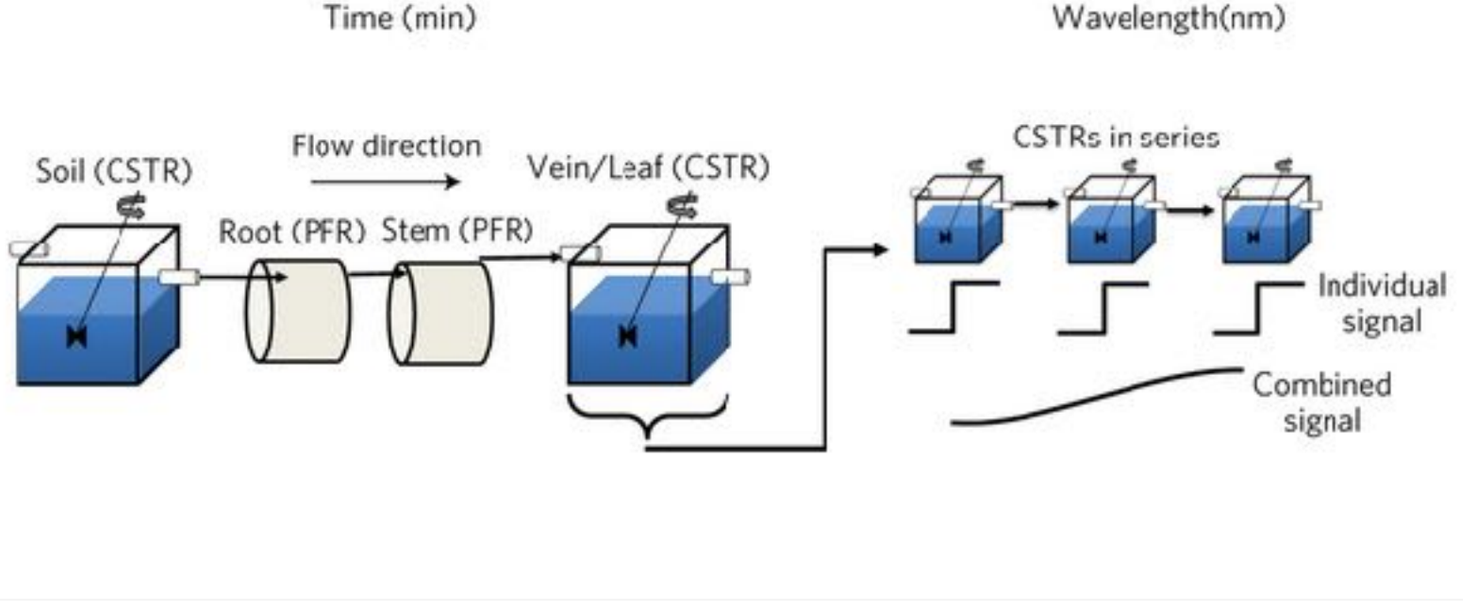

c
B-SWCNT/P-SWCNT ratio
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0
20
40
60
80
100
Time (min)
B/P (Control)
B/P (Picric acid)
RTD model


d
B-SWCNT/P-SWCNT ratio
1.0
0.9
0.8
0.7
0.6
0.5
0.4
Control
Picric acid

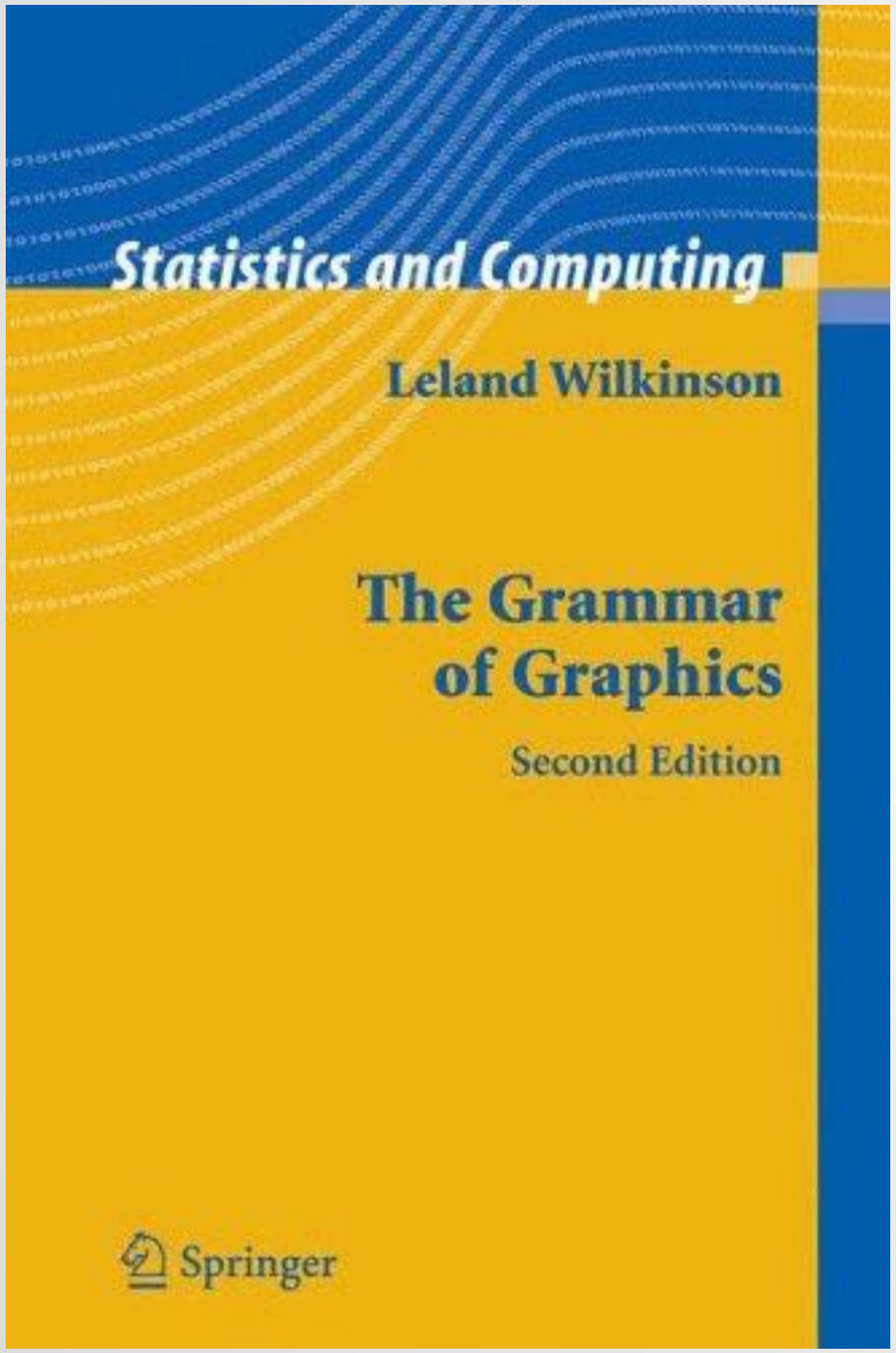

e
B-SWCNT/P-SWCNT ratio
1.0
0.9
0.8
0
20
40
60
80
100
Time (min)
B/P (Picric acid)
B/P (Control)
RTD model


f
Intensity(a.u.)
4,000
3,000
980
1,000
1,020
Wavelength(nm)
2 min
4 min
6 min
8 min
10 min
12 min
14 min
16 min
18 min
20 min
22 min
24 min
26 min
28 min
30 min
32 min
34 min
36 min
38 min
40 min


g
Normalized I_{max}
1.2
1.1
1.0
0.9
0
10
20
30
40
Time (min)
Dopamine-1
Dopamine-2
Control-1
Control-2
RTD model

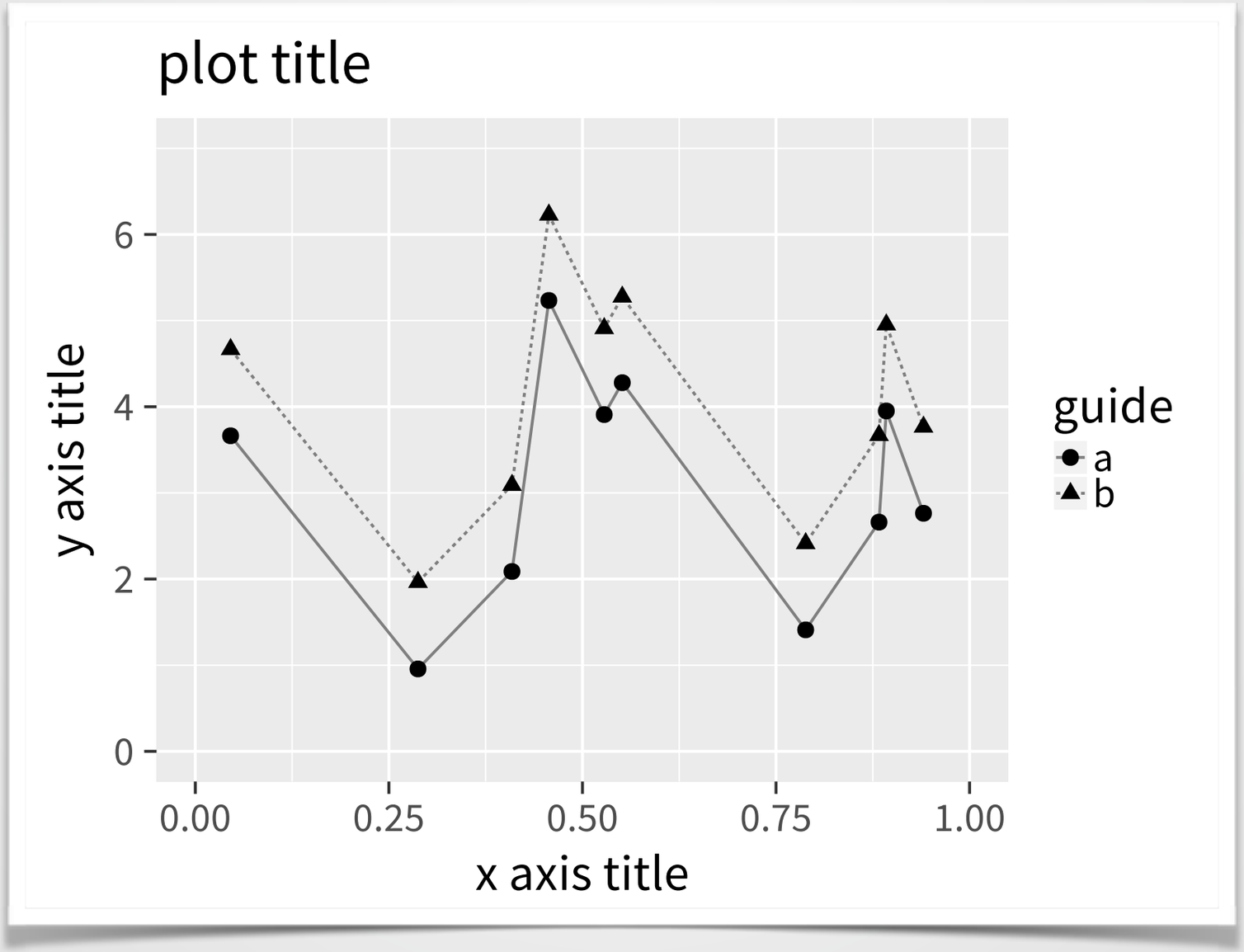

h
Soil (CSTR)
Flow direction
Vein/Leaf (CSTR)
Root (PFR)
Stem (PFR)
CSTRs in series
Individual signal
Combined signal

2 GRAMMAR OF GRAPHICS



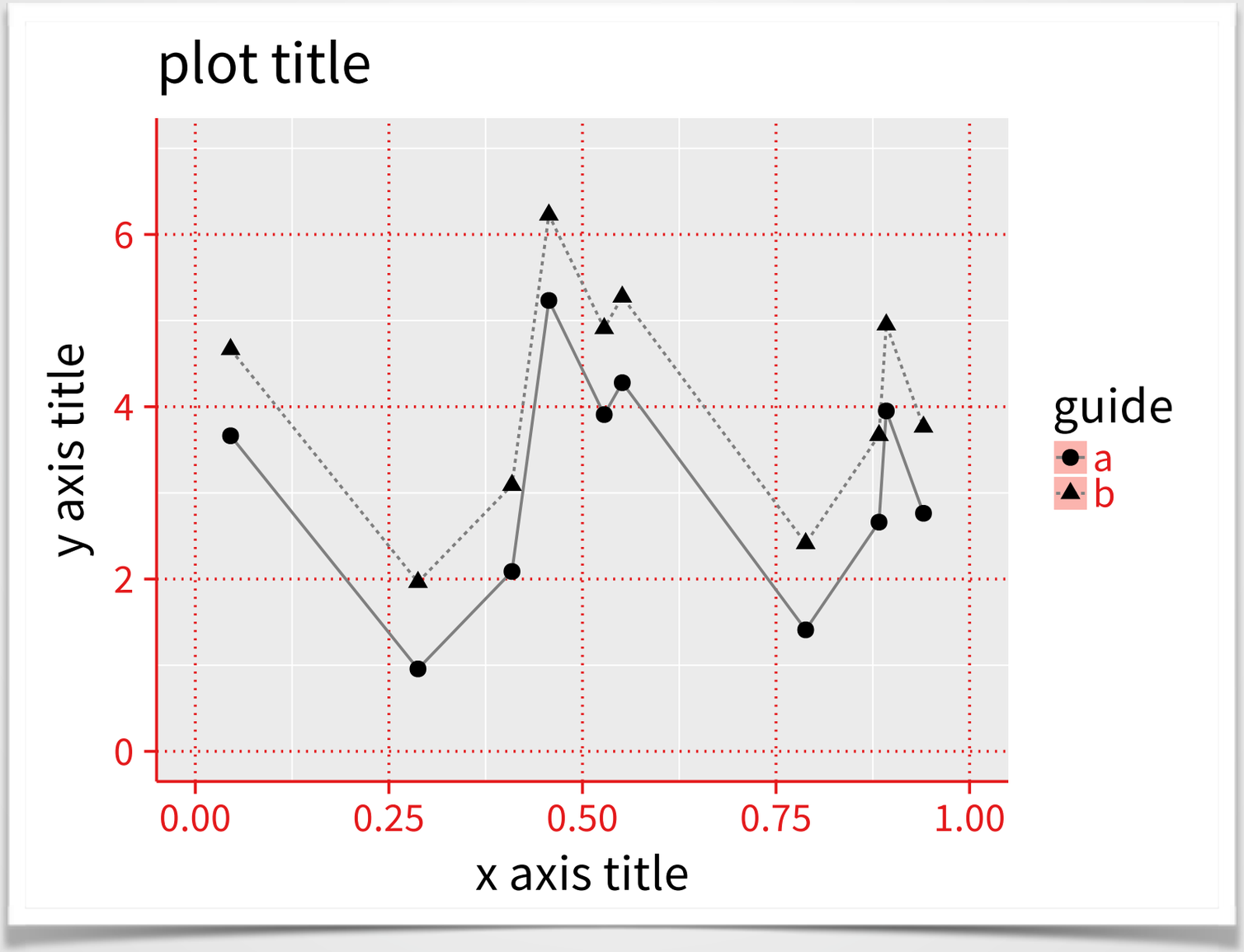
> If charts are maps of abstract worlds the guiding principles of graphics usage could be derived from the psychology of perception.

ANATOMY OF A PLOT

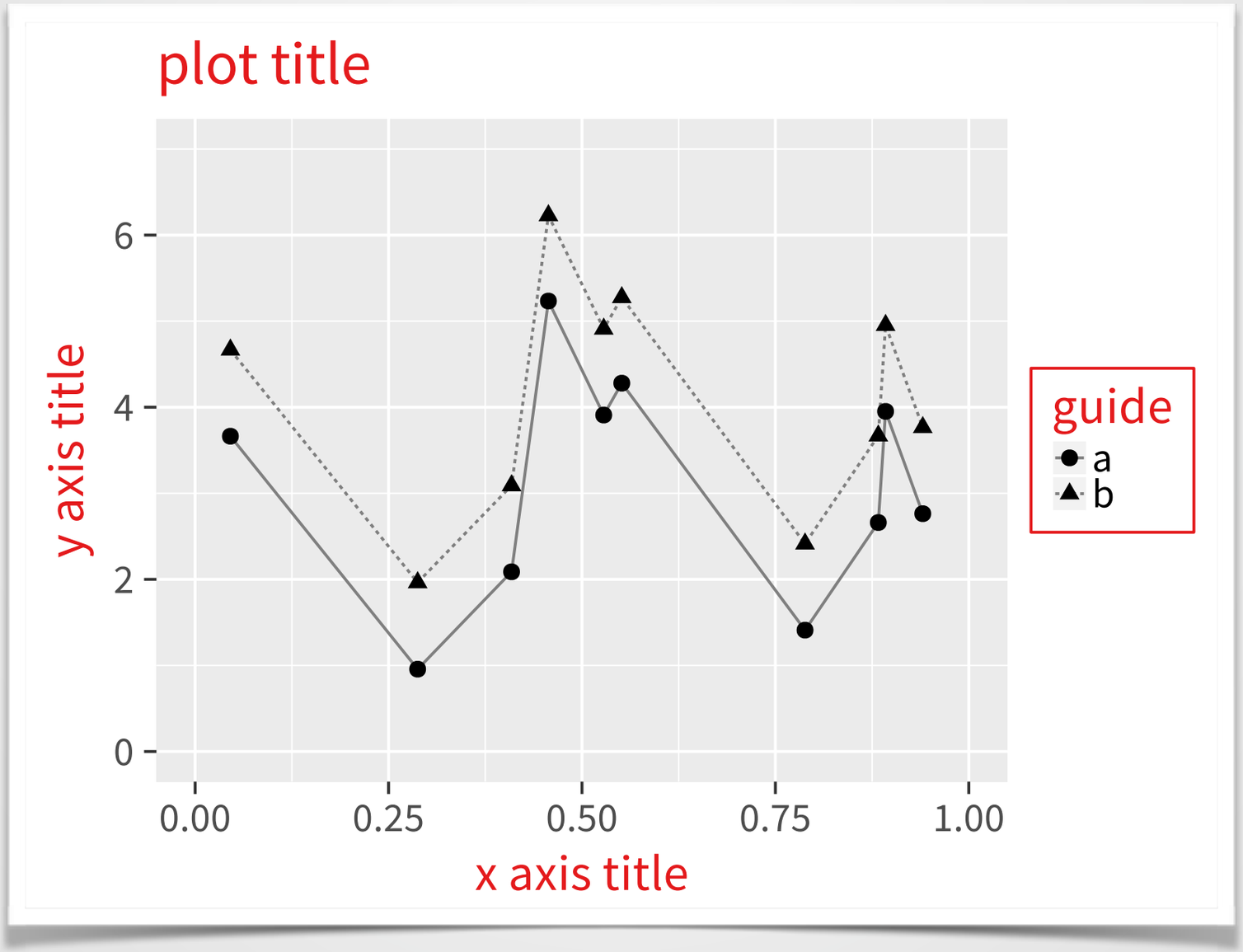


ANATOMY OF A PLOT • *THE DATA*

ANATOMY OF A PLOT • *GUIDES*

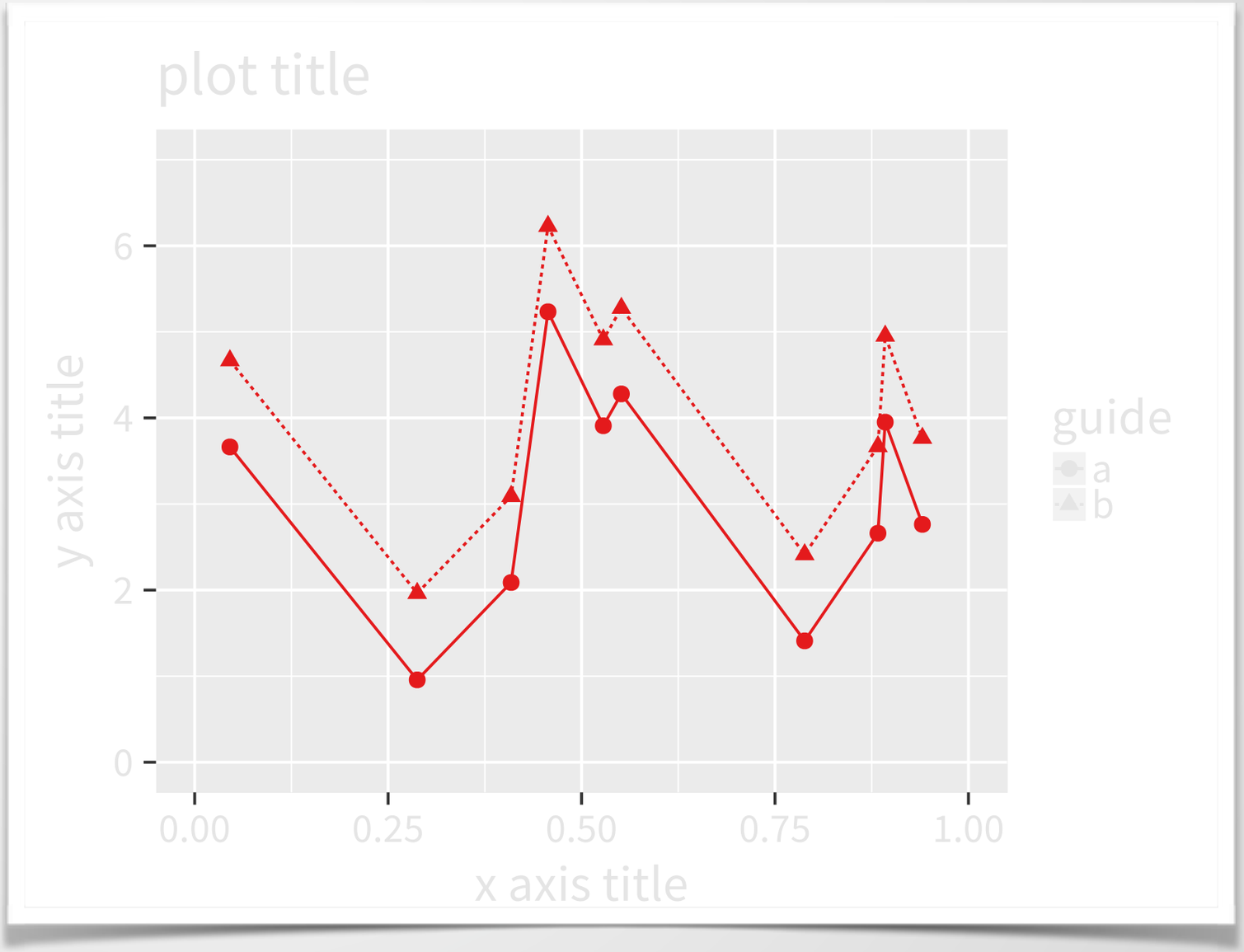


ANATOMY OF A PLOT • *ANNOTATIONS*



GRAMMAR OF GRAPHICS – MAPPING DATA

- position
- length
- angle
- area
- colour
- shape
- line type, size, time, …



EXPRESSIVITY, LEGIBILITY, REPRODUCIBILITY

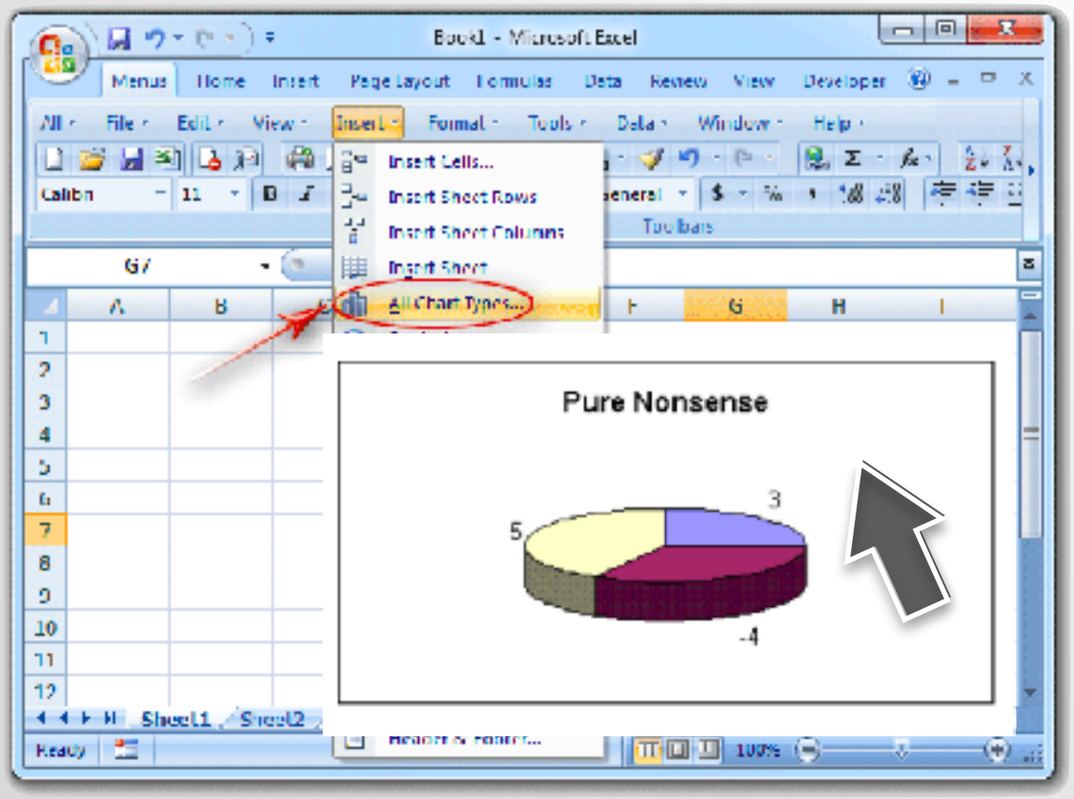
Point & Click

Yeah but, no but, yeah but, no but ! ! !

yeah but . . . I swear * * * * * * * ! ! ! ? ! ! !

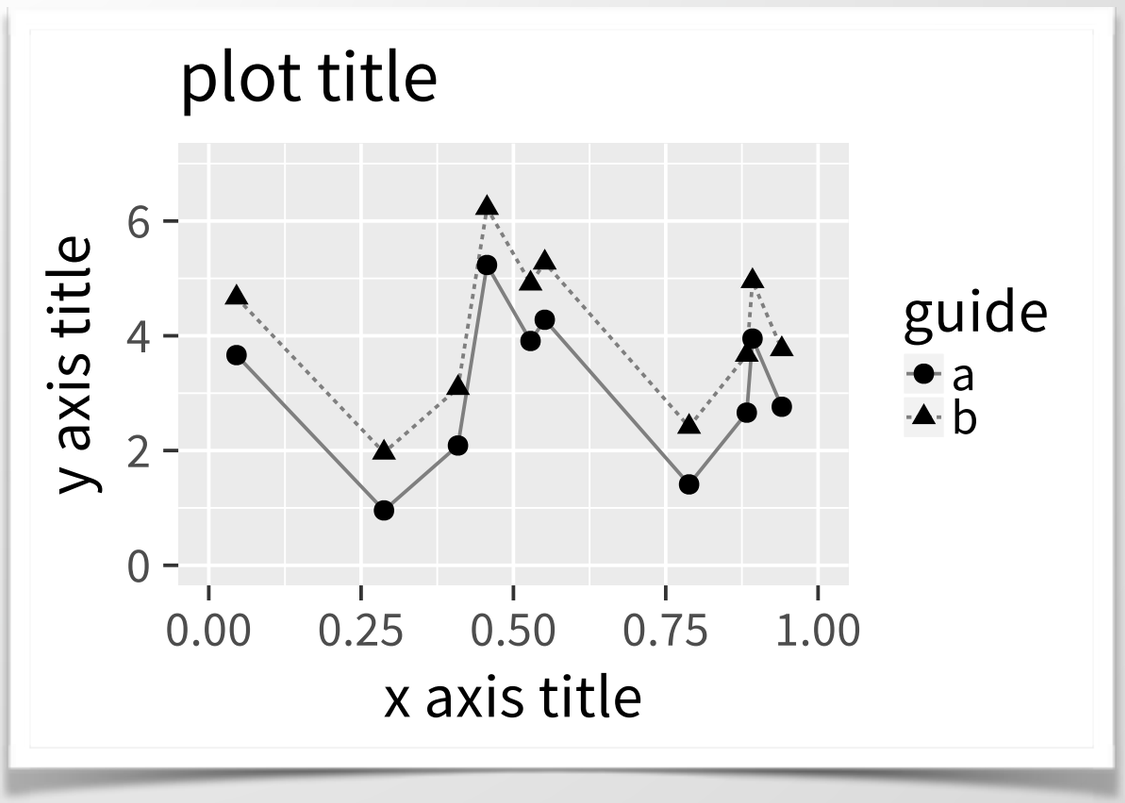
. . . but yeah _(ツ)_/ **COMPUTER SAYS NO**

Ctrl-Z



Grammar of Graphics

```
plot(data, map(x, y)) +
  layer(point, map(colour = z))    +
  layer(line,  map(linetype = t)) +
  theme(fontsize = 12)
```

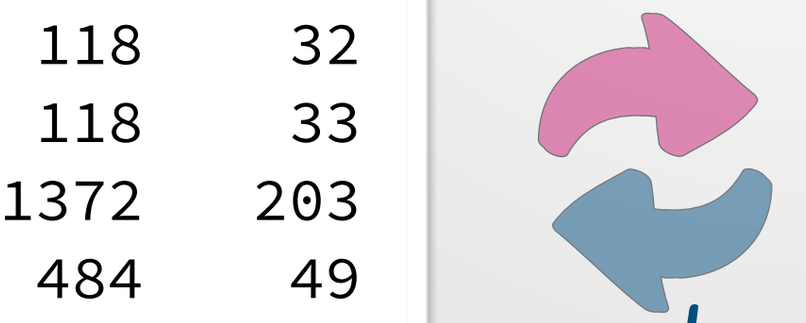


MAPPING DATA TO GLYPHS

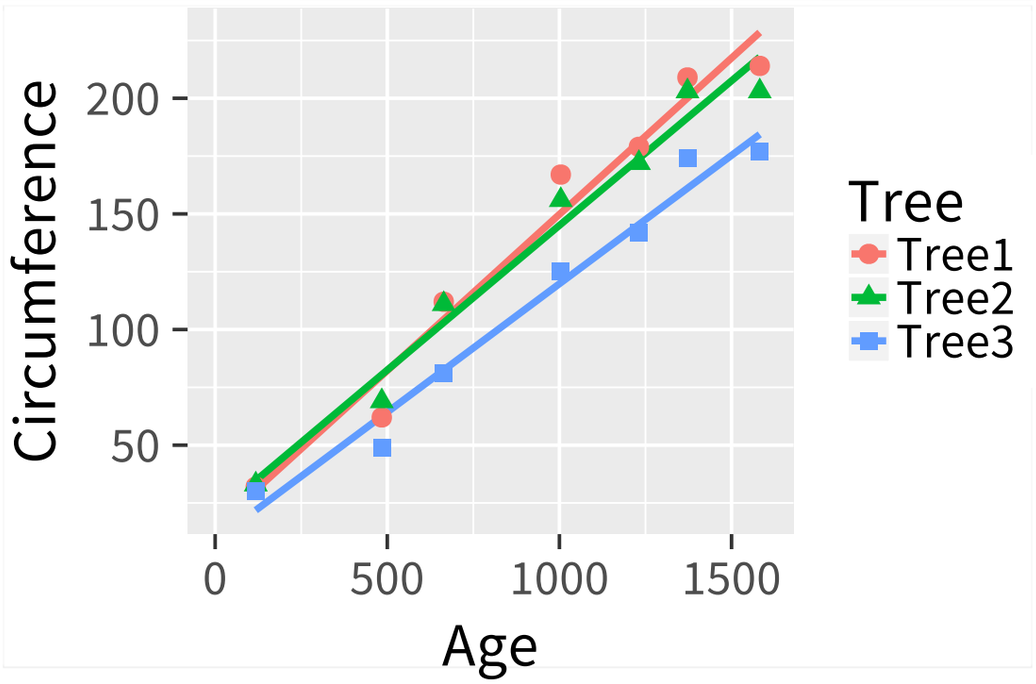
```
plot(data = d,
     mapping = map(x = age,
                   y = circumference)) +
  layer(type = point,
        mapping = map(shape  = Tree,
                      colour = Tree))  +
  layer(type = line,
        mapping = map(colour = Tree))
```

	Tree	age	circ.
1	Tree1	1582	214
2	Tree1	118	32
3	Tree2	118	33
4	Tree2	1372	203
5	Tree3	484	49
6	Tree3	1372	174
7	Tree3	1004	125

mapping

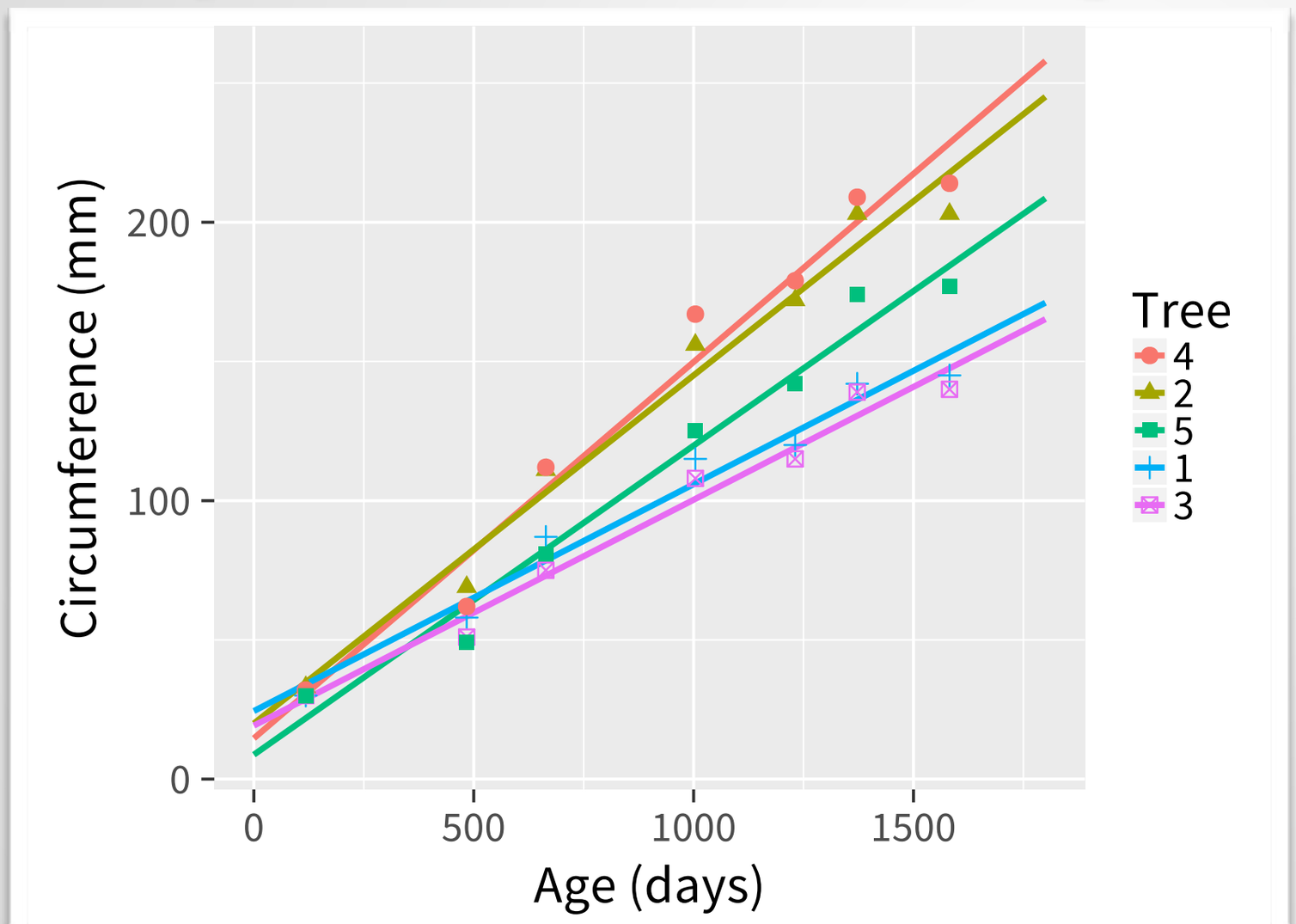


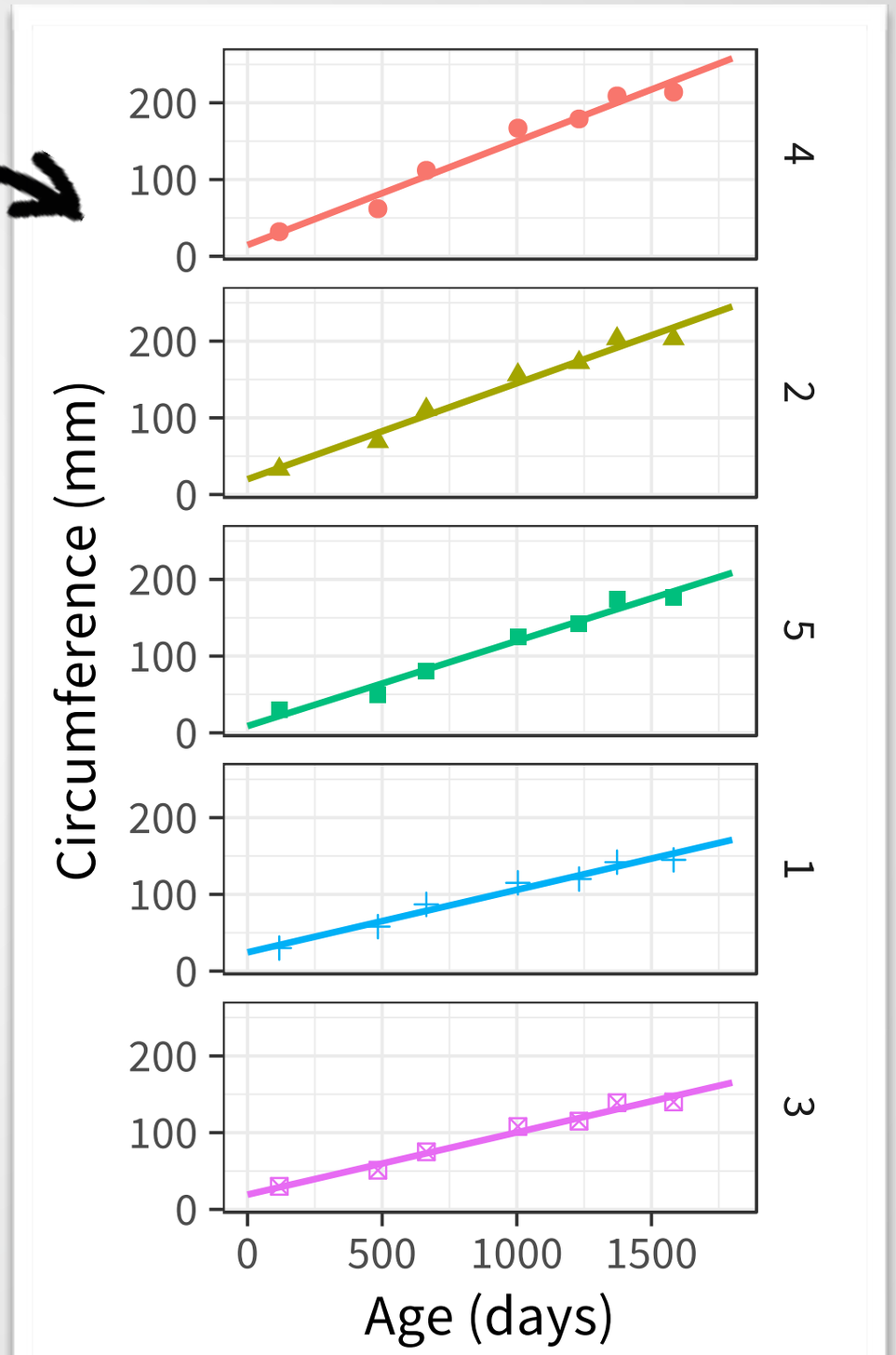
guides



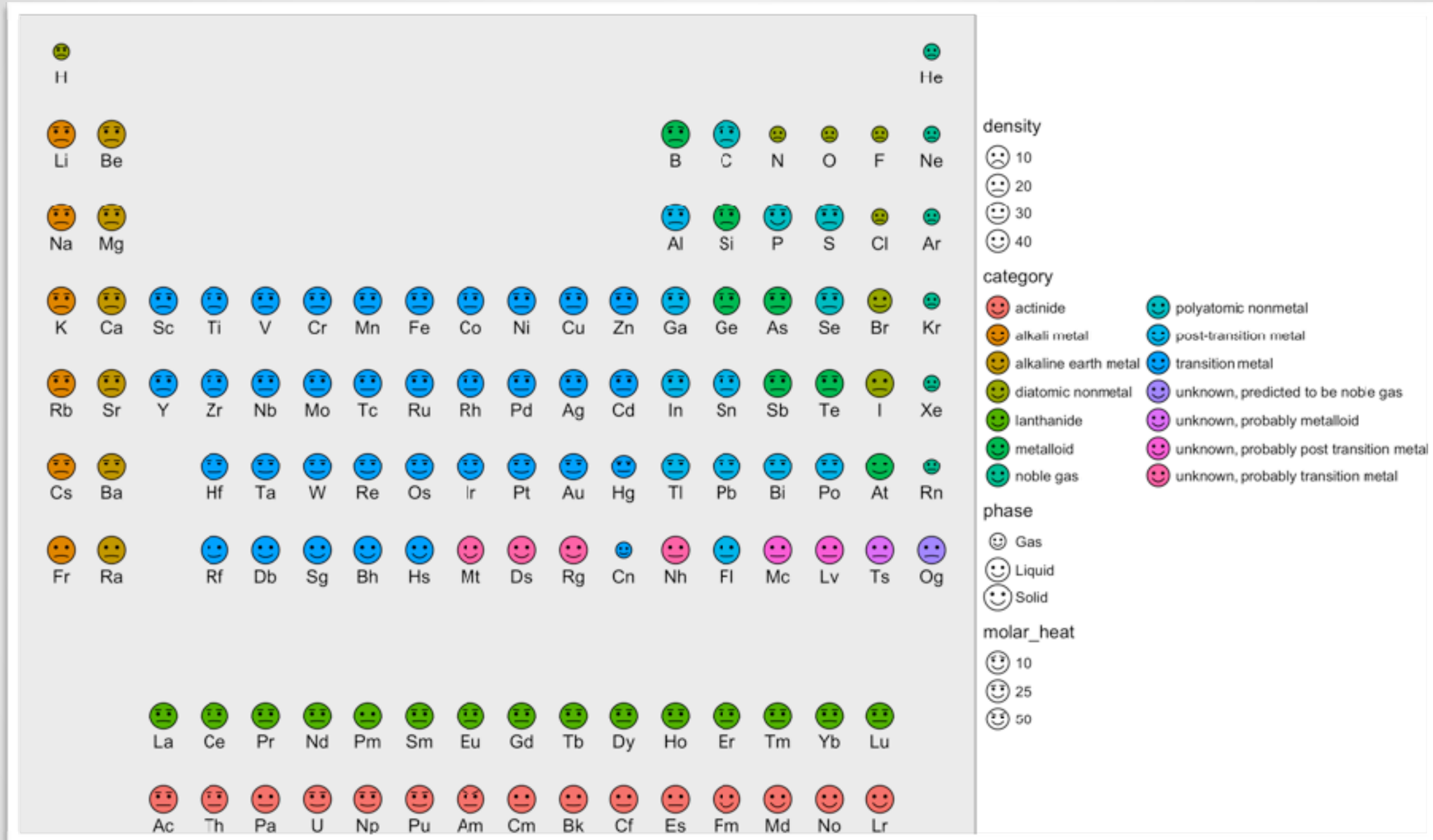
GRAPHICAL EXPLORATIONS

```
last_plot() +
  facet_grid(Tree ~ .) +
  theme_publication
```





MAPPING DATA TO VISUAL ATTRIBUTES



CONSIDER DIFFERENT VISUAL ATTRIBUTES

credit: **@nicgaston**

But different representations of the exact same data can lead to different understanding and, more importantly, to different decisions.

—R. Kosara

BENEFITS OF SCRIPTING GRAPHICS

- **EXPLORING MORE POSSIBILITIES**
  - Save time
  - Try multiple variations
- **CONSISTENCY**
  - Reproducible code & aesthetics
  - Self-documenting analysis

SUMMARY • KEY POINTS

- **SHOW THE DATA '*AS NATURE INTENDED*'**
  - Maximise data-to-ink ratio (*no chart junk*)
  - Sort and organise (*meaningful order*)
  - Consider transformations (*log*, *difference*, …)

- **HELP THE READER**
  - Proximity of things to compare
  - Axes aligned to ease comparisons
  - Deliberate use of colour and labels

TIP #1 | AVOID RESCALING IMAGES

Donec leo. Morbi vulputate convallis est. Integer aliquet. Pellentesque aliquet sodales urna.

Columnwidth: 3.18143in
Textwidth: 6.50127in

Include the figures without rescaling,

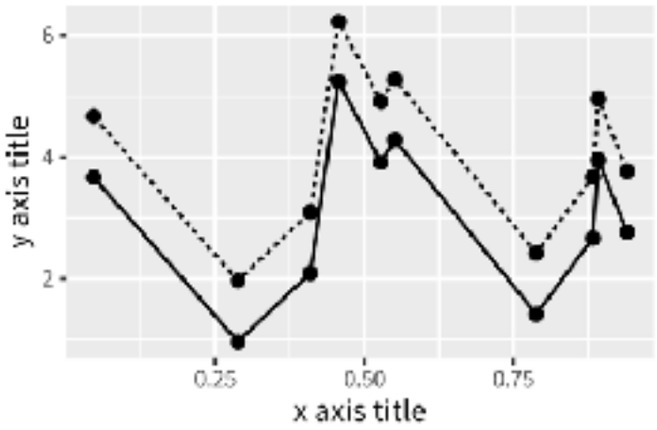


Figure 1: Nunc sed pede. Praesent vitae lectus. Praesent neque justo, vehicula eget, interdum id, facilisis et, nibh. Phasellus at purus et libero lacinia dictum. Fusce aliquet. Nulla eu ante placerat leo semper dictum.

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Etiam lobortis facilisis sem. Nullam

lectus velit ultrices augue, a dignissim nibh lectus placerat pede. Vivamus nunc nunc, molestie ut, ultricies vel, semper in, velit. Ut porttitor. Praesent in sapien. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Duis fringilla tristique neque. Sed interdum libero ut metus. Pellentesque placerat. Nam rutrum augue a leo. Morbi sed elit sit amet ante lobortis sollicitudin. Praesent blandit blandit mauris. Praesent lectus tellus, aliquet aliquam, luctus a, egestas a, turpis. Mauris lacinia lorem sit amet ipsum. Nunc quis urna dictum turpis accumsan semper.

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Etiam lobortis facilisis sem. Nullam nec mi et neque pharetra sollicitudin. Praesent imperdiet mi nec ante. Donec ullamcorper, felis non sodales commodo, lectus velit ultrices augue, a dignissim nibh lectus placerat pede. Vivamus nunc nunc, molestie ut, ultricies vel, semper in, velit. Ut porttitor. Praesent in sapien. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Duis fringilla tristique neque. Sed interdum libero ut metus. Pellentesque placerat. Nam rutrum augue a leo. Morbi sed elit sit amet ante lobortis sollicitudin. Praesent blandit blandit mauris. Praesent lectus tellus, aliquet ali-

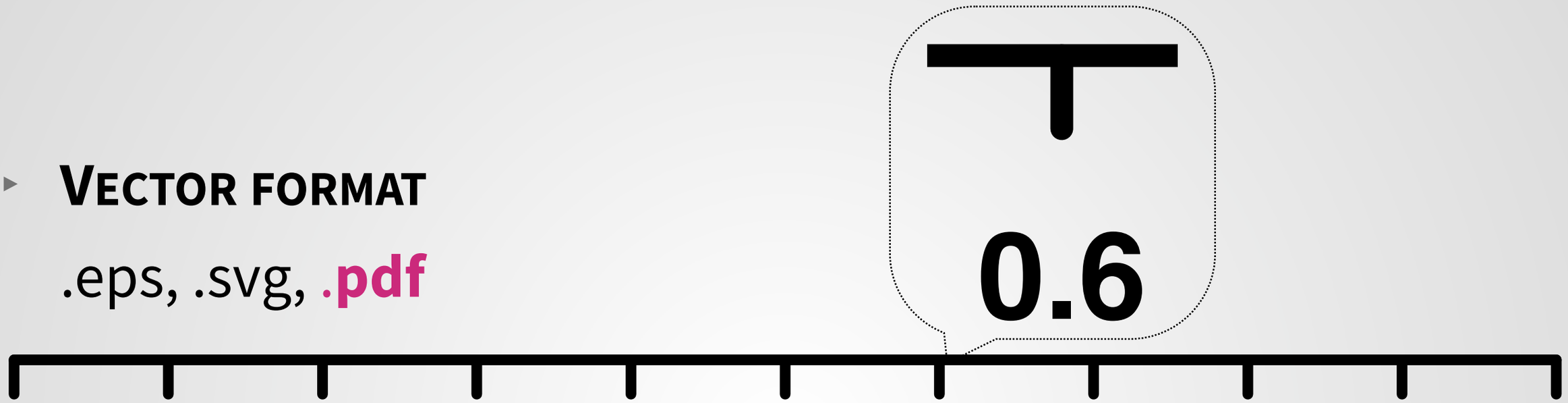
LaTeX tip

```
\usepackage{layouts}
\printinunitsof{in}\prntlen{\columnwidth}
\printinunitsof{in}\prntlen{\textwidth}
```

TIP #2 | FILE FORMATS

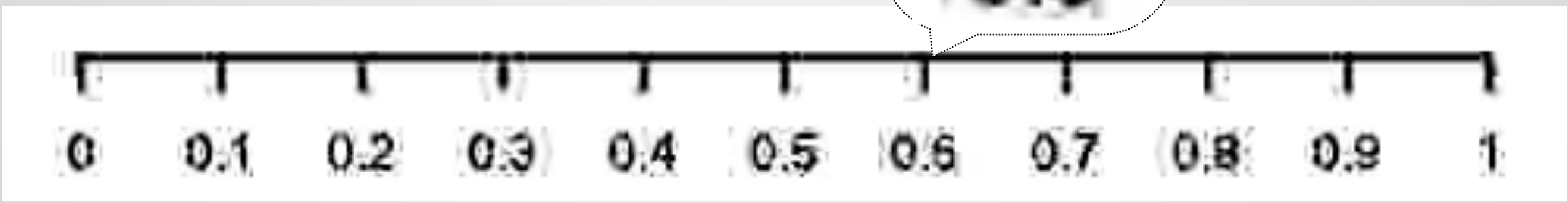
- **VECTOR FORMAT**

  .eps, .svg, **.pdf**

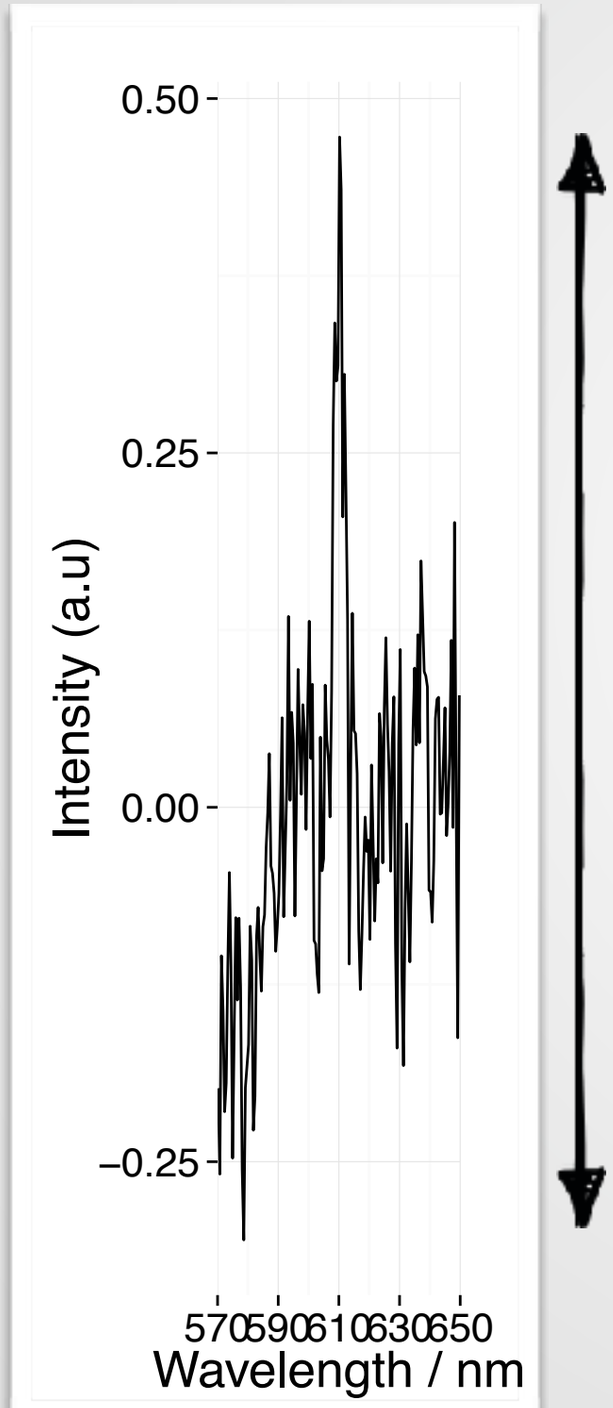


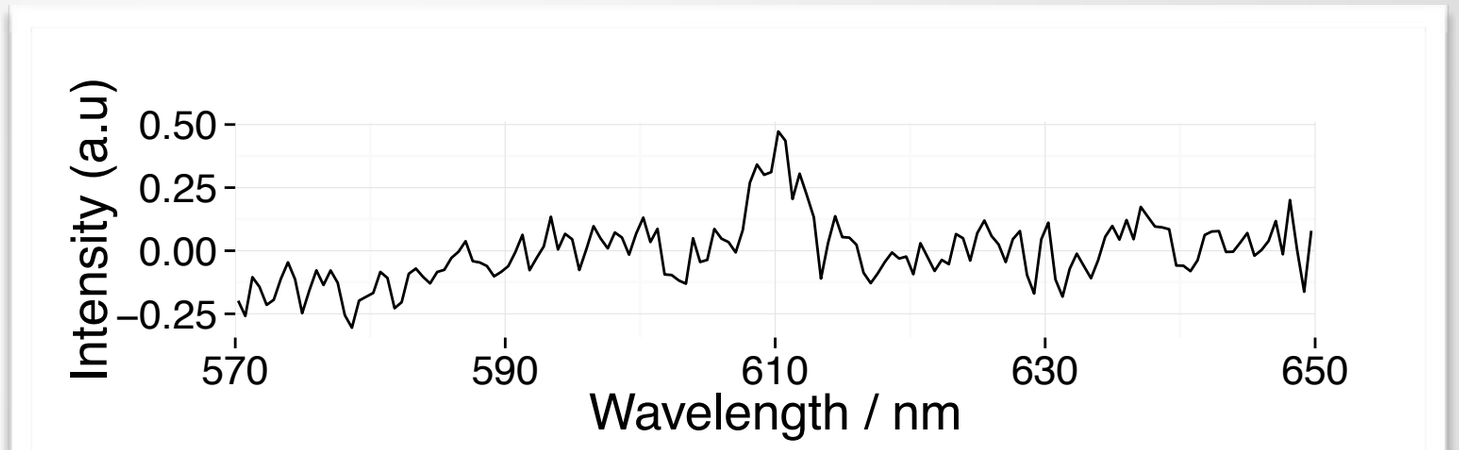
- **RASTER FORMAT**

  .jpg, .tiff, **.png**



TIP #3 | ASPECT RATIO





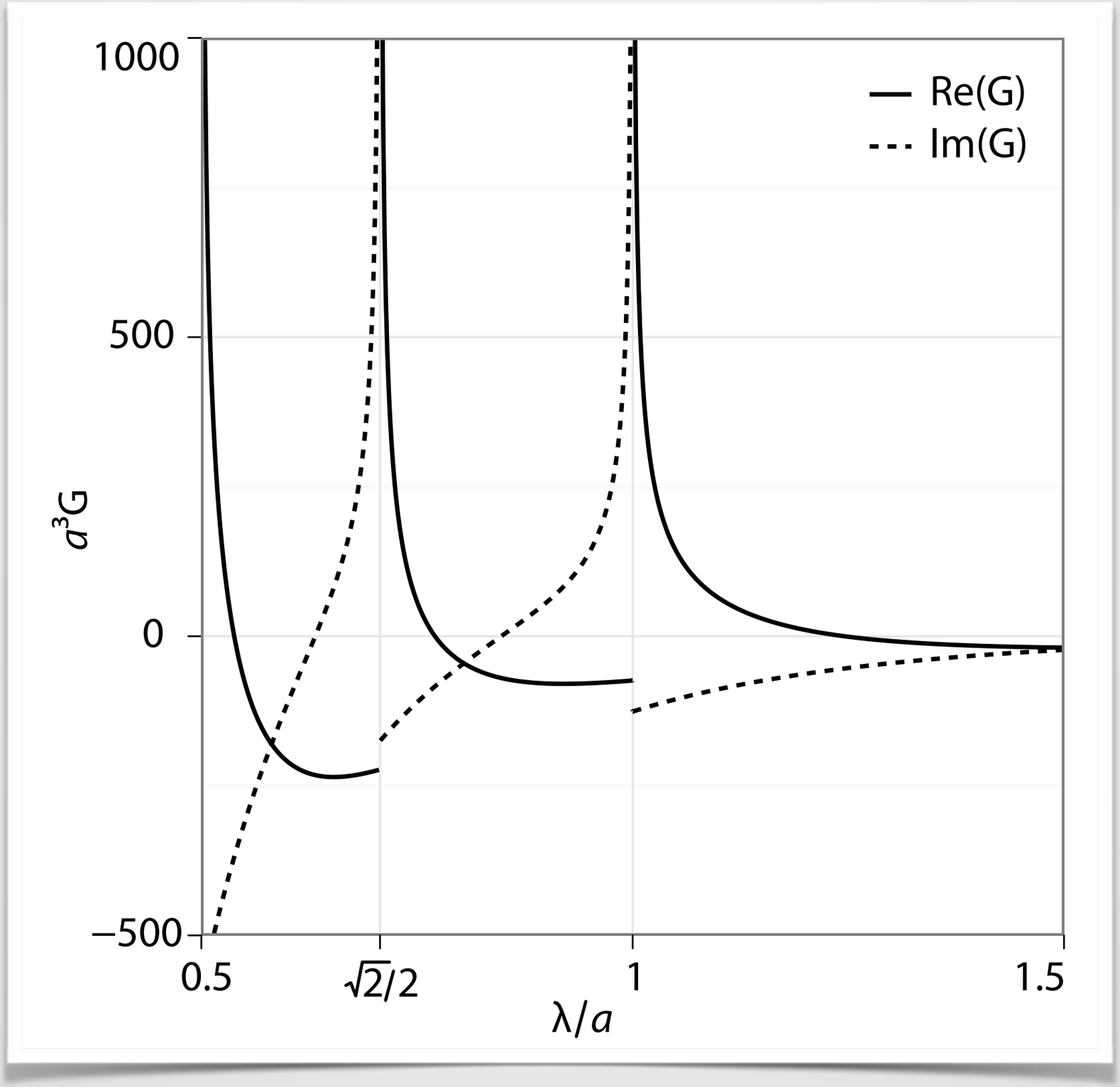
Try

- "banking" at 45°
- standard ratios

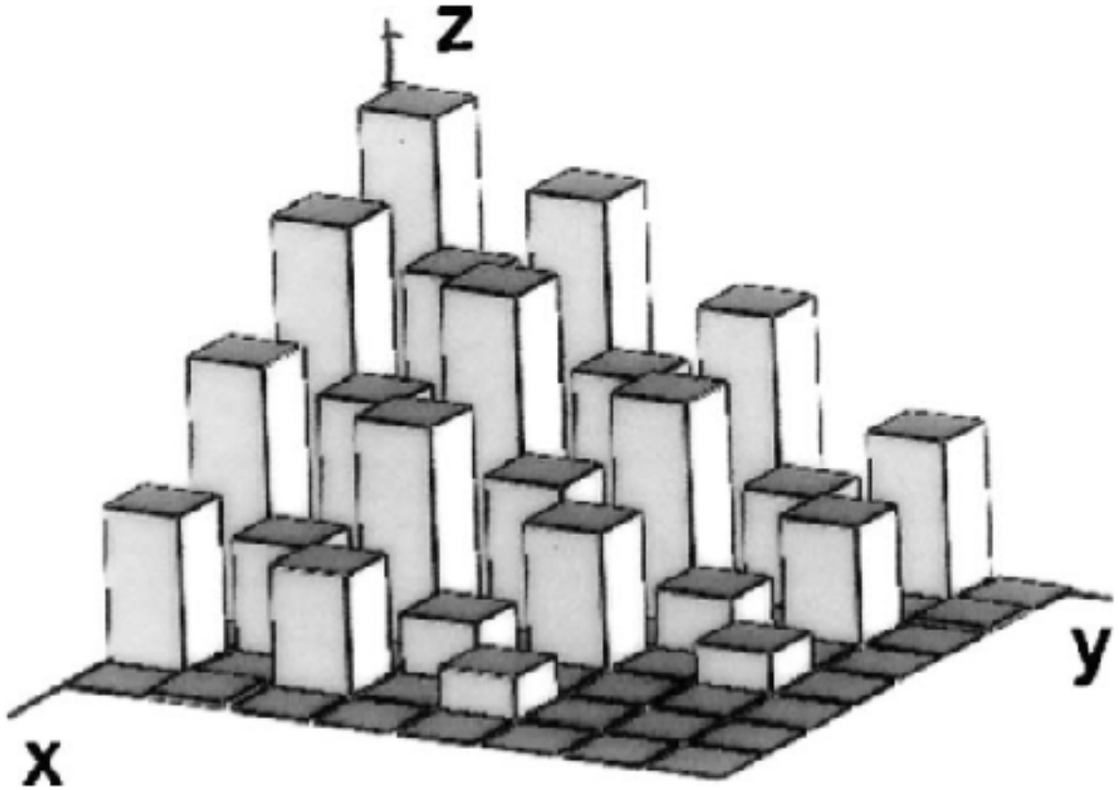
TIP #2 | ASPECT RATIO

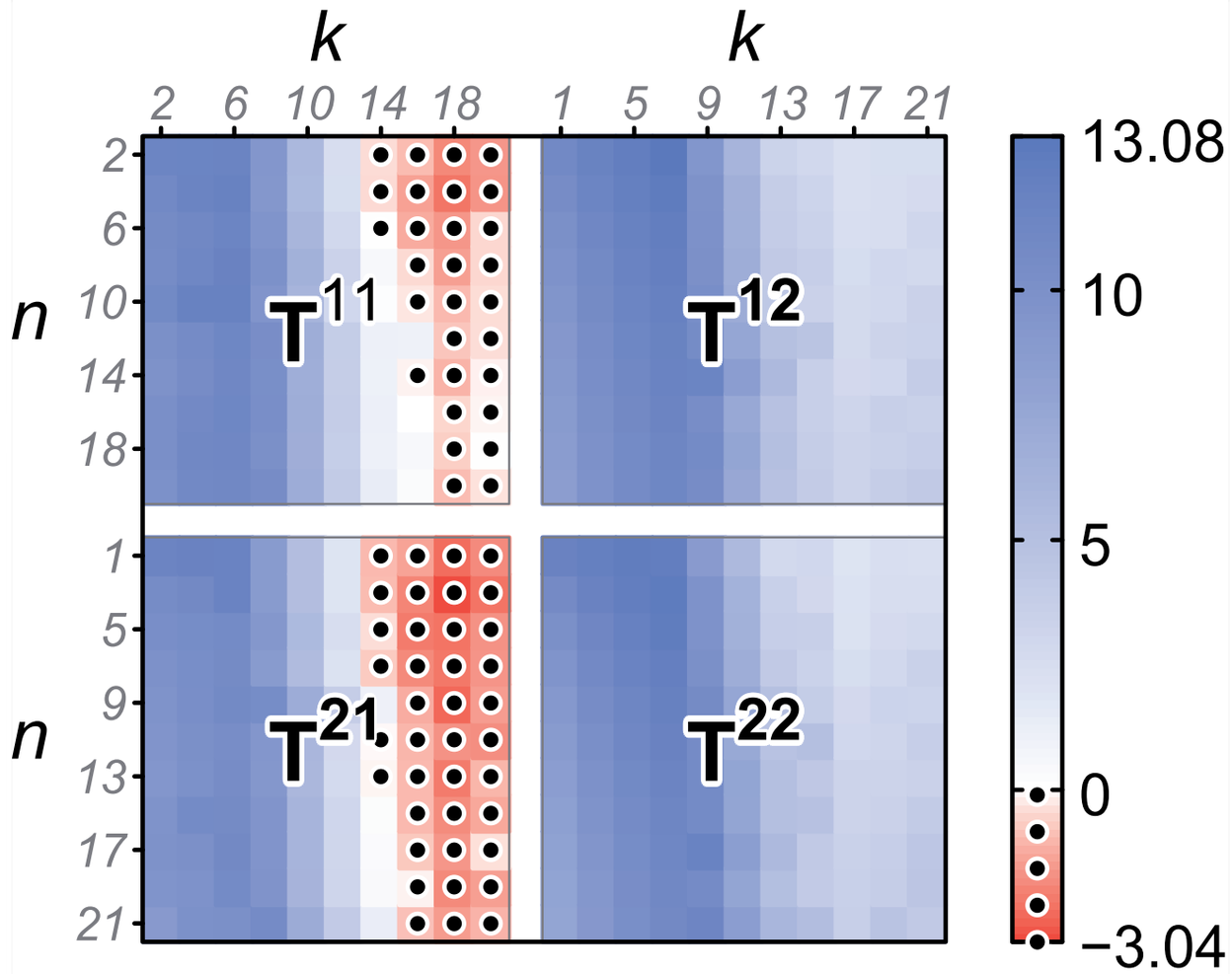
https://xkcd.com/1732/

TIP #4 | DATA-TO-INK RATIO — IS MORE

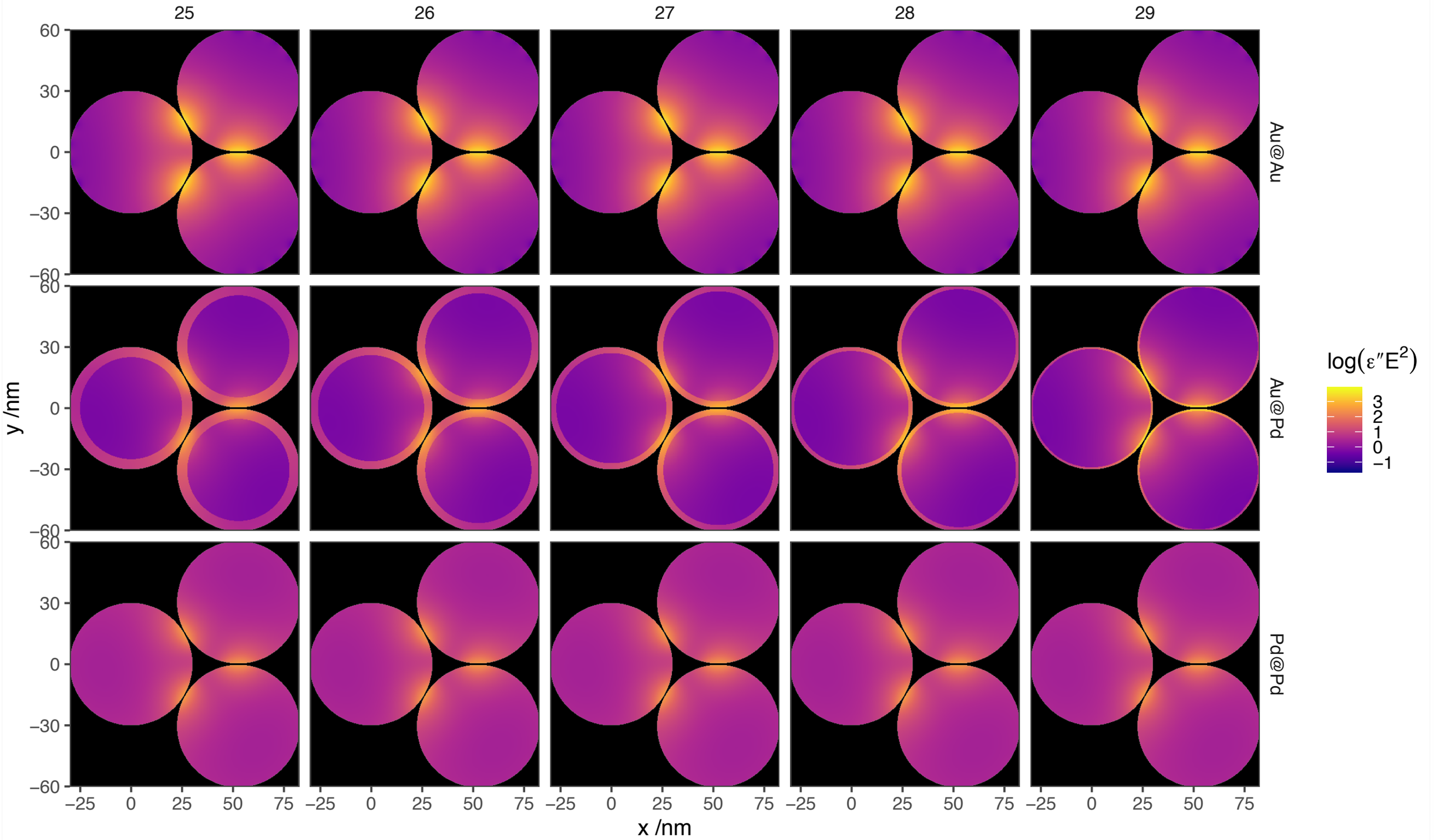


TIP #5 | FAKE 3D IS OFTEN DETRIMENTAL

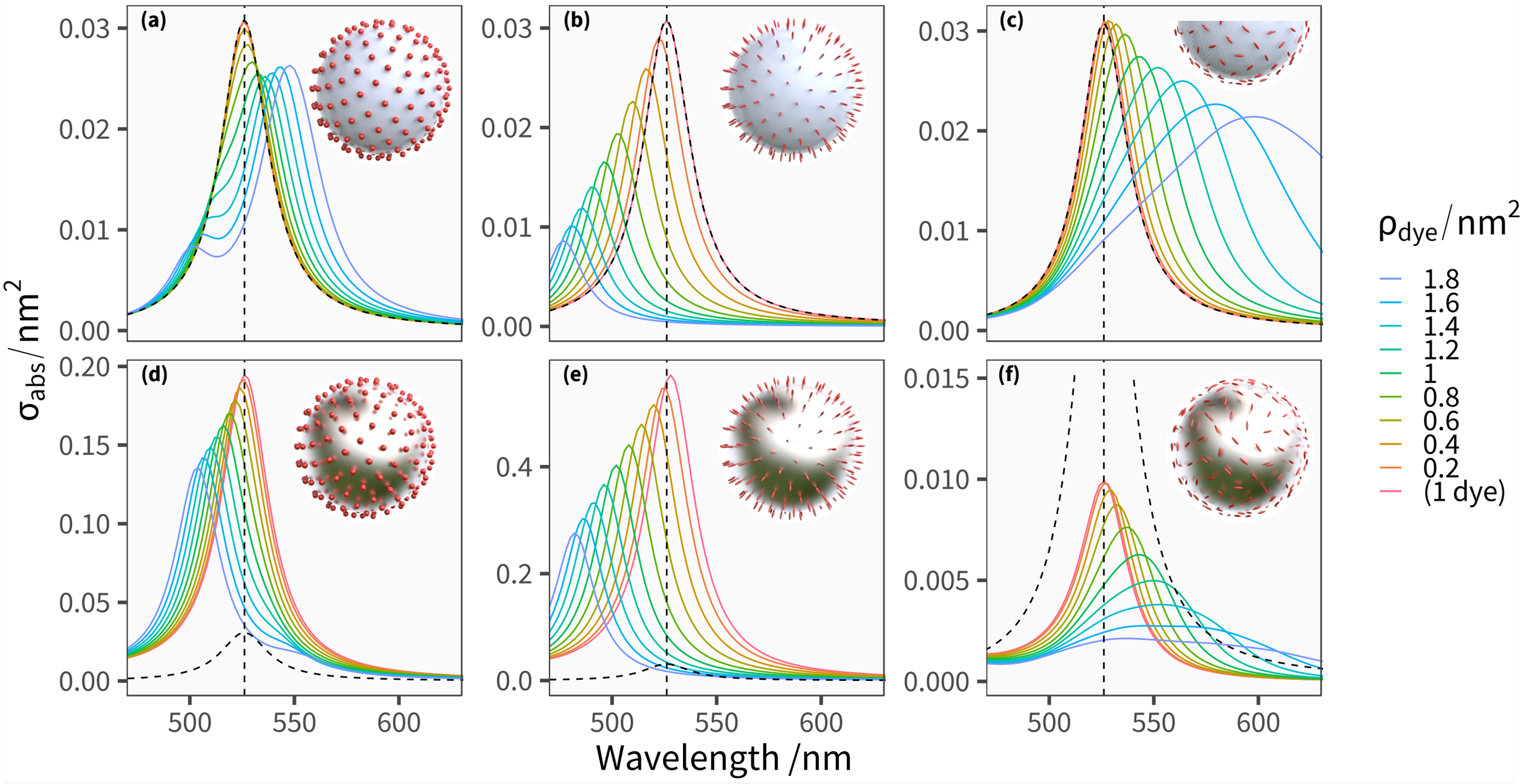




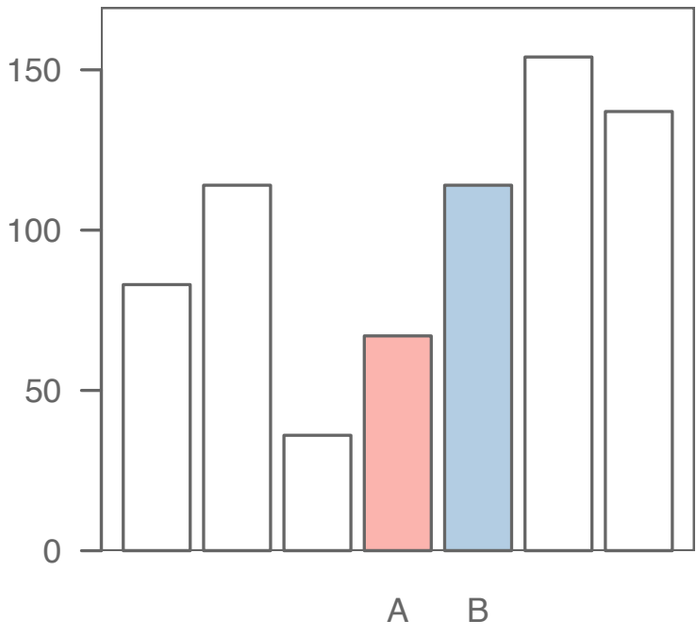
TIP #6 | SMALL MULTIPLES

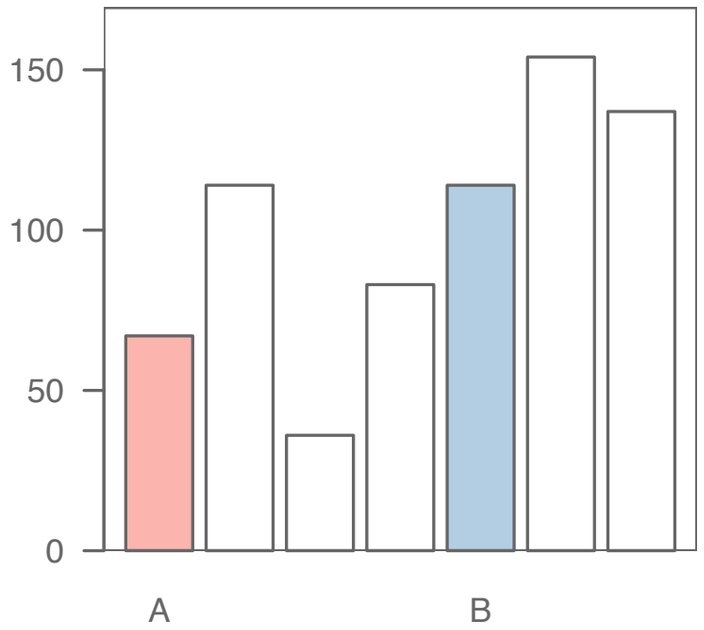


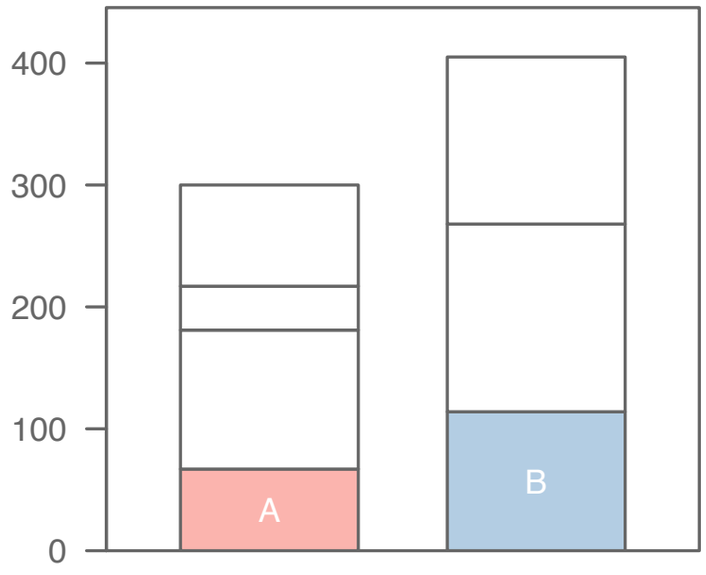
TIP #6 | SMALL MULTIPLES

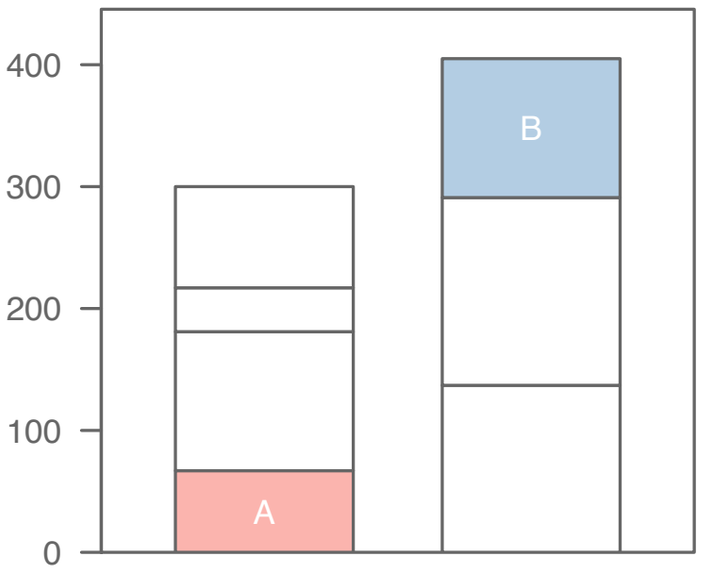


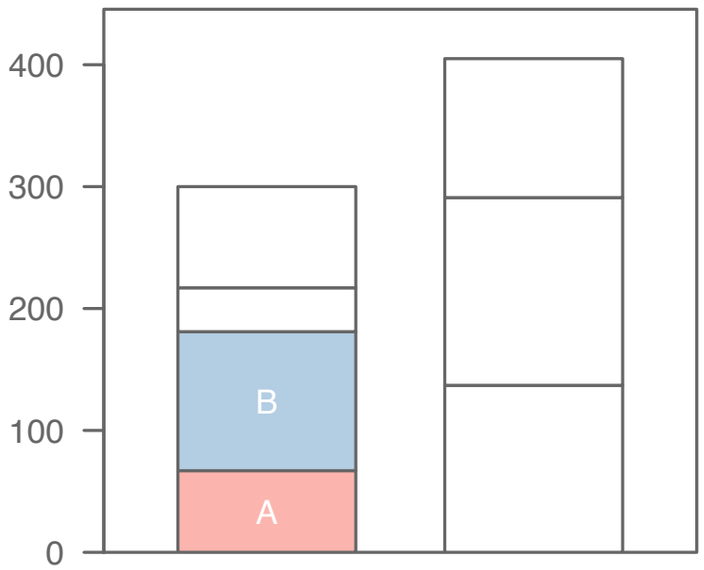
TIP #7 | MAKE IMPORTANT COMPARISONS EASIER

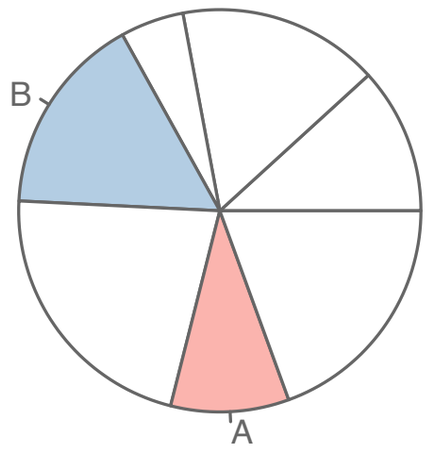




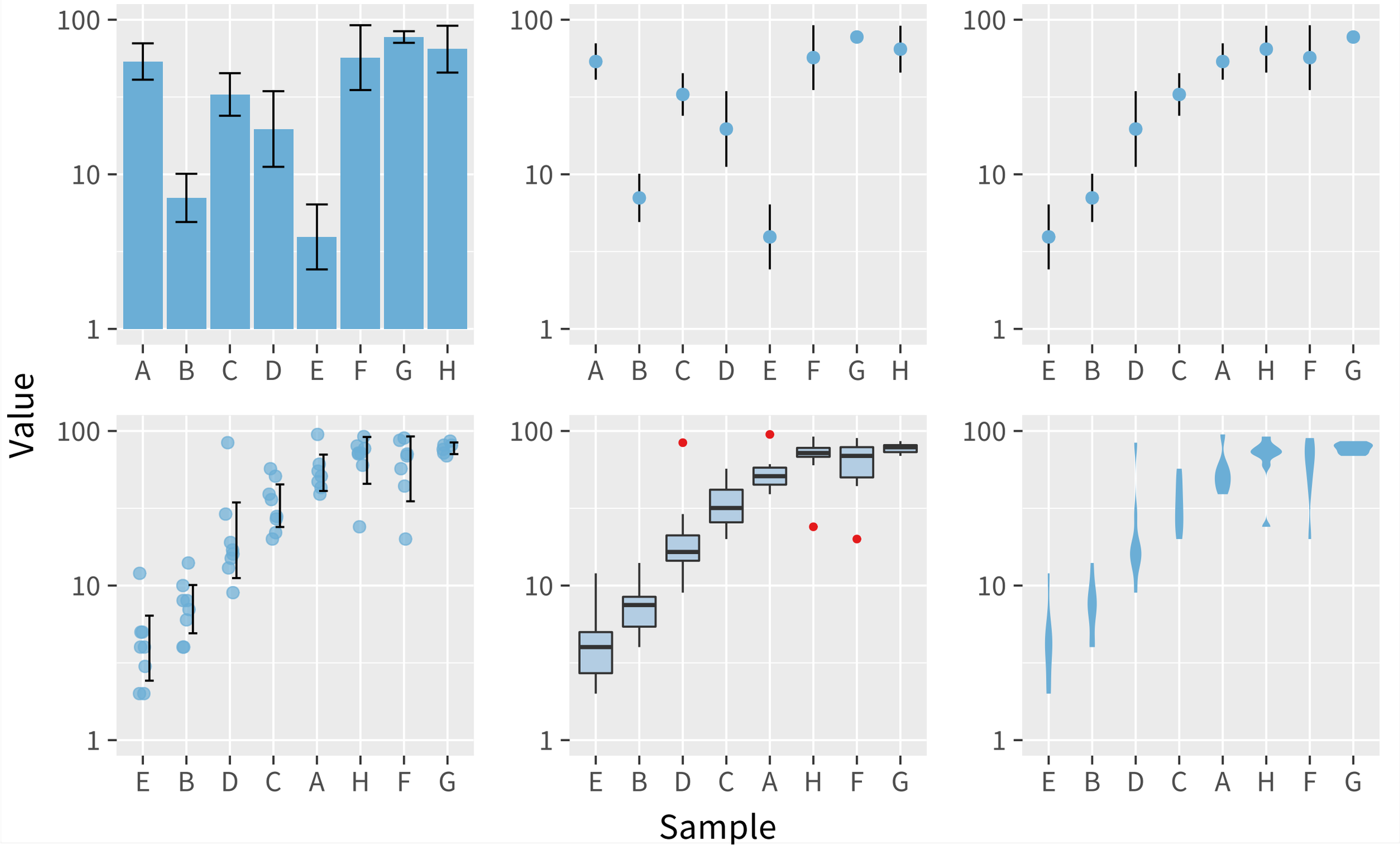




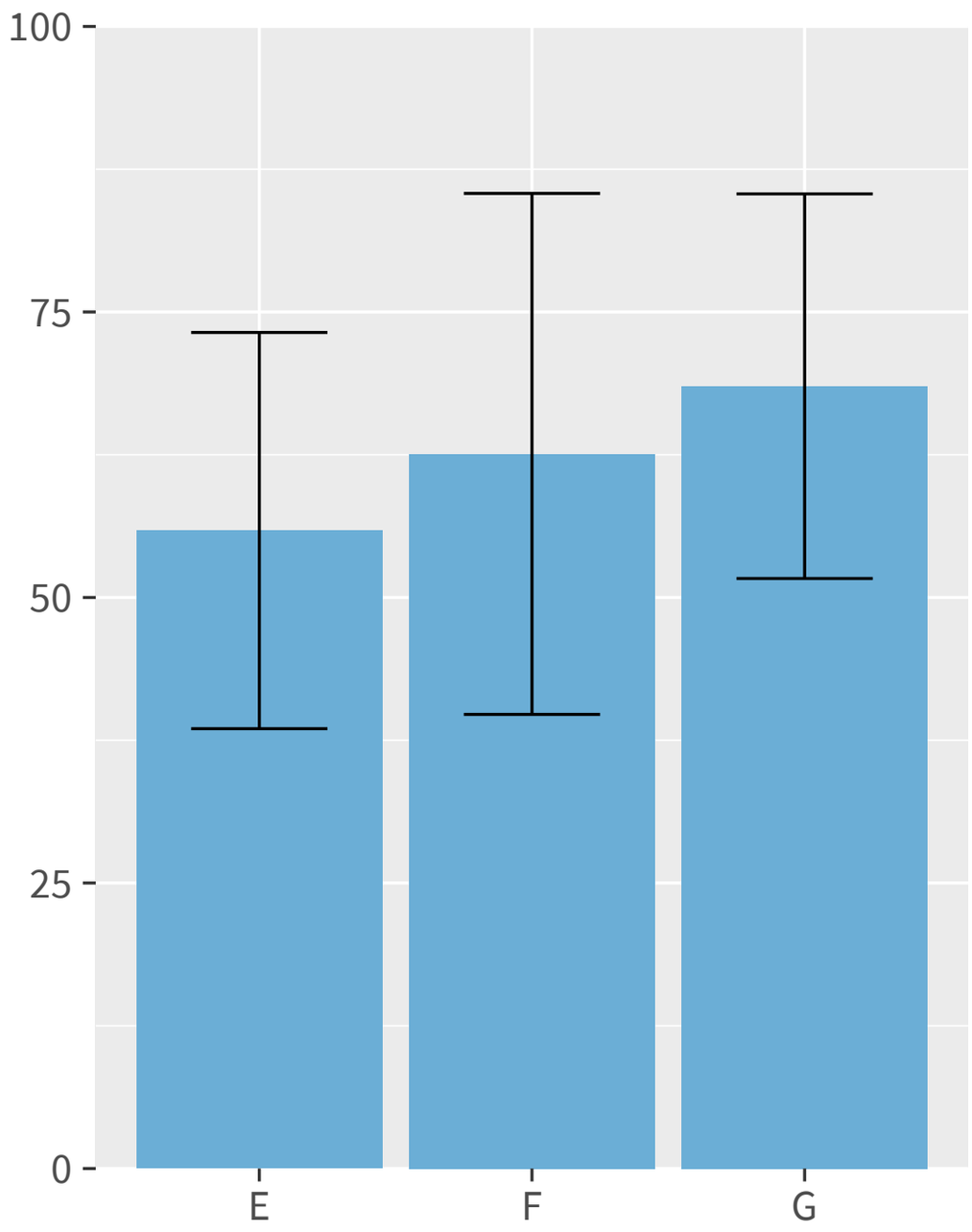


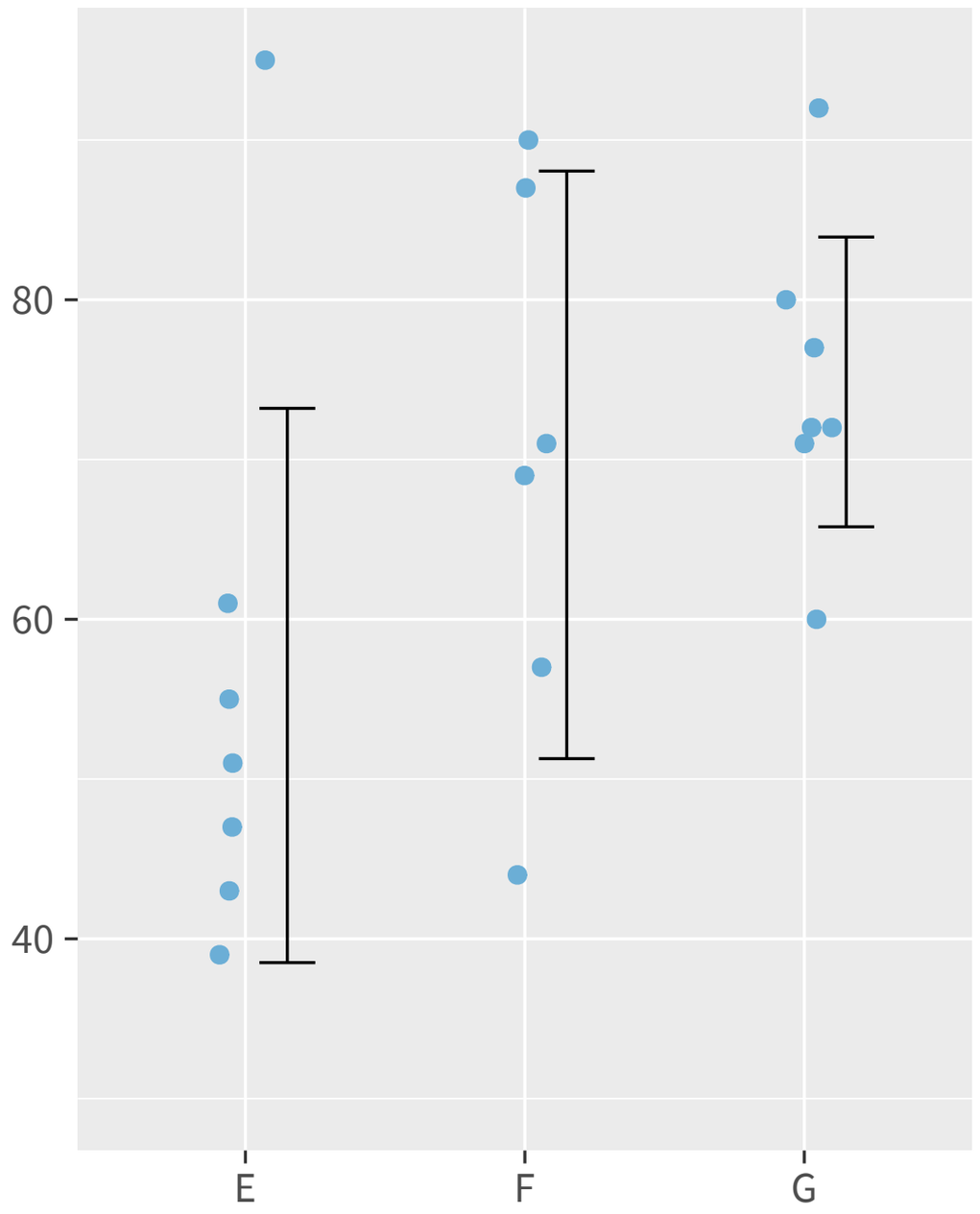


TIP #8 | DYNAMITE PLOT ALTERNATIVES

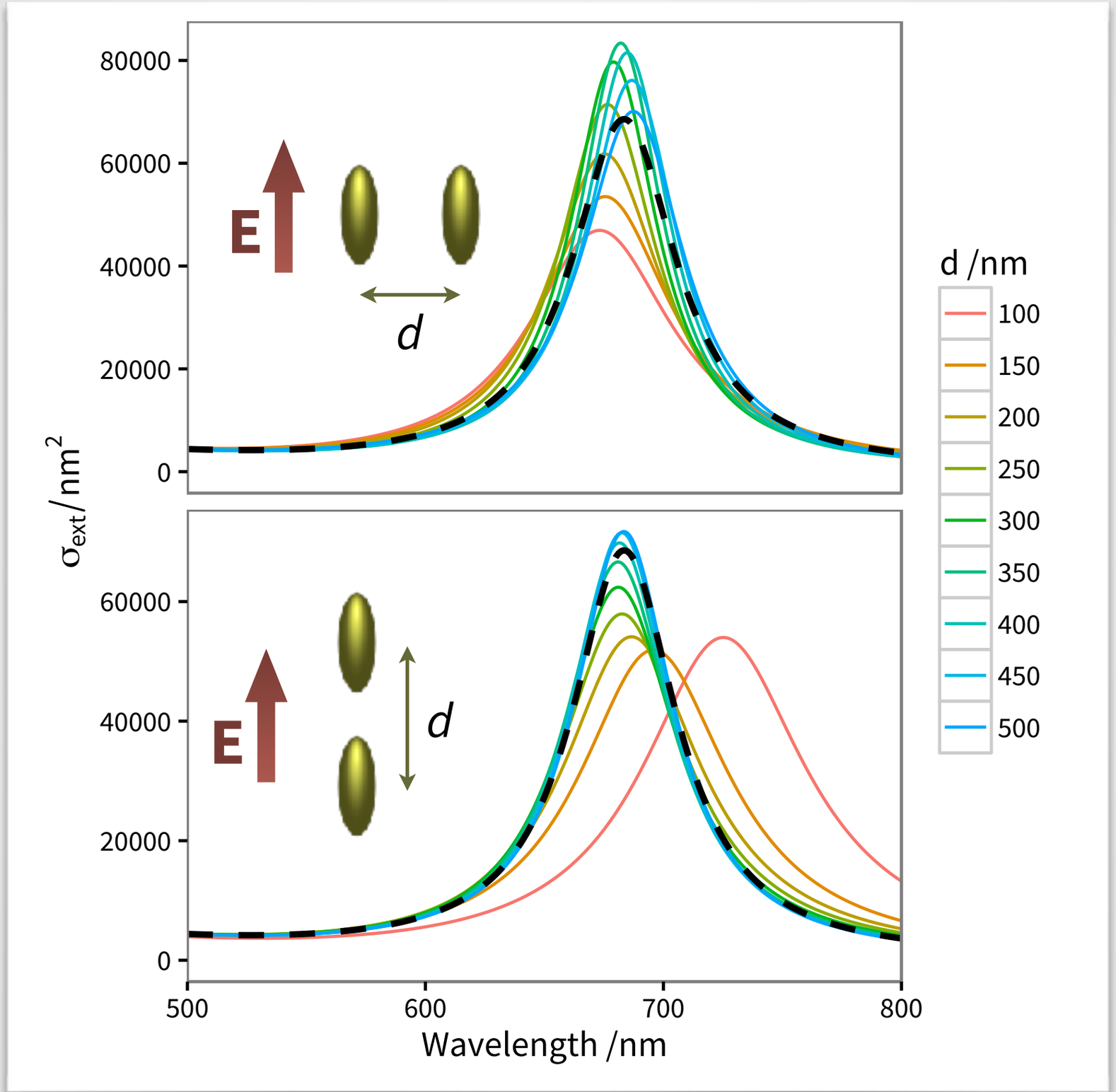


ALWAYS INCLUDE 0? IT DEPENDS





TIP #9 | CONTEXTUAL ANNOTATIONS



TIP #10 | USING COLOURS

- **USE COLOUR TO SYMBOLISE**

  Be logical & follow conventions

- **USE COLOUR TO PRIORITISE INFORMATION**

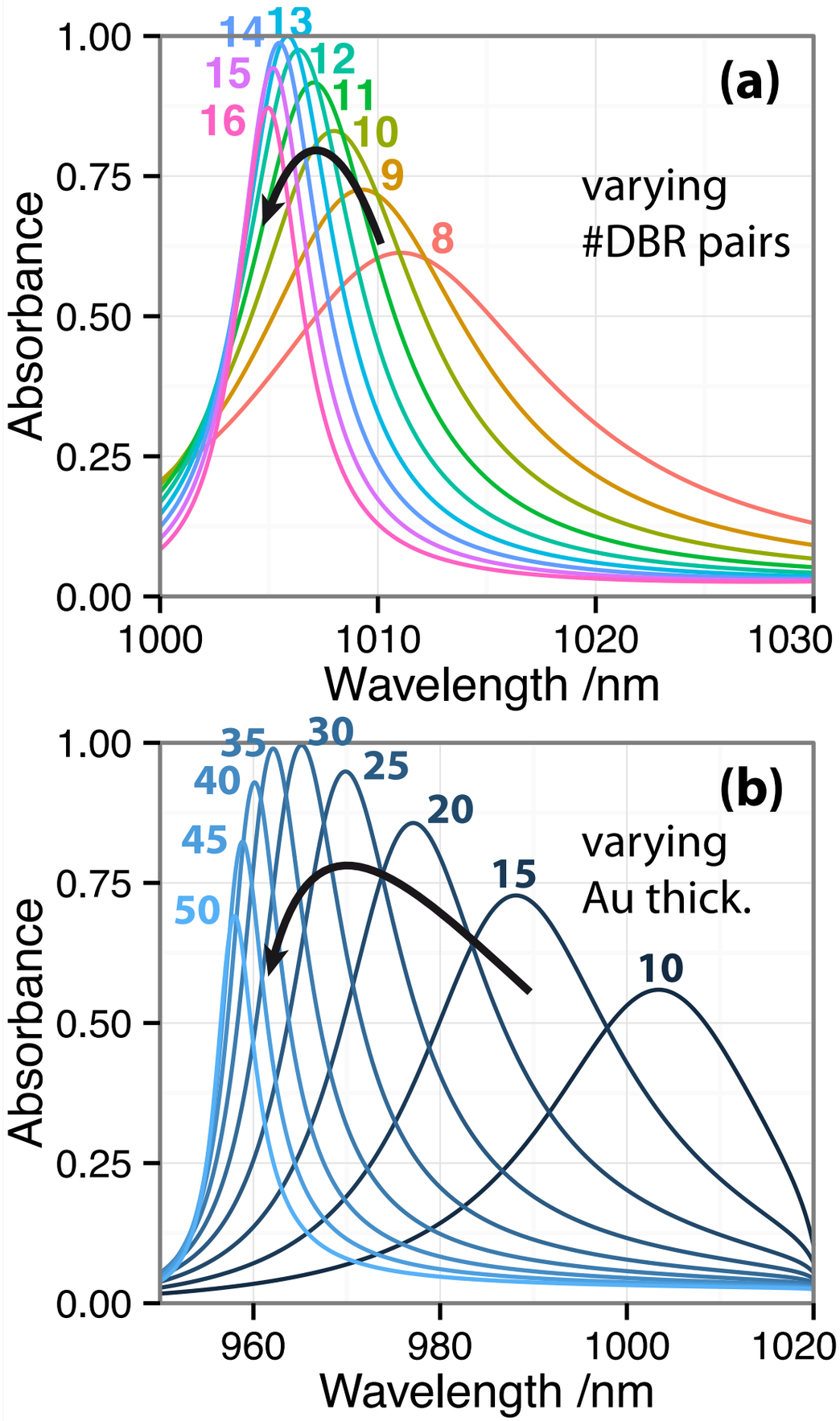
  Smaller areas brighter, larger areas lighter

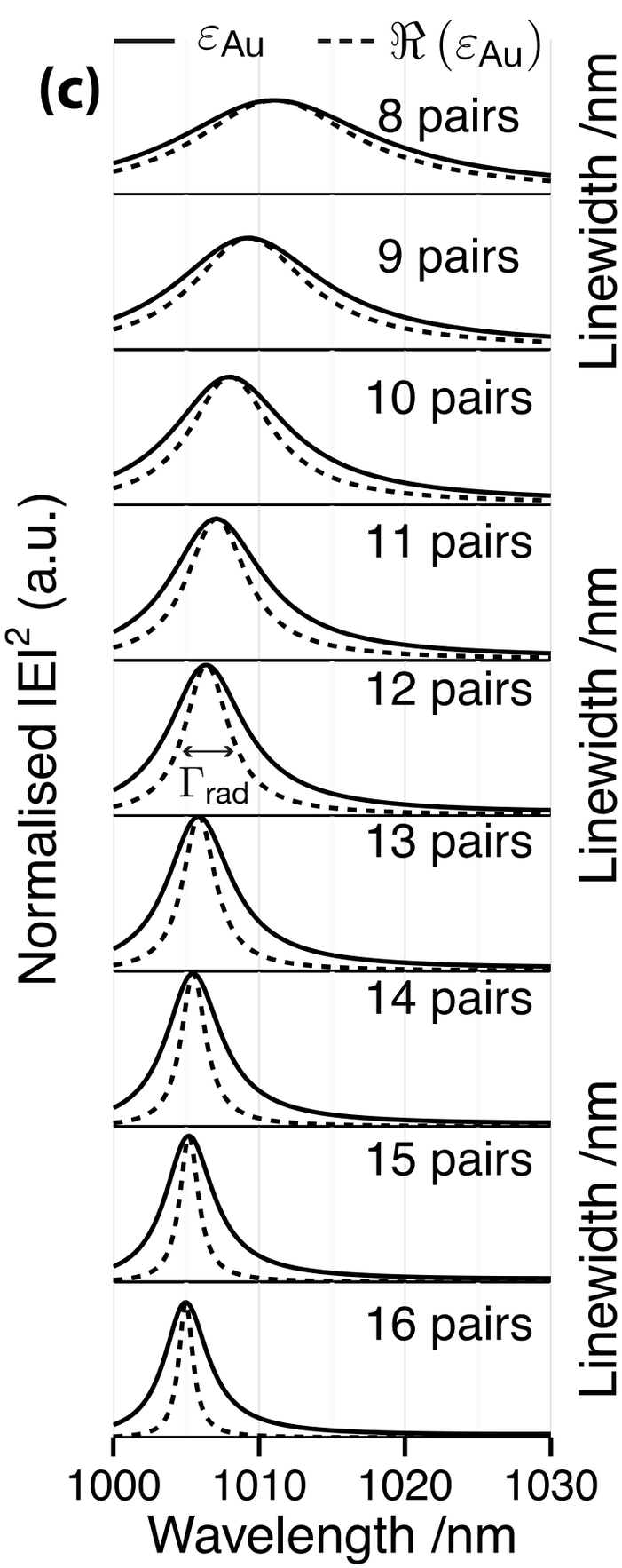
- **USE COLOUR TO IDENTIFY A RECURRING THEME**

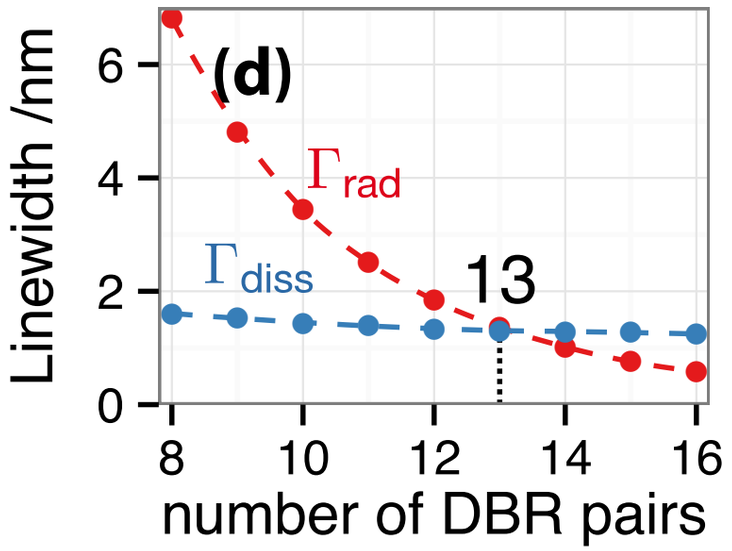
  Be consistent

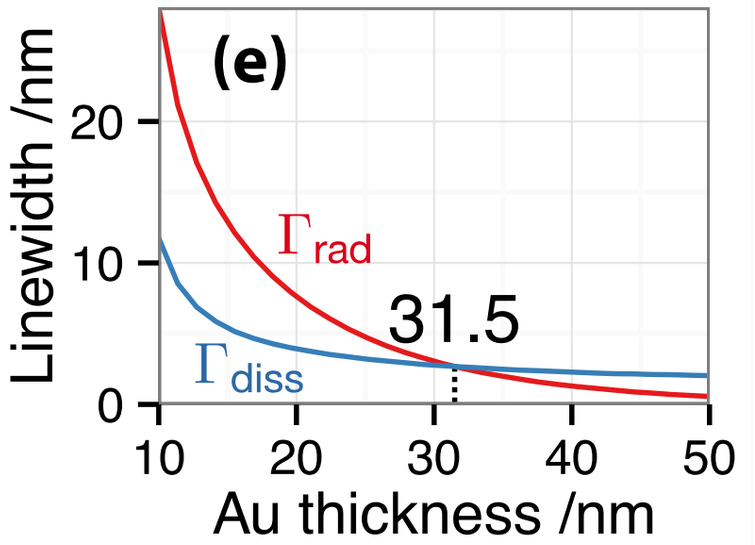
Use colour to explain, never just to decorate. Do not make something pretty for the sake of prettiness or because colour is available.

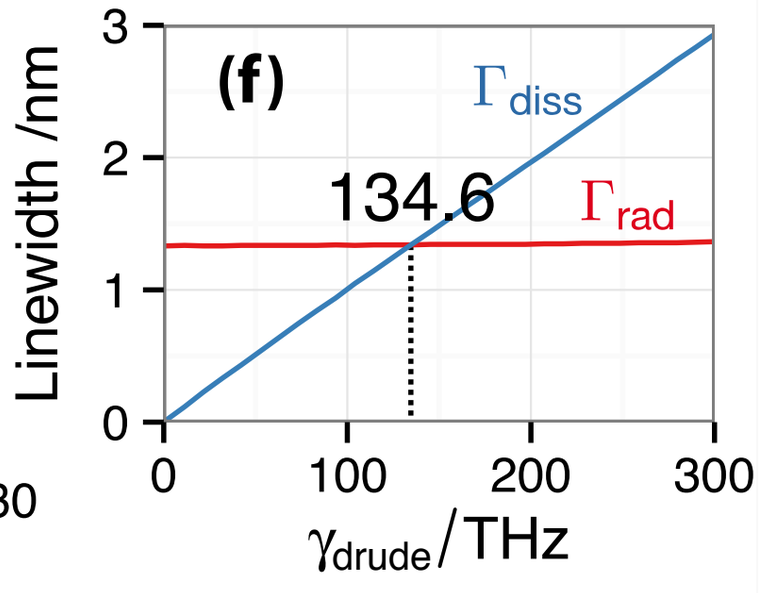
–Jan White


(a)
varying
#DBR pairs
Absorbance
Wavelength /nm
(b)
varying
Au thick.
Absorbance
Wavelength /nm


(c)
ε_{Au}
$\Re(\varepsilon_{Au})$
8 pairs
9 pairs
10 pairs
11 pairs
12 pairs
13 pairs
14 pairs
15 pairs
16 pairs
Γ_{rad}
Normalised |E|² (a.u.)
Wavelength /nm


(d)
Γ_{rad}
Γ_{diss}
13
Linewidth /nm
number of DBR pairs


(e)
Γ_{rad}
Γ_{diss}
31.5
Linewidth /nm
Au thickness /nm

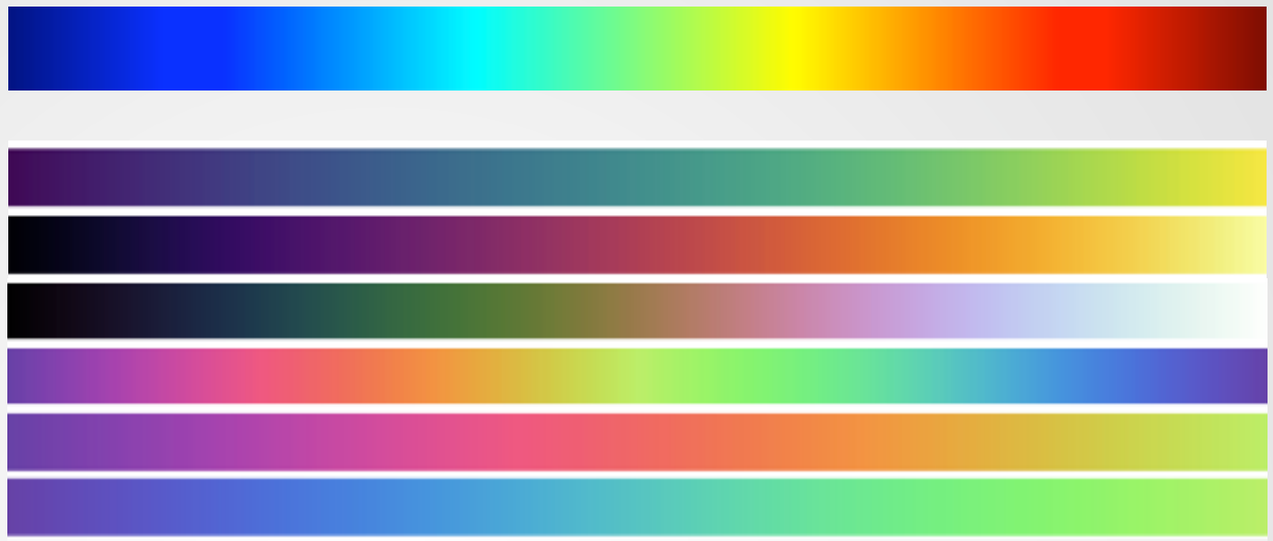

(f)
Γ_{diss}
Γ_{rad}
134.6
Linewidth /nm
γ_{drude}/THz

CHOOSING COLOUR PALETTES

rainbow

viridis

cubehelix



Paired

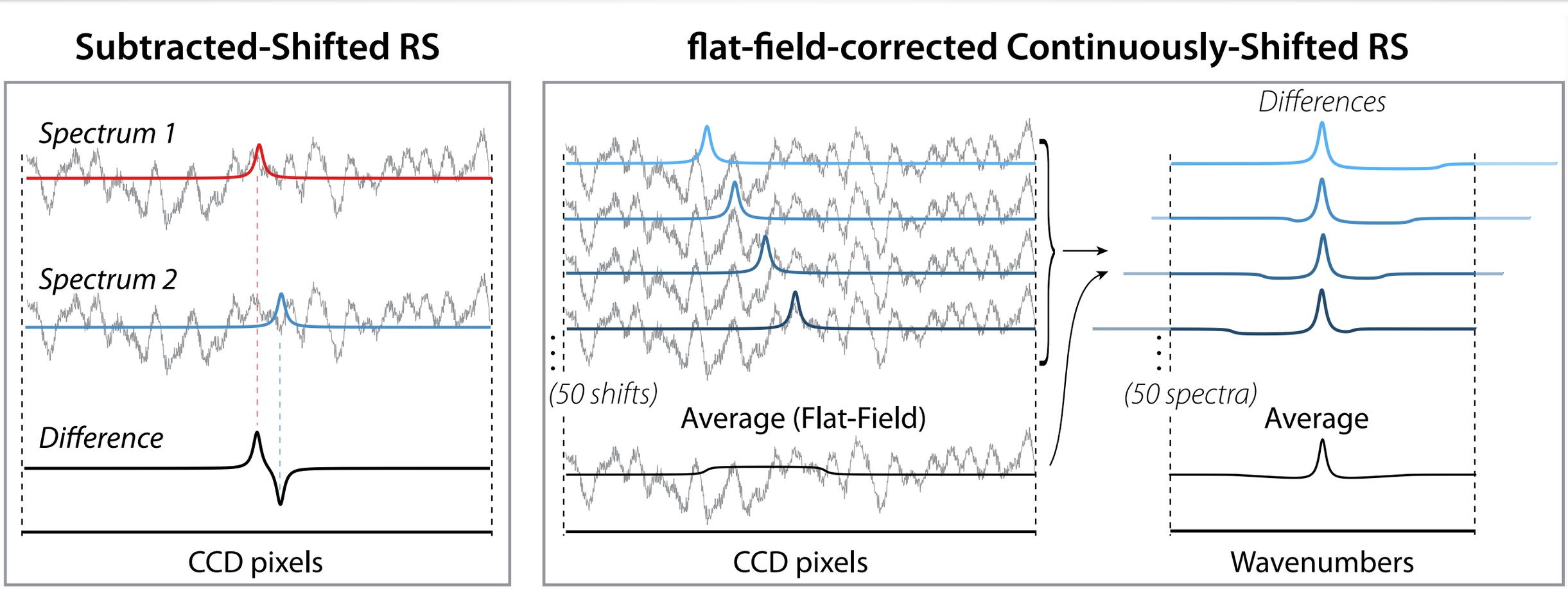
Sequence

Continuous

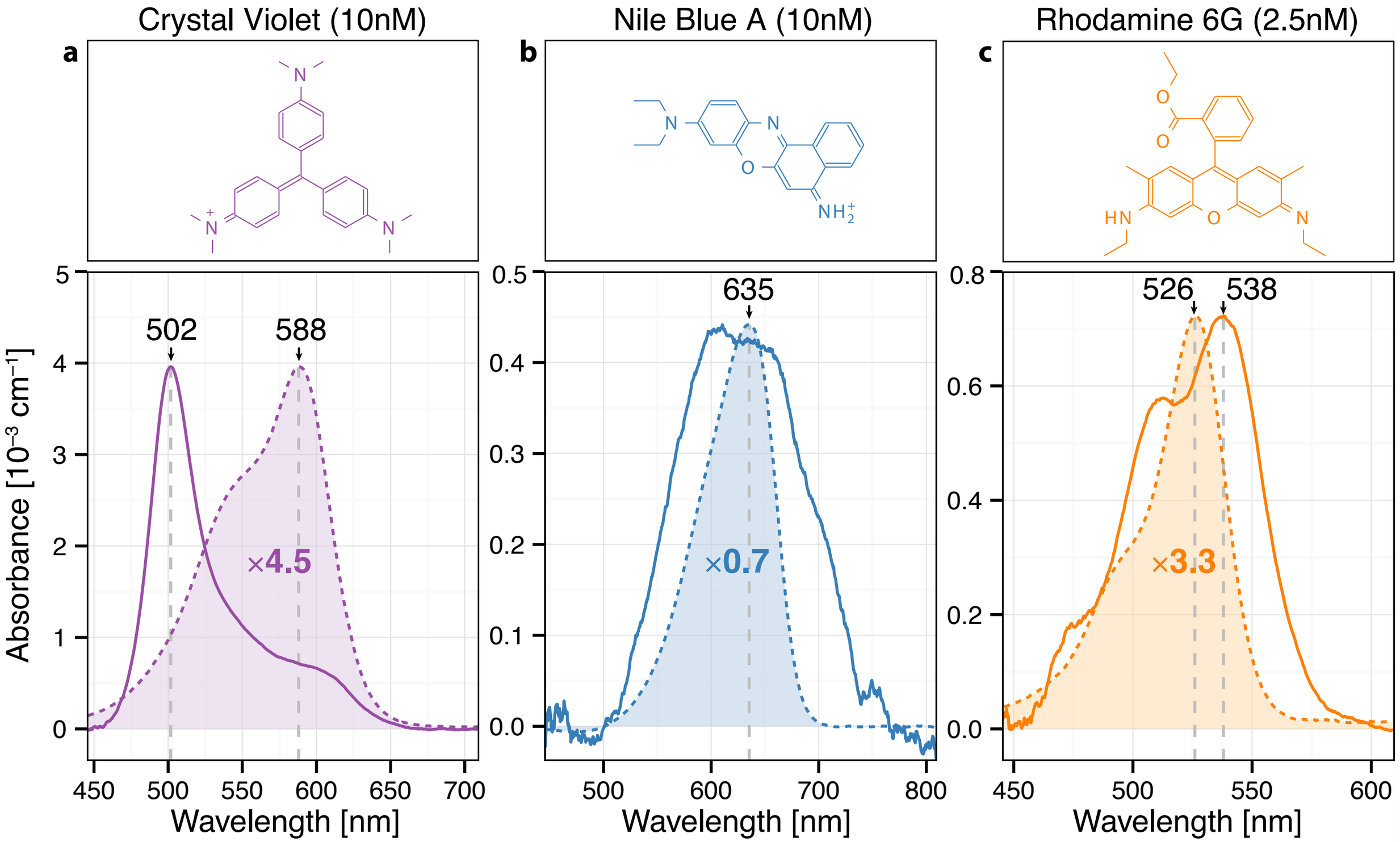
Diverging

Note: ~**8%** of males, 0.5% of females, are **COLOUR BLIND**

COLOUR HELPS IDENTIFY, FOCUS, ORGANISE



COLOUR AND CONTEXT



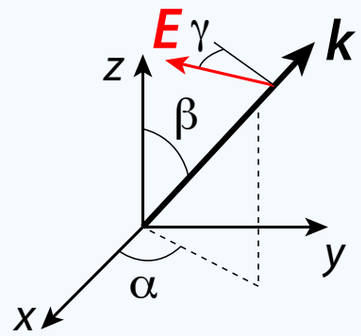
CLUSTER **MATERIAL** **INCIDENCE**

positions
x
y
z
sizes
a
b
c
angles
φ
θ
ψ

N_r

λ

N_l

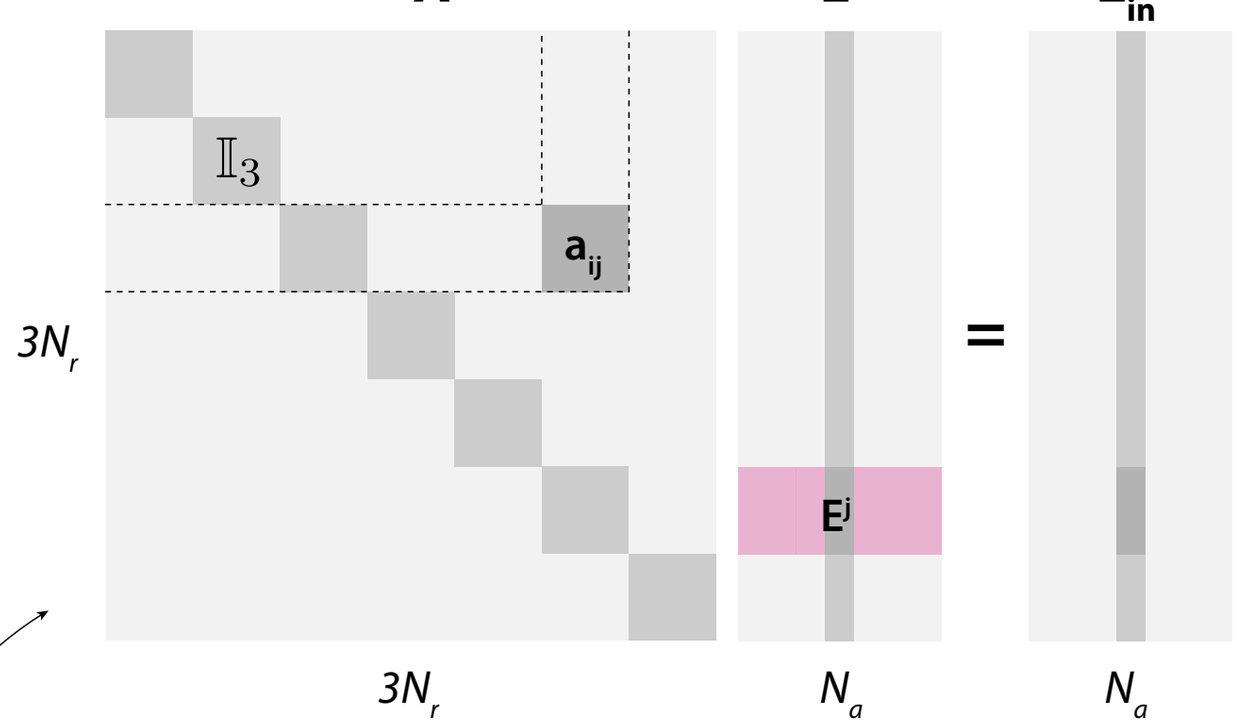


Incidence
α
β
γ

N_a

$\varepsilon(\lambda)$ or $\bar{\alpha}(\lambda)$

CDA SYSTEM



POLARISABILITY

Alpha

$3N_r$

$\alpha_j^a(\lambda)$
$\alpha_j^b(\lambda)$
$\alpha_j^c(\lambda)$

N_l

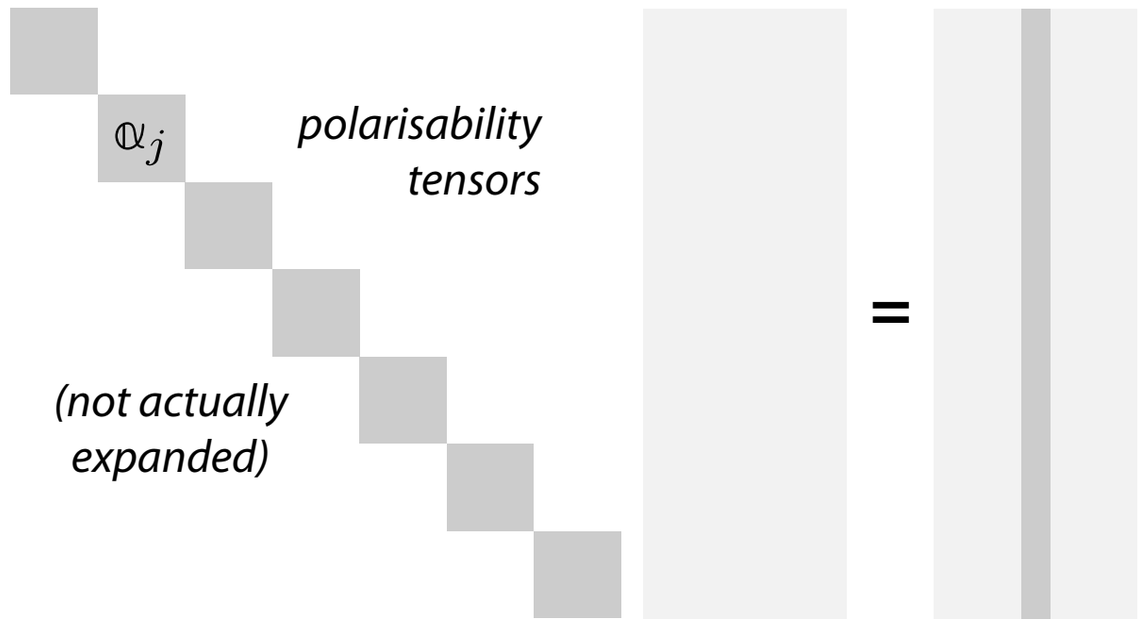
Rotation
(φ, θ, ψ)

R^{-1} $\begin{matrix}\alpha_j^a\\ \alpha_j^b\\ \alpha_j^c\end{matrix}$ R = $\mathbb{\alpha}_j$

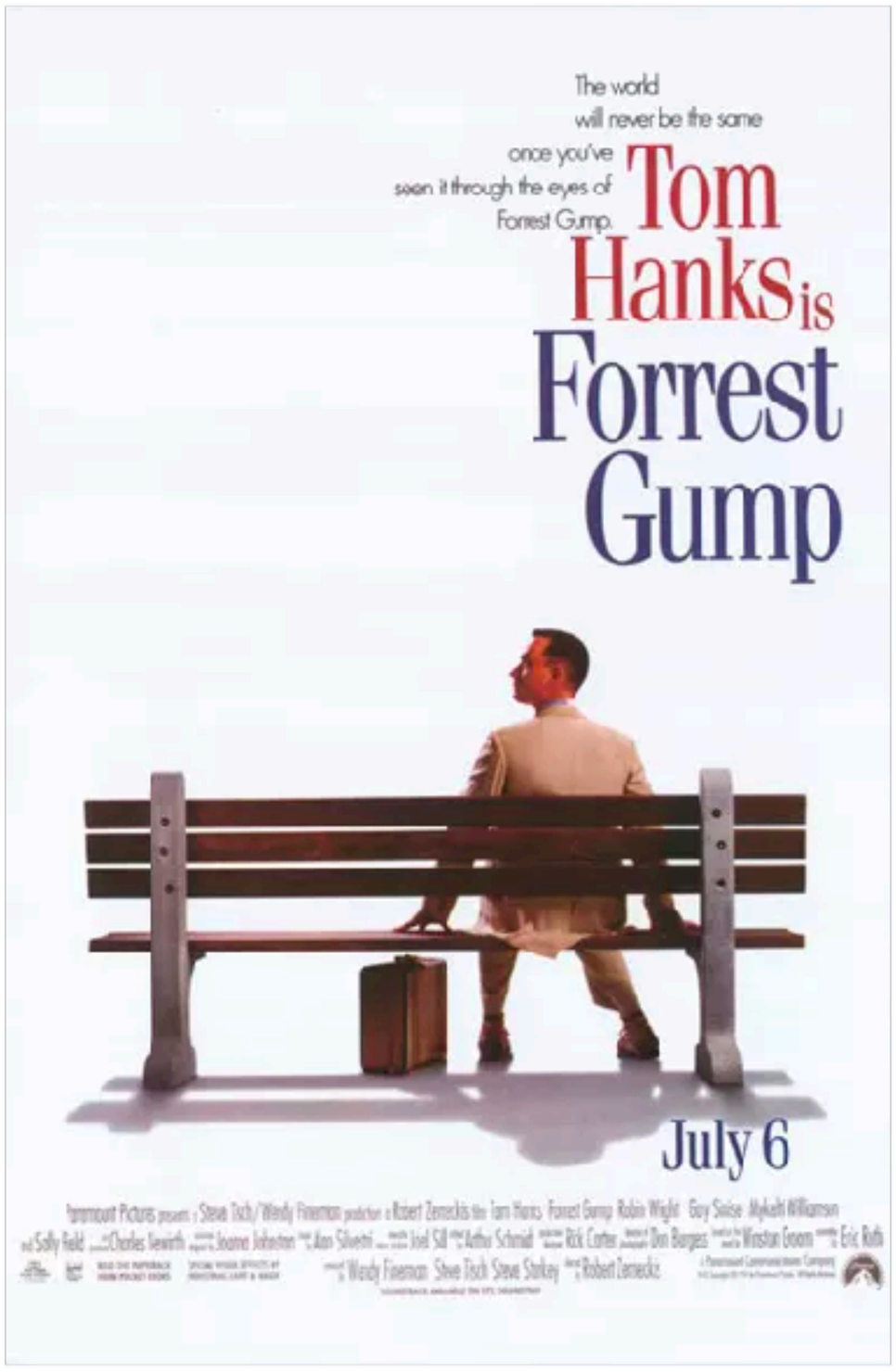
3
3
N_r

AlphaBlocks

DIPOLE MOMENTS



4 POSTERS & MISC. GRAPHICS



WHAT IS THE POSTER FOR?

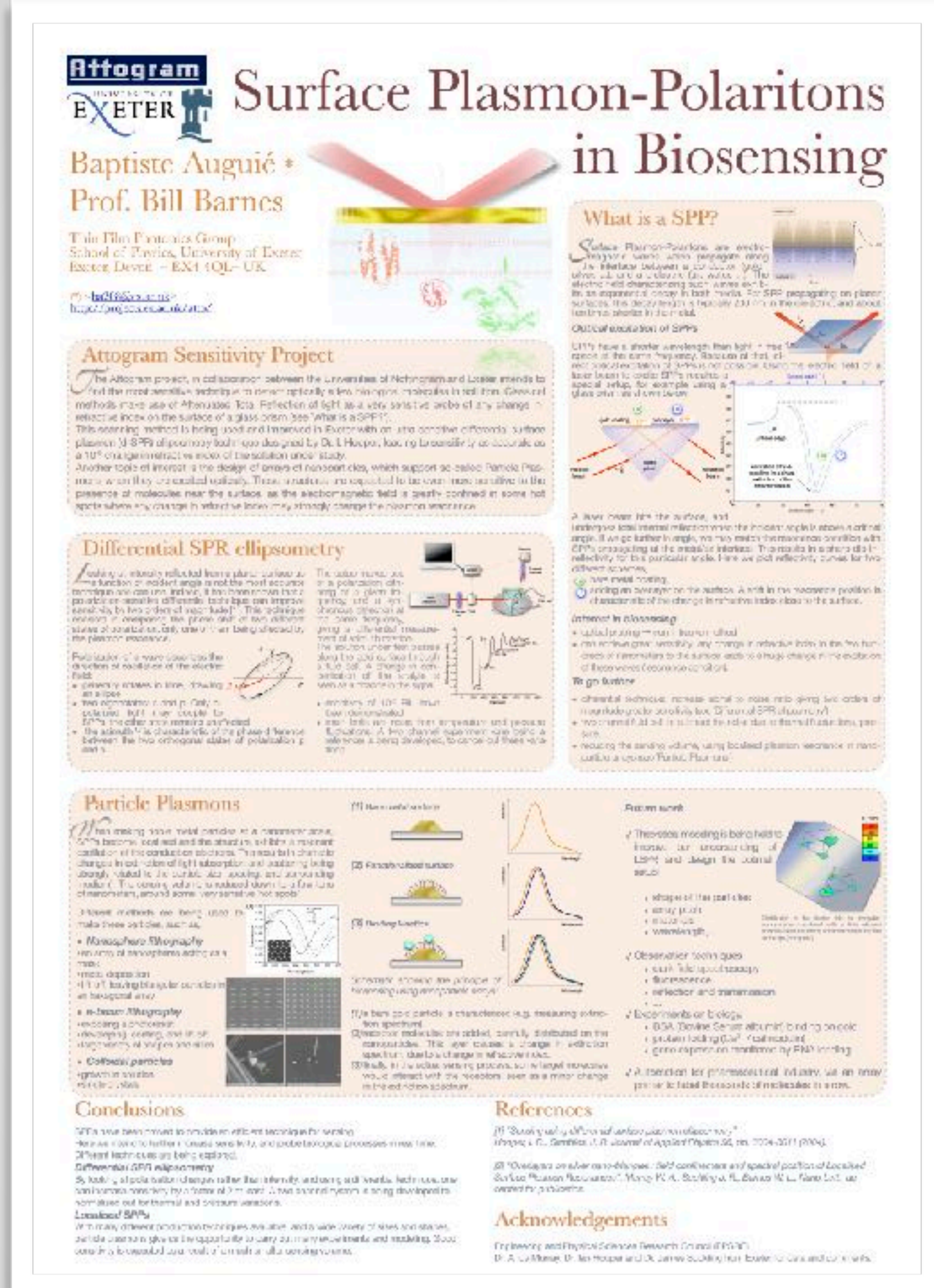
WHAT GOOD IS A POSTER?

- **POSTERS CAN BE EFFECTIVE FOR**
  - Lab advertisement (appealing, introductory)
  - Discussing our research less formally
  - Showing the "big picture" – *e.g. xkcd.com/980*

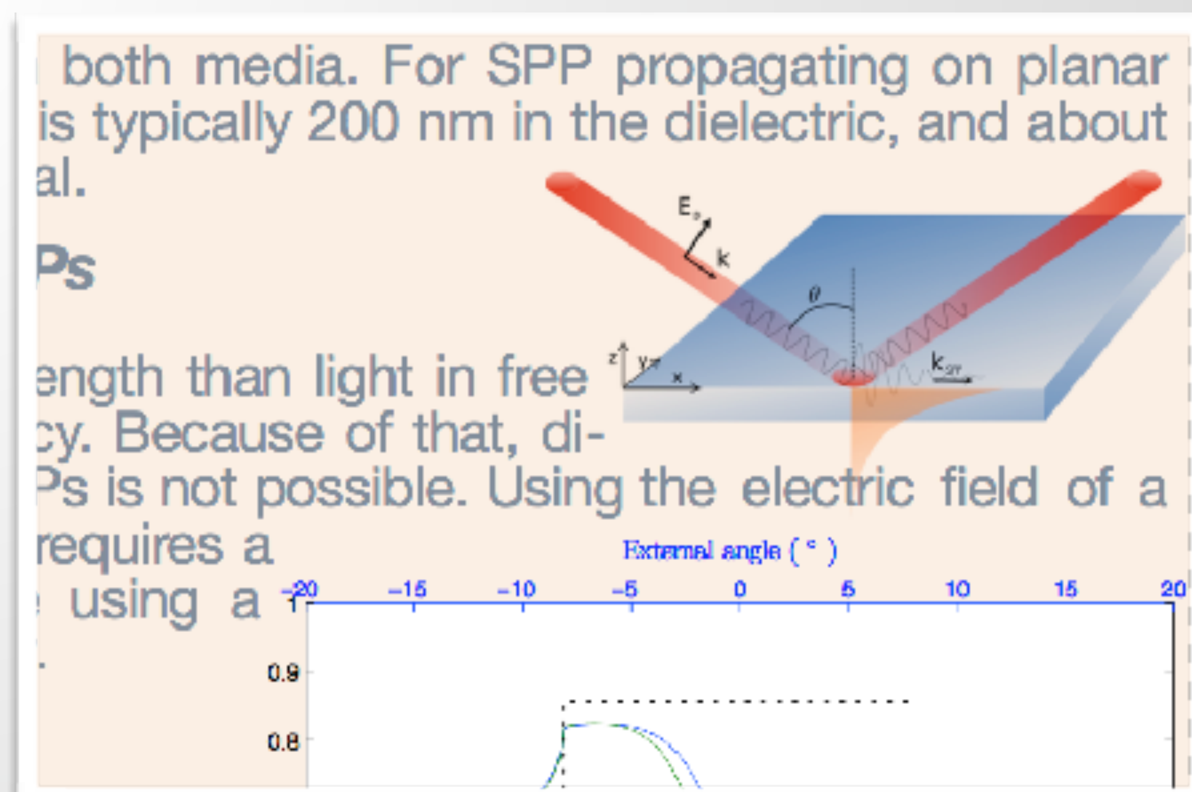
- **POSTER USE IS VARIED**
  - Interactive discussion vs individual viewing
  - Serious vs introductory – *consider your audience*
  - ¿A lesser oral presentation?

THE TEMPTATION OF THE AVAILABLE RICHES IS IRRESISTIBLE

—Jan White


Attogram
EXETER
Surface Plasmon-Polaritons in Biosensing
Baptiste Auguié *
Prof. Bill Barnes
What is a SPP?
Attogram Sensitivity Project
Differential SPR ellipsometry
Particle Plasmons
Conclusions
References
Acknowledgements


(*) <ba208@ex.ac.uk>
http://projects.ex.ac.uk/atto/
Attogram Sensitivity
The Attogram project, in collaboration b
find the most sensitive technique to det
methods make use of Attenuated Total Re
refractive index on the surface of a glass pr


both media. For SPP propagating on planar
is typically 200 nm in the dielectric, and about
al.
Ps
ength than light in free
cy. Because of that, di-
Ps is not possible. Using the electric field of a
requires a
using a
External angle (°)
-20
-15
-10
-5
0
5
10
15
20
0.9
0.8

POSTER PRESENTATION GUIDELINES

- **TELL A COMPELLING STORY**
  - Focus on main points
  - Attract the viewer's attention
  - Use few words, lists
- **TEST FOR EFFECTIVENESS** – print, discuss, iterate
- **MAKE THE BEST USE OF THE MEDIUM**
  - Complement with discussion (*prepare it*)
  - Consider other supports (*tablet, 3D model, …*)
  - Be original, but not distracting (*message first*)

POSTER TIPS

- **FONTS**
  - Few styles, consistent
  - 24pt minimum
  - Appropriate (e.g. Helvetica, not Zapfino or Comic Sans)
- **STRUCTURE**
  - Not an abstract: be concise
  - Results first: get the attention
  - Good flow: reading order must be obvious

POSTER TIPS

- **FOCUS ON WHAT'S IMPORTANT**
  - Use *only* what's required for your story
  - Find a beautiful illustration
  - Be consistent and structured

- **FACILITATE THE COMMUNICATION**
  - Choose meaningful colours and illustrations
  - Design with balance (not *too big*, *use of negative space*)
  - Be ready to present and engage

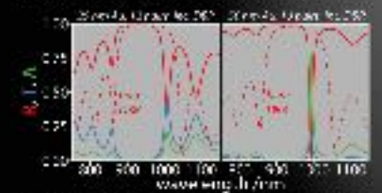
CRITICAL COUPLING OF LIGHT to TAMM SURFACE-PLASMONS

Baptiste Auguié, Viviana Villafañe, Axel Bruchhausen, Alejandro Fainstein

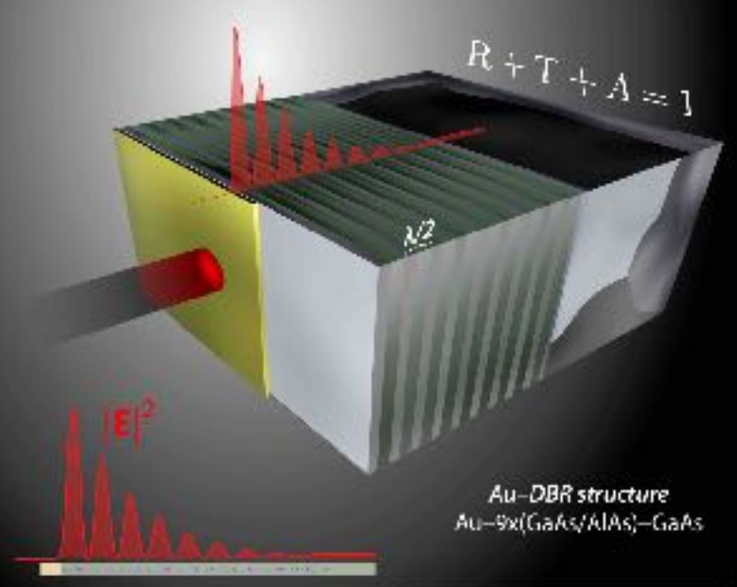
Centro Atómico Bariloche e Instituto Balseiro, San Carlos de Bariloche, 8400 Rio Negro, Argentina

Introduction

Tamm plasmons [1] (TP) are electromagnetic modes confined between a Distributed Bragg Reflector (DBR) and a noble metal (e.g. gold). In contrast to surface plasmons, they may be excited at normal incidence, and present a high-quality factor, making them promising candidates for enhanced light-matter interaction, nonlinear optics, optomechanical coupling [2,3]. Upon excitation of a TP, a dip in reflectivity is observed, which may be optimized to reach 0% (critical coupling), and optical energy is redistributed in transmission and absorption [4].



In this work, we describe the conditions that yield vanishing reflectivity at the TP resonance, and further discriminate the regime of total absorption.



Critical coupling

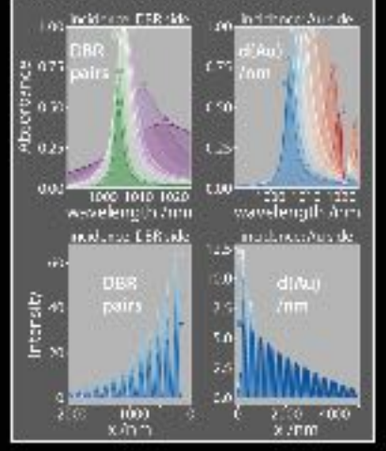
- **transparency**, T=1, only in a dispersionless symmetric resonator

$$Q = \frac{|\omega_{res}|}{|\omega_{abs}| - |\omega_{res}|} = \frac{Q_{abs} Q_{res}}{Q_{abs} - Q_{res}}$$

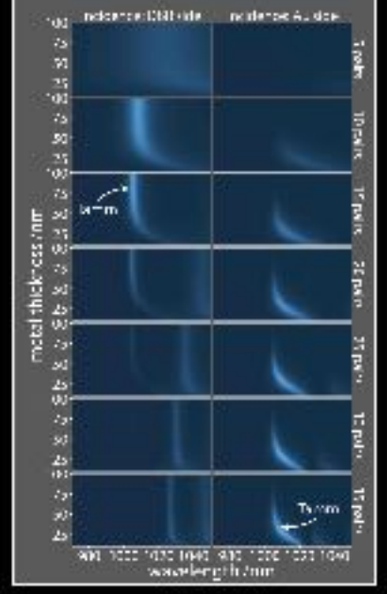
- If $Q_{abs} = Q_{res}$, **critical coupling**, where

$$\omega_{res}'' = \omega_{abs}''$$

- If $Q_{abs} = Q_{res}$, **complete absorption**

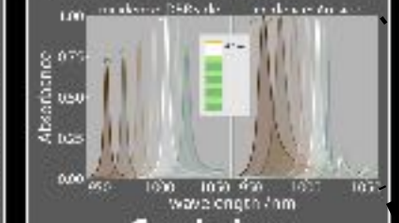


- Optimal TP excitation requires different parameters for either side
- from DBR: ~15 pairs, and thick Au layer
- from Au: ~55nm, and ~6 DBR pairs



Tuning

- The TP mode shifts with the dielectric layer thickness next to the Au layer



Conclusions

- The theory of open resonators and critical coupling sheds light on some counter-intuitive features of Tamm modes
- A regime of complete absorption can be reached, with optimal field enhancement
- Applications may include thermal emitters, optical communications, and sensing

References

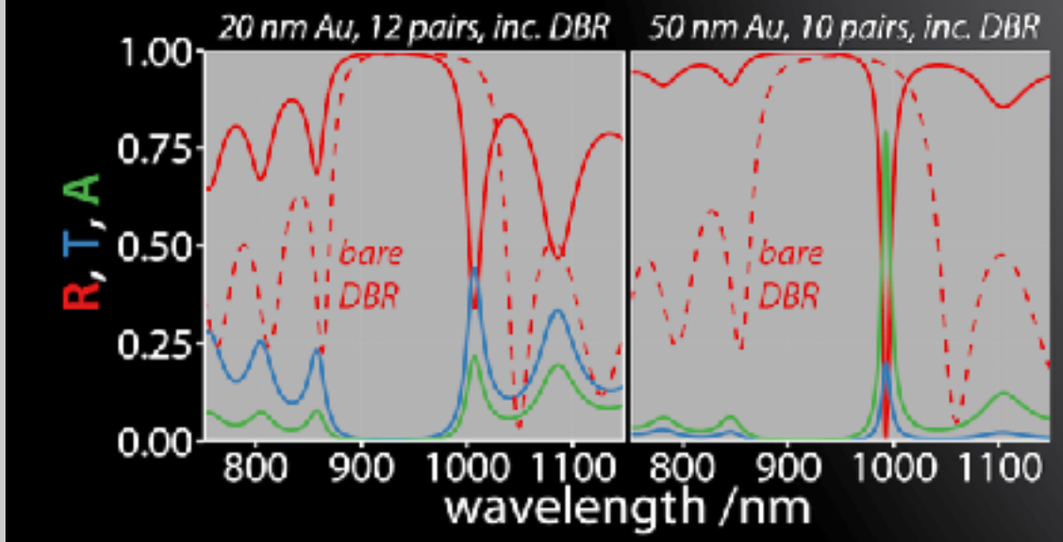
[1] Phys Rev B 75(1), 2007

[2] Opt Lett 38(7), 2013

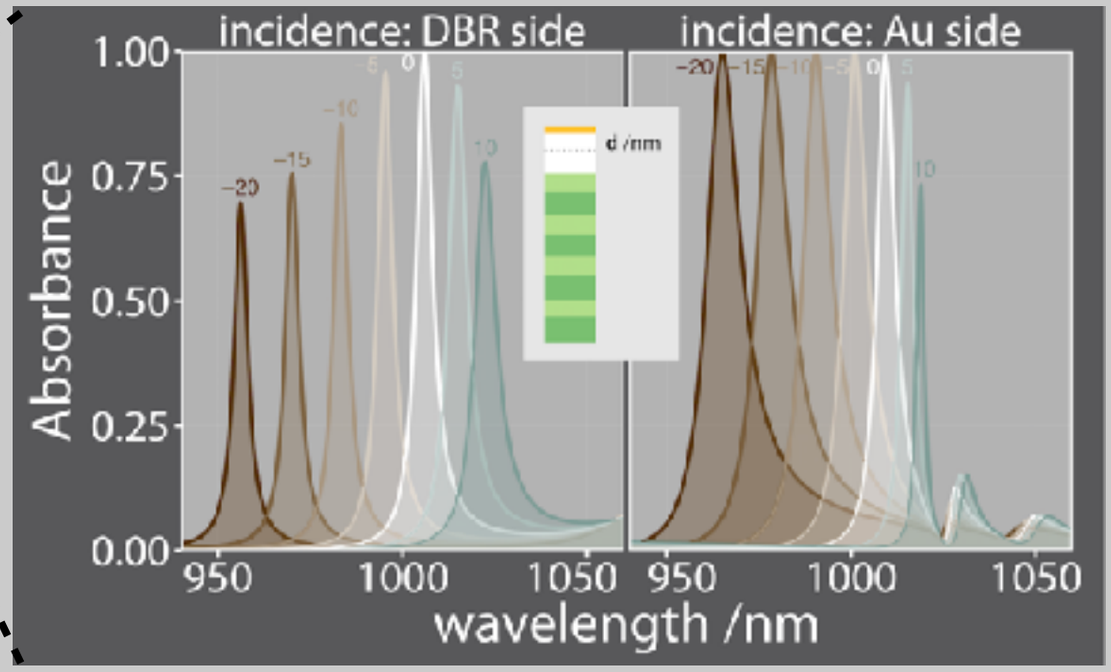
[3] App Phys Lett 100(11), 2012

[4] Rev Mod Phys 80(4), 2008

0% (***critical coupling***), and optical energy is re-distributed in transmission and absorption [4].



In this work, we describe the conditions that



Radiative Correction for Electromagnetic Scattering

Eric Le Ru, Walter Somerville, Baptiste Auguié

The MacDiarmid Institute for Advanced Materials and Nanotechnology
School of Chemical and Physical Sciences
Victoria University, Wellington, New Zealand

Motivation— With the recent increased interest in the optical properties of nano-particles, there has been a strong incentive to develop simple methods to solve the electromagnetic (EM) scattering problem for sub-wavelength objects of general shape and composition. The quasi-static approximation is particularly well suited for the rapid and accurate modelling of such small scatterers. However, because this approximation intrinsically neglects radiation, it cannot satisfy the conservation of energy. The recurring issue of defining a rigorous self-reaction correction has thus resurfaced in this particular context. To date, this correction has been introduced only heuristically, and only for the simplest cases. We propose a formalism in which such radiative corrections (RC) to EM scattering can be justified *rigorously* and *generalized* to any other cases including point or body scatterers, and to any multipolar order.

— The Case of a Point Dipole —

- Power extracted by such a dipole from the EM field is $P_{ext} = \frac{1}{2}\omega\mathrm{Im}(\alpha_1)|E_{incl}|^2$

- Also the power absorbed P_{abs} in the electrostatics approximation

- Energy conservation $P_{ext} = P_{abs} + P_{sca}$ is violated for optical properties

Self-field correction, polarizability

$$\left(\alpha^{RC}\right)^{-1} = \alpha_0^{-1} - G$$

- Enforces energy conservation, but G is infinite...

- Common prescription: use the finite, imaginary part

$$\alpha = \frac{\alpha_0}{1 - i\frac{k_0^3}{6\pi\varepsilon_0\varepsilon_1}\alpha_0}$$

— T-Matrix for Light Scattering —

Relates field expansions of incident and scattered fields in a basis of vector spherical wavefunctions.

$$\begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} = \mathbf{T}\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}$$

With

$$\mathbf{E}_{inc}(\mathbf{r}) = E_0 \sum_\nu a_\nu \mathbf{N}_\nu^{(1)}(k_1\mathbf{r}) + b_\nu \mathbf{N}_\nu^{(3)}(k_1\mathbf{r}),$$

$$\mathbf{E}_{sca}(\mathbf{r}) = E_0 \sum_\nu p_\nu \mathbf{N}_\nu^{(3)}(k_1\mathbf{r}) + q_\nu \mathbf{N}_\nu^{(3)}(k_1\mathbf{r}).$$

Link with S-matrix: $\mathbf{S} = \mathbf{I} + 2\mathbf{T}$

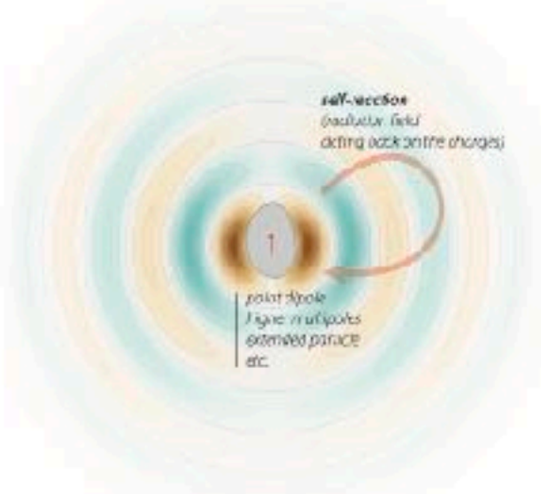
Cayleigh transform

We define a reactance matrix, K

$$\mathbf{K} = i(\mathbf{I} - \mathbf{S})(\mathbf{I} + \mathbf{S})^{-1}$$

Energy conservation

$$\mathbf{T} - \mathbf{T}^\dagger = -2\mathbf{T}^\dagger\mathbf{T} \Leftrightarrow \mathbf{S}\mathbf{S}^\dagger = \mathbf{I} \Leftrightarrow \mathbf{K} = \mathbf{K}^\dagger$$



Artistic representation of self-reaction

— Rigorous RC in the T-matrix Framework —

- Energy conservation is expressed as $\mathbf{K} = \mathbf{K}^\dagger$ (non-absorbing)

- Absorbing particles: $i\mathbf{K} - \mathbf{K}^\dagger$ is Hermitian positive semi-definite ($\mathbf{K}$ is dissipative) (generalizes $\mathrm{Im}(K) \geq 0$ for a response function K, to matrices)

- Given an (truncated, approximate...) expression for K, we obtain a radiation-corrected T-matrix, automatically satisfying energy conservation.

$$\mathbf{T}^{-1} = -i\mathbf{K}^{-1} - \mathbf{I}$$

Example of a point dipole

Using the approximate T-matrix from electrostatics, $\mathbf{K}_d^{(1)} = -i\mathbf{T}_d^{(1)} = \frac{\varepsilon_1^3}{6\pi\varepsilon_0\varepsilon_2}\alpha_0$

We justify $\alpha = \frac{\alpha_0}{1 - i\frac{k_1^3}{6\pi\varepsilon_0\varepsilon_1}\alpha_0}$

Recent examples scattered in the literature

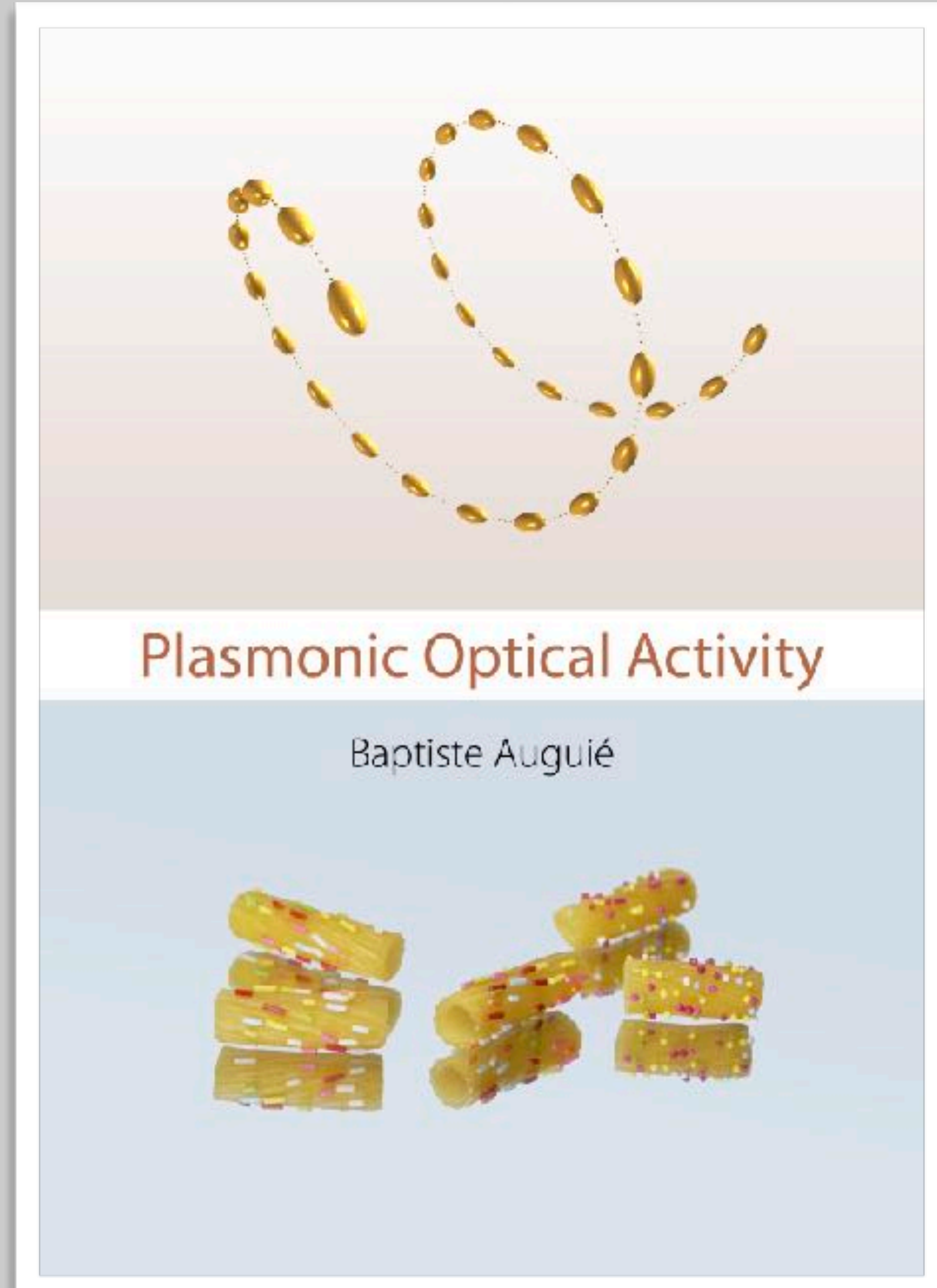
General multipole correction from Mie theory [5] $\alpha_n = \left[1 - \frac{(n+1)k^{2n+1}}{n(2n-1)!!(2n+1)!!}\alpha_n\right]^{-1}\alpha_n$

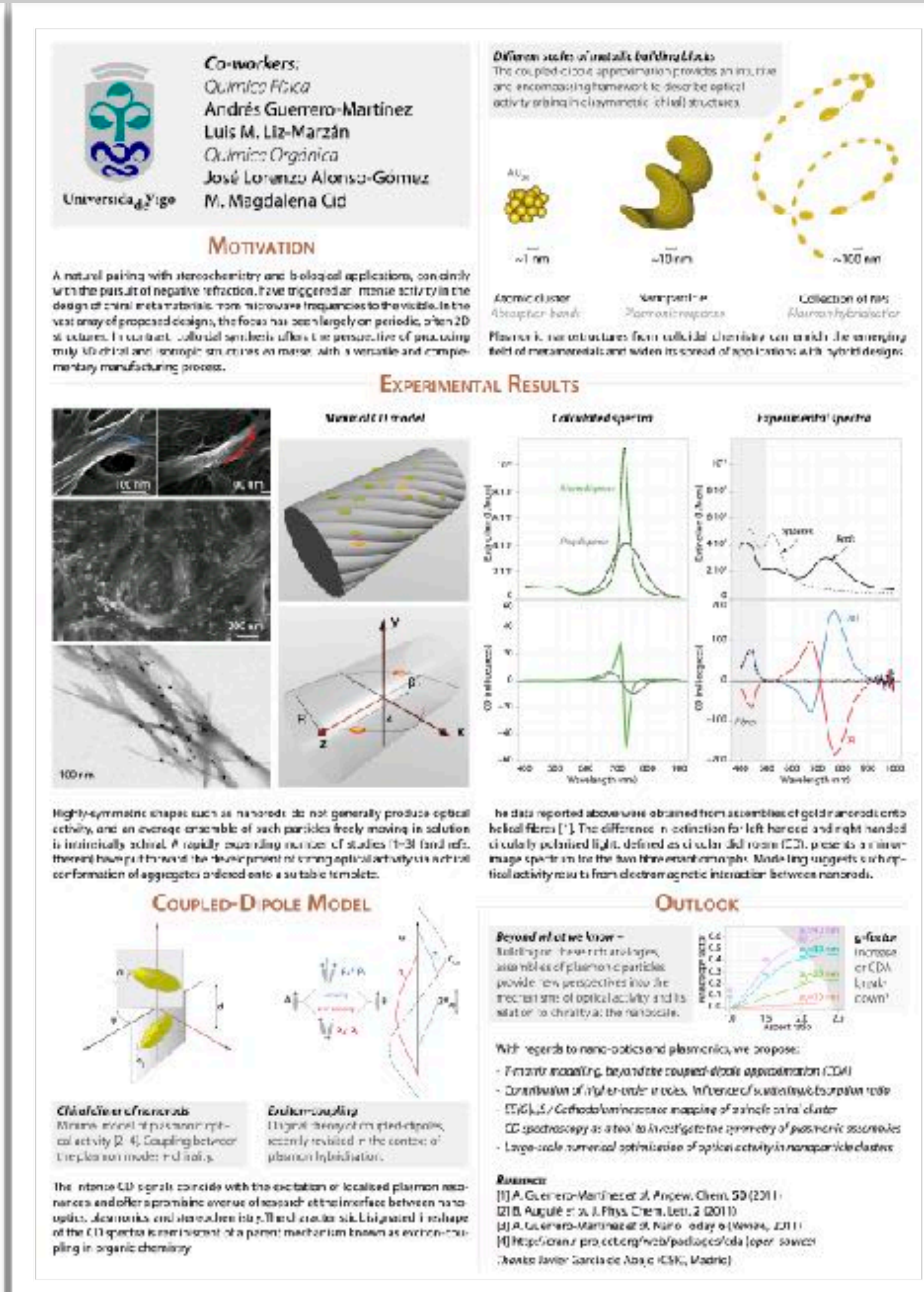
Non-anisotropic/achiral scatterers [6] also [7] with magnetoelectric coupling $\alpha^{-1} - (\alpha^{-1})^\dagger = -\frac{ik^3}{3\pi}\begin{pmatrix} 1/\varepsilon_0 & 0 \\ 0 & 1/\mu_0 \end{pmatrix}$

Outlook— Using this formalism, radiative corrections to EM scattering can be justified rigorously and directly generalized to point or body scatterers, and to any multipolar order. Notably, these results trivially reproduce, and make a connection to, several independent results for special cases that were scattered in the recent literature.
Remarkably, the use of the K matrix avoids the appearance of any infinities in the derivation of the radiative corrections, which we believe may have implications beyond EM theory.

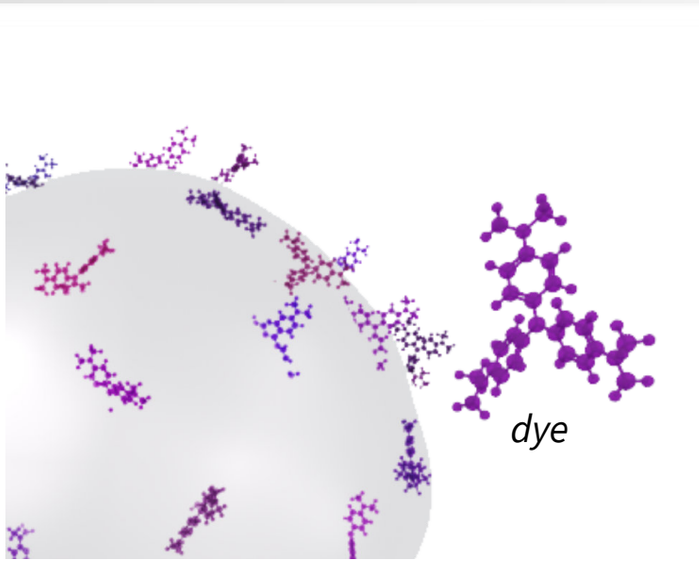
References

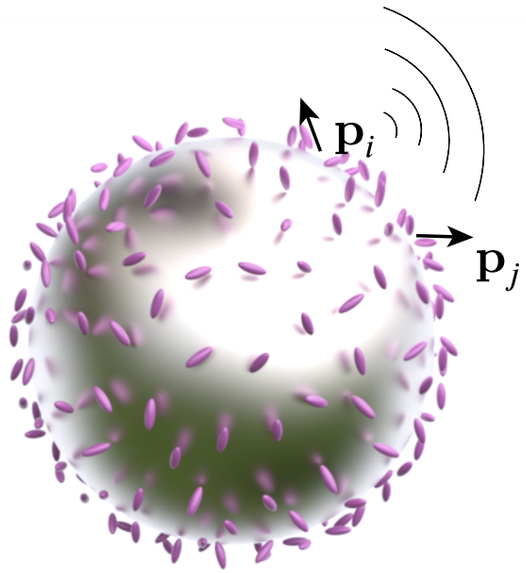
[1] P. de Vries *et al*, Rev. Mod. Phys. **70**, 447 (1998)
[2] A. Wokaun *et al*, Phys. Rev. Lett. **48**, 957 (1983)
[3] M. I. Mishchenko, L. D. Travis, and A. A. Lacis, *Scattering, absorption and emission of light by small particles*, 3rd ed. (Cambridge Univ. Press, 2002)
[4] R. G. Newton, *Scattering theory of waves and particles* (McGraw-Hill, New York, 1966)
[5] G. Colas des Francs, Int. J. Mol. Sci. **10**, 3913 (2009)
[6] P. A. Belov *et al*, Tech. Phys. Lett. **29**, 718 (2003)
[7] I. Sersic *et al*, Phys. Rev. E **83**, 245102 (2011)

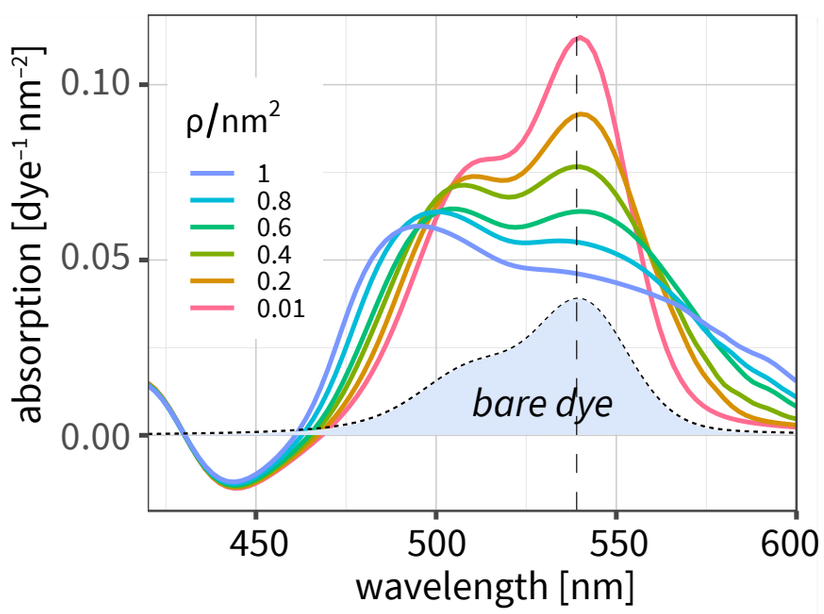

Plasmonic Optical Activity
Baptiste Auguié


Co-workers:
Química Física
Andrés Guerrero-Martínez
Luis M. Liz-Marzán
Química Orgánica
José Lorenzo Alonso-Gómez
M. Magdalena Cid
Universida de Vigo
Motivation
Experimental Results
Coupled-Dipole Model
Outlook
~1 nm
~10 nm
~100 nm
Collection of NPs
With regards to nano-optics and plasmonics, we propose:
[1] A. Guerrero-Martínez et al. Angew. Chem. 50 (2011)
[2] B. Auguié et al. J. Phys. Chem. Lett. 2 (2011)

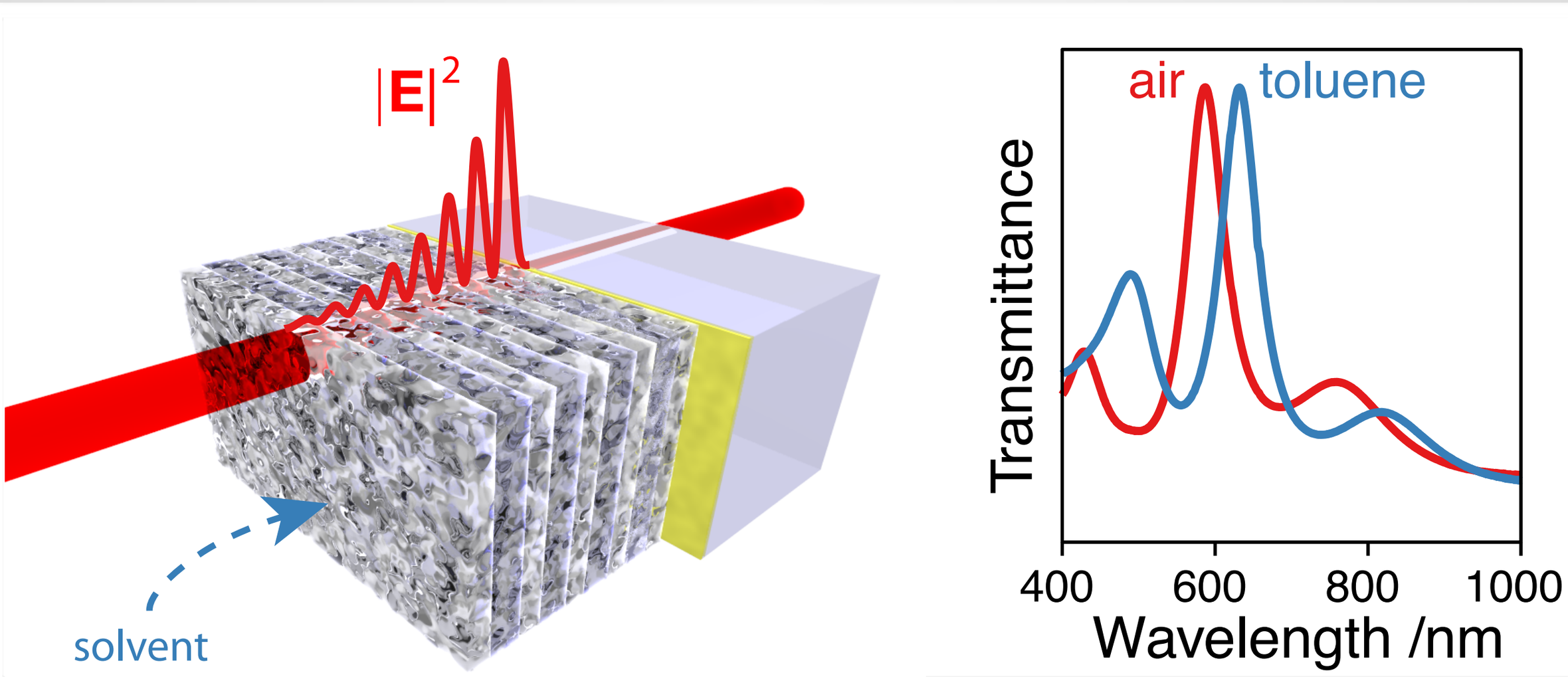
5 TABLE OF CONTENTS GRAPHICS







5 TABLE OF CONTENTS GRAPHICS



If progress is to be made in graphics, we must be prepared to set aside old procedures when better ones are developed, just as is done in other areas of science.

—W.S. Cleveland

5 RESOURCES

- J.L. Doumont • *Trees, maps, and theorems*
- Jan White • *Graphic design for the electronic age*
- Edward Tufte • *The visual display of quantitative information*
- serialmentor.com/dataviz
- socviz.co
- ft.com/vocabulary
- data-to-viz.com

ADDITIONAL LINKS

- https://github.com/kbroman/Talk_Graphs
- http://www.perceptualedge.com/examples.php
- http://colinpurrington.com/2012/example-of-bad-scientific-poster/
- http://tools.medialab.sciences-po.fr/iwanthue/
- Aspect ratio: http://vis.berkeley.edu/papers/banking/
- http://earthobservatory.nasa.gov/blogs/elegantfigures/2013/08/06/subtleties-of-color-part-2-of-6/
- Show the data, don't conceal them https://doi.org/10.1111/j.1476-5381.2011.01251.x

SOFTWARE SUGGESTIONS

- **PLOTS**
  - Python, R, ...
  - D3, Vega-lite, plot.ly (interactive)
  - Tableau (expensive)

- **SCHEMATICS & LAYOUT**
  - Inkscape (open-source)
  - Adobe Illustrator, Indesign (expensive)

from Data to Viz

'From Data to Viz' is a classification of chart types based on input data format. It will help you find the perfect chart in three simple steps:

1. Identify what type of data you have.
2. Go to the corresponding decision tree and follow it down to a set of possible charts.
3. Choose the chart from the set that will suit your data and your needs best.

Dataviz is a world with endless possibilities and this project does not claim to be exhaustive. However it should provide you with a good starting point. For an interactive version and much more visit:

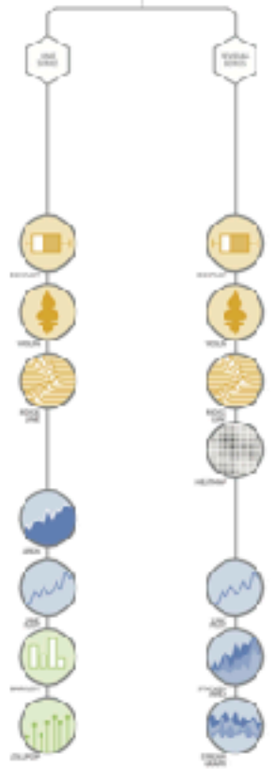
data-to-viz.com

CATEGORIC

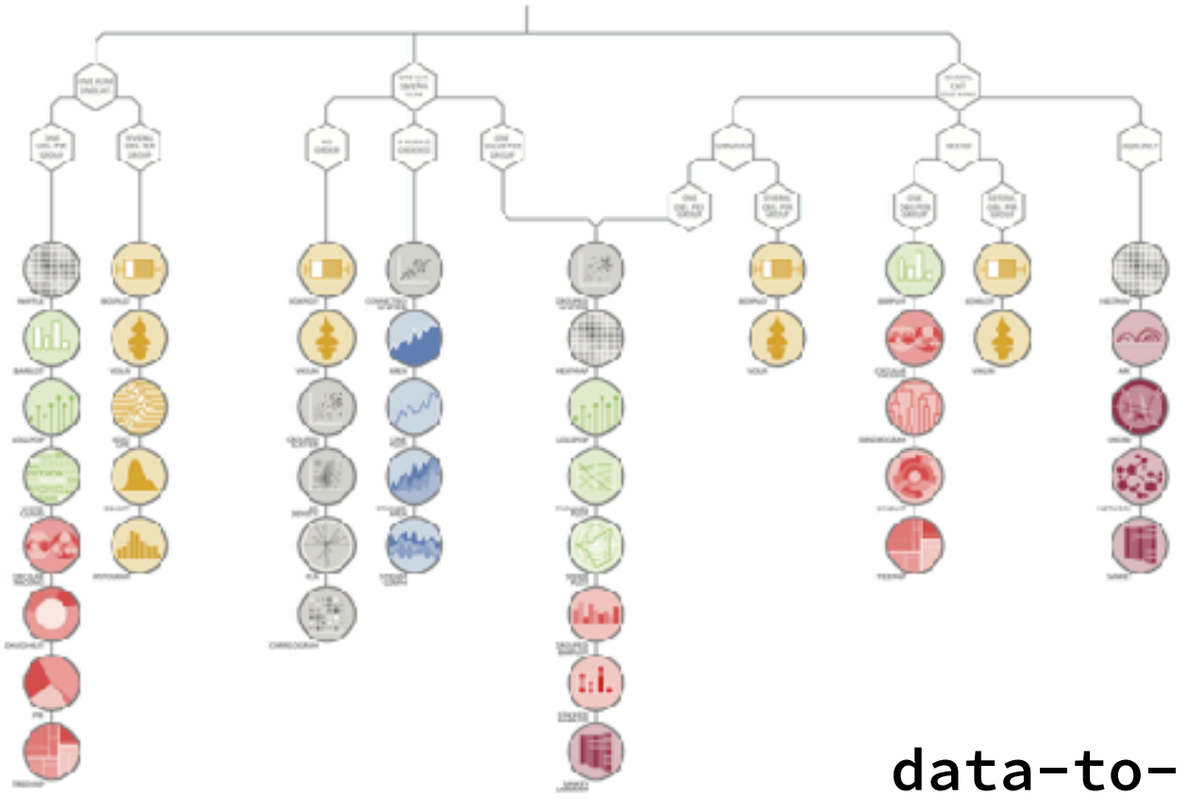
RELATIONAL

MAP

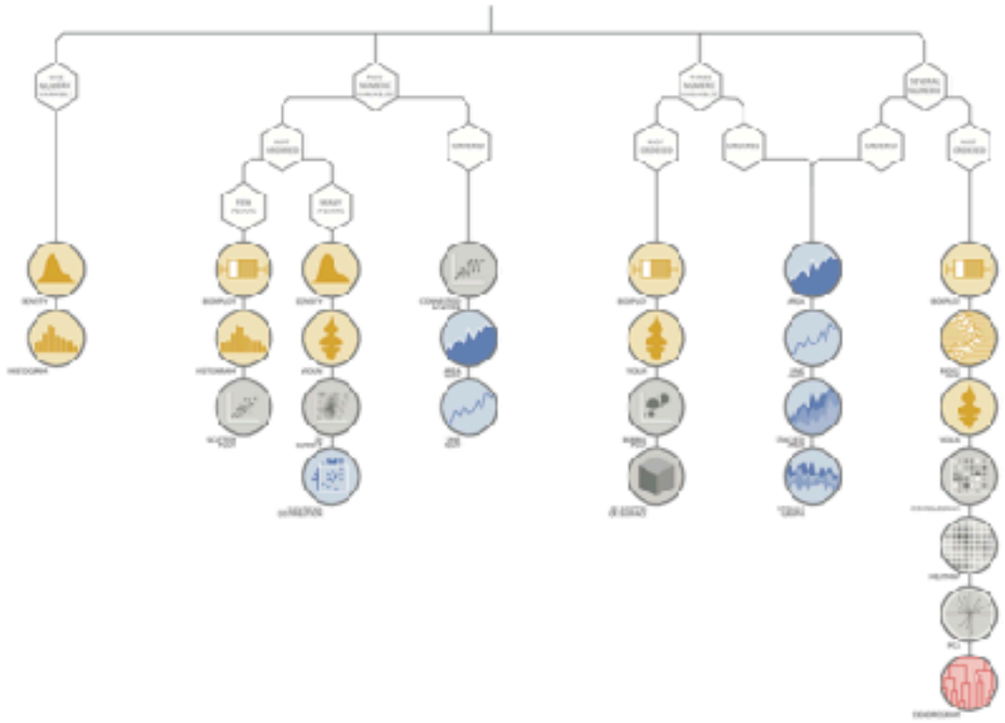
TIME SERIES



CATEGORIC AND NUMERIC



NUMERIC



WHAT DO YOU WANT TO SHOW?

- Distribution
- Correlation
- Ranking
- Part of a whole
- Evolution
- Maps
- Flow

data-to-viz.com

Deviation

Emphasise variations (+/-) from a fixed reference point. Typically the reference point is zero but it can also be a target or a long-term average. Can also be used to show sentiment (positive/neutral/negative).

Example FT uses
Trade surplus/deficit, climate change

Diverging bar

A simple standard bar chart that can handle both negative and positive magnitude values.

Diverging stacked bar

Perfect for presenting survey results which involve sentiment (eg disagree/neutral/agree).

Spine chart

Splits a single value into 2 contrasting components (eg Male/Female).

Surplus/deficit filled line

The shaded area of these charts allows a balance to be shown – either against a baseline or between two series.

XY heatmap

A good way of showing the patterns between 2 categories of data, less good at showing fine differences in amounts.

Correlation

Show the relationship between two or more variables. Be mindful that, unless you tell them otherwise, many readers will assume the relationships you show them to be causal (i.e. one causes the other).

Example FT uses
Inflation & unemployment, income & life expectancy

Scatterplot

The standard way to show the relationship between two continuous variables, each of which has its own axis.

Line + Column

A good way of showing the relationship between an amount (columns) and a rate (line).

Connected scatterplot

Usually used to show how the relationship between 2 variables has changed over time.

Bubble

Like a scatterplot, but adds additional detail by sizing the circles according to a third variable.

Slope

Perfect for showing how ranks have changed over time or vary between categories.

Lollipop chart

Lollipops draw more attention to the data value than standard bar/column and can also show rank and value effectively.

Ranking

Use where an item's position in an ordered list is more important than its absolute or relative value. Don't be afraid to highlight the points of interest.

Example FT uses
Wealth, deprivation, league tables, constituency election results

Ordered bar

Standard bar charts display the ranks of values much more easily when sorted into order.

Ordered column

See above.

Ordered proportional symbol

Use when there are big variations between values and/or seeing fine differences between data is not so important.

Dot strip plot

Dots placed in order on a strip are a space-efficient method of laying out ranks across multiple categories.

Distribution

Show values in a dataset and how often they occur. The shape (or 'skew') of a distribution can be a memorable way of highlighting the lack of uniformity or equality in the data.

Example FT uses
Income distribution, population (age/sex) distribution

Histogram

The standard way to show a statistical distribution - keep the gaps between columns small to highlight the 'shape' of the data.

Boxplot

Summarise multiple distributions by showing the median (centre) and range of the data

Violin plot

Similar to a box plot but more effective with complex distributions (data that cannot be summarised with simple average).

Population pyramid

A standard way for showing the age and sex breakdown of a population distribution; effectively, back to back histograms.

Dot strip plot

Good for showing individual values in a distribution, can be a problem when too many dots have the same value.

Dot plot

A simple way of showing the change or range (min/max) of data across multiple categories.

Barcode plot

Like dot strip plots, good for displaying all the data in a table,they work best when highlighting individual values.

Cumulative curve

A good way of showing how unequal a distribution is: y axis is always cumulative frequency, x axis is always a measure.

Change over Time

Give emphasis to changing trends. These can be short (intra-day) movements or extended series traversing decades or centuries: Choosing the correct time period is important to provide suitable context for the reader.

Example FT uses
Share price movements, economic time series

Line

The standard way to show a changing time series. If data are irregular, consider markers to represent data points.

Column

Columns work well for showing change over time - but usually best with only one series of data at a time.

Line + column

A good way of showing the relationship over time between an amount (columns) and a rate (line).

Stock price

Usually focused on day-to-day activity, these charts show opening/closing and hi/low points of each day.

Slope

Good for showing changing data as long as the data can be simplified into 2 or 3 points without missing a key part of story.

Area chart

Use with care – these are good at showing changes to total, but seeing change in components can be very difficult.

Fan chart (projections)

Use to show the uncertainty in future projections - usually this grows the further forward to projection.

Connected scatterplot

A good way of showing changing data for two variables whenever there is a relatively clear pattern of progression.

Calendar heatmap

A great way of showing temporal patterns (daily, weekly, monthly) – at the expense of showing precision in quantity.

Priestley timeline

Great when date and duration are key elements of the story in the data.

Circle timeline

Good for showing discrete values of varying size across multiple categories (eg earthquakes by contintent).

Seismogram

Another alternative to the circle timeline for showing series where there are big variations in the data.

Part-to-whole

Show how a single entity can be broken down into its component elements. If the reader's interest is solely in the size of the components, consider a magnitude-type chart instead.

Example FT uses
Fiscal budgets, company structures, national election results

Stacked column

A simple way of showing part-to-whole relationships but can be difficult to read with more than a few components.

Proportional stacked bar

A good way of showing the size and proportion of data at the same time – as long as the data are not too complicated.

Pie

A common way of showing part-to-whole data – but be aware that it's difficult to accurately compare the size of the segments.

Donut

Similar to a pie chart – but the centre can be a good way of making space to include more information about the data (eg. total).

Treemap

Use for hierarchical part-to-whole relationships; can be difficult to read when there are many small segments.

Voronoi

A way of turning points into areas – any point within each area is closer to the central point than any other centroid.

Sunburst

Another way of visualisaing hierarchical part-to-whole relationships. Use sparingly (if at all) for obvious reasons.

Arc

A hemicycle, often used for visualising political results in parliaments.

Gridplot

Good for showing % information, they work best when used on whole numbers and work well in multiple layout form.

Venn

Generally only used for schematic representation.

Waterfall

Can be useful for showing part-to-whole relationships where some of the components are negative.

Magnitude

Show size comparisons. These can be relative (just being able to see larger/bigger) or absolute (need to see fine differences). Usually these show a 'counted' number (for example, barrels, dollars or people) rather than a calculated rate or per cent.

Example FT uses
Commodity production, market capitalisation

Column

The standard way to compare the size of things. Must always start at 0 on the axis.

Bar

See above. Good when the data are not time series and labels have long category names.

Paired column

As per standard column but allows for multiple series. Can become tricky to read with more than 2 series.

Paired bar

See above.

Proportional stacked bar

A good way of showing the size and proportion of data at the same time – as long as the data are not too complicated.

Proportional symbol

Use when there are big variations between values and/or seeing fine differences between data is not so important.

Isotype (pictogram)

Excellent solution in some instances – use only with whole numbers (do not slice off an arm to represent a decimal).

Lollipop chart

Lollipop charts draw more attention to the data value than standard bar/column – does not HAVE to start at zero (but preferable).

Radar chart

A space-efficient way of showing value pf multiple variables– but make sure they are organised in a way that makes sense to reader.

Parallel coordinates

An alternative to radar charts – again, the arrngement of the variables is important. Usually benefits from highlighting values.

Spatial

Used only when precise locations or geographical patterns in data are more important to the reader than anything else.

Example FT uses
Locator maps, population density, natural resource locations, natural disaster risk/impact, catchment areas, variation in election results

Basic choropleth (rate/ratio)

The standard approach for putting data on a map – should always be rates rather than totals and use a sensible base geography.

Proportional symbol (count/magnitde)

Use for totals rather than rates – be wary that small differences in data will be hard to see.

Flow map

For showing unambiguous movement across a map.

Contour map

For showing areas of equal value on a map. Can use deviation colour schemes for showing +/- values

Equalised cartogram

Converting each unit on a map to a regular and equally-sized shape – good for representing voting regions with equal value.

Scaled cartogram (value)

Stretching and shrinking a map so that each area is sized according to a particular value.

Dot density

Used to show the location of individual events/locations – make sure to annotate any patterns the reader should see.

Heat map

Grid-based data values mapped with an intensity colour scale. As choropleth map – but not snapped to an admin/political unit.

Flow

Show the reader volumes or intensity of movement between two or more states or conditions. These might be logical sequences or geographical locations.

Example FT uses
Movement of funds, trade, migrants, lawsuits, information; relationship graphs.

Sankey

Shows changes in flows from one condition to at least one other; good for tracing the eventual outcome of a complex process.

Waterfall

Designed to show the sequencing of data through a flow process, typically budgets. Can include +/- components.

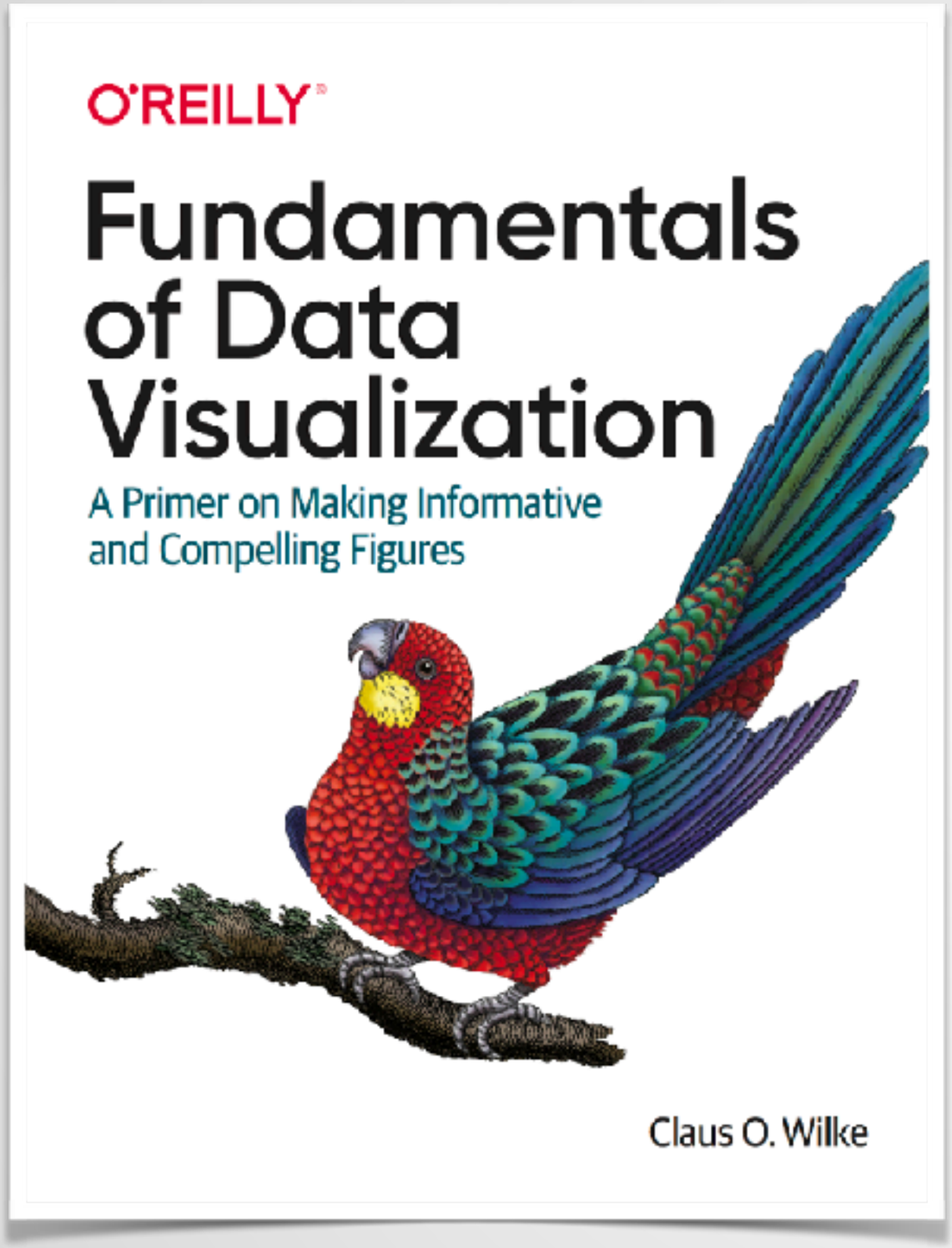
Chord

A complex but powerful diagram which can illustrate 2-way flows (and net winner) in a matrix.

Network

Used for showing the strength and inter-connectdness of relationships of varying types.

ft.com/vocabulary



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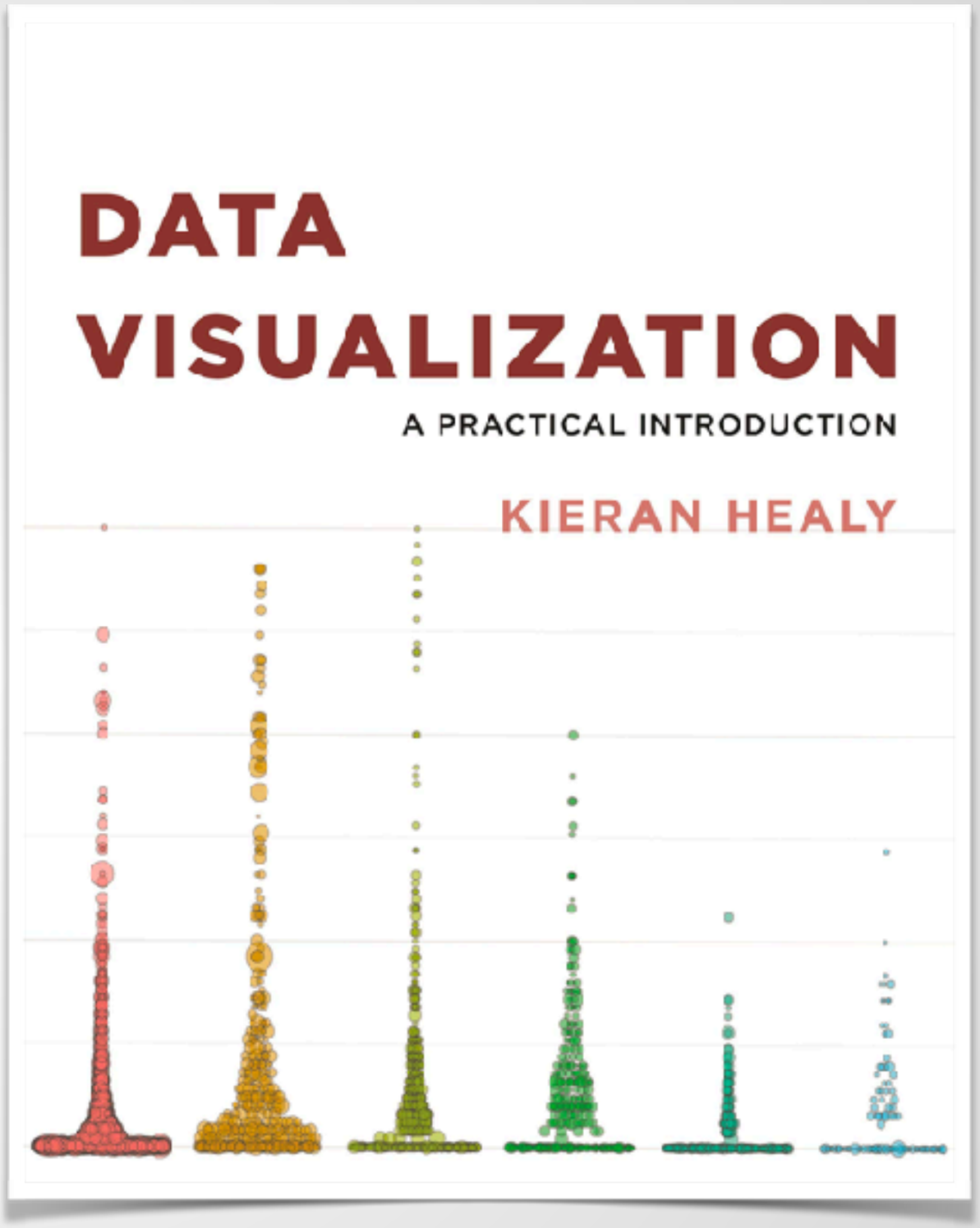

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