Baptiste Auguié

~ presents ~

Here Be Dragons

Unexpected Journey Through The Land Of Graphics

MY GOAL: challenge us
to think differently
about 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, 1983

MOTIVATION • A NEW MEDIUM

(SOME ILLUSTRATIONS)

`worrydream.com/TenBrighterIdeas/`

`jasondavies.com/maps/transition/`

`mbostock.github.io/d3/talk/20111116/#17`

OUTLINE

- **A PHILOSOPHY OF GRAPHICS**
  - *The good, the bad, and the ugly*
  - *Tips and guidelines*
- **A GRAMMAR OF GRAPHICS**
  - *Elements of theory*
  - *Glimpse of the future*
- **A VISION FOR GRAPHICS**
  - *Aesthetics and impact*
  - *TOC figures, slides, posters*

Tools don't matter

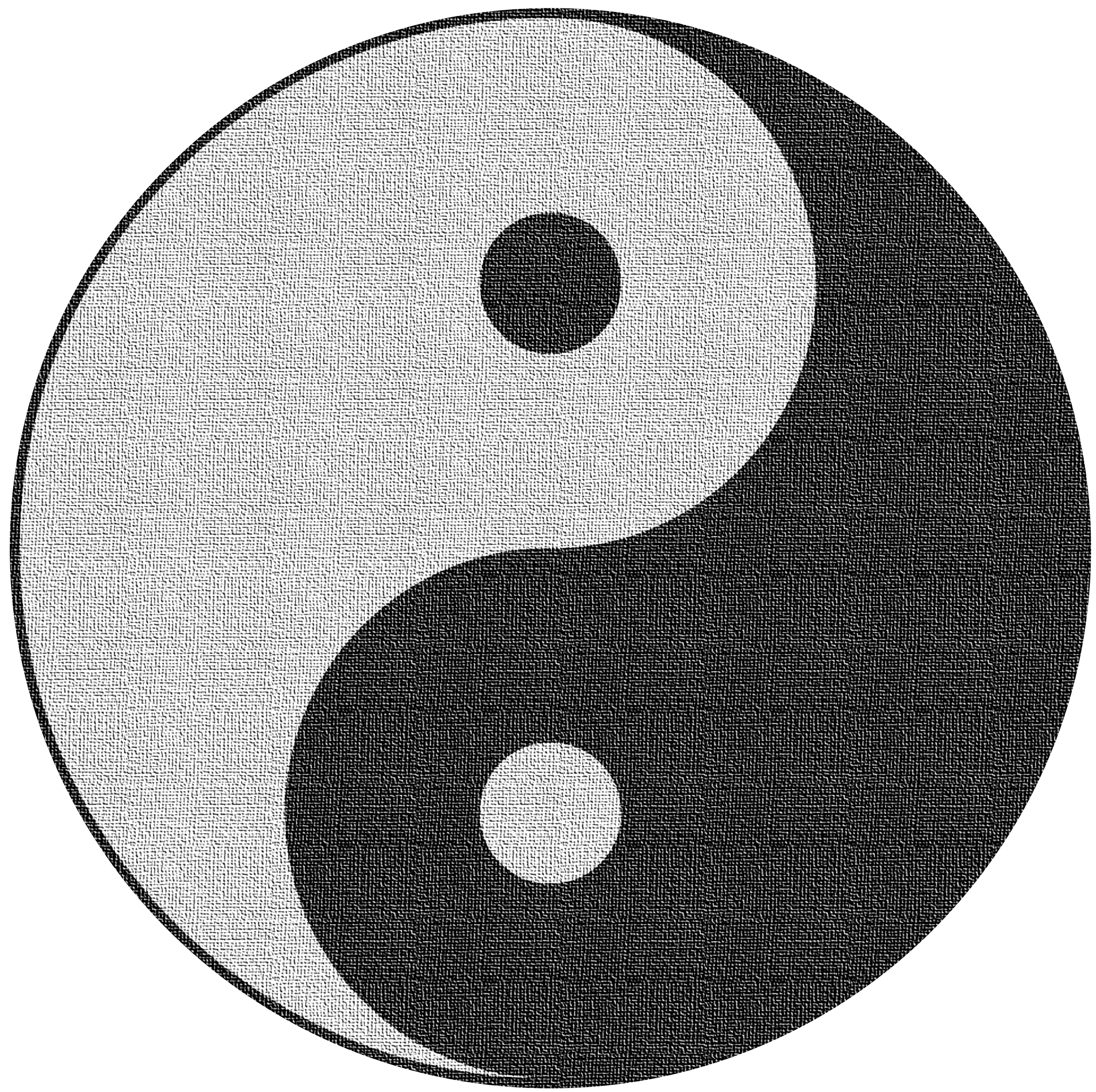
(but they do)

Tatsuo Horiuchi

Excel artist

Part I • A philosophy of graphics

Analytic

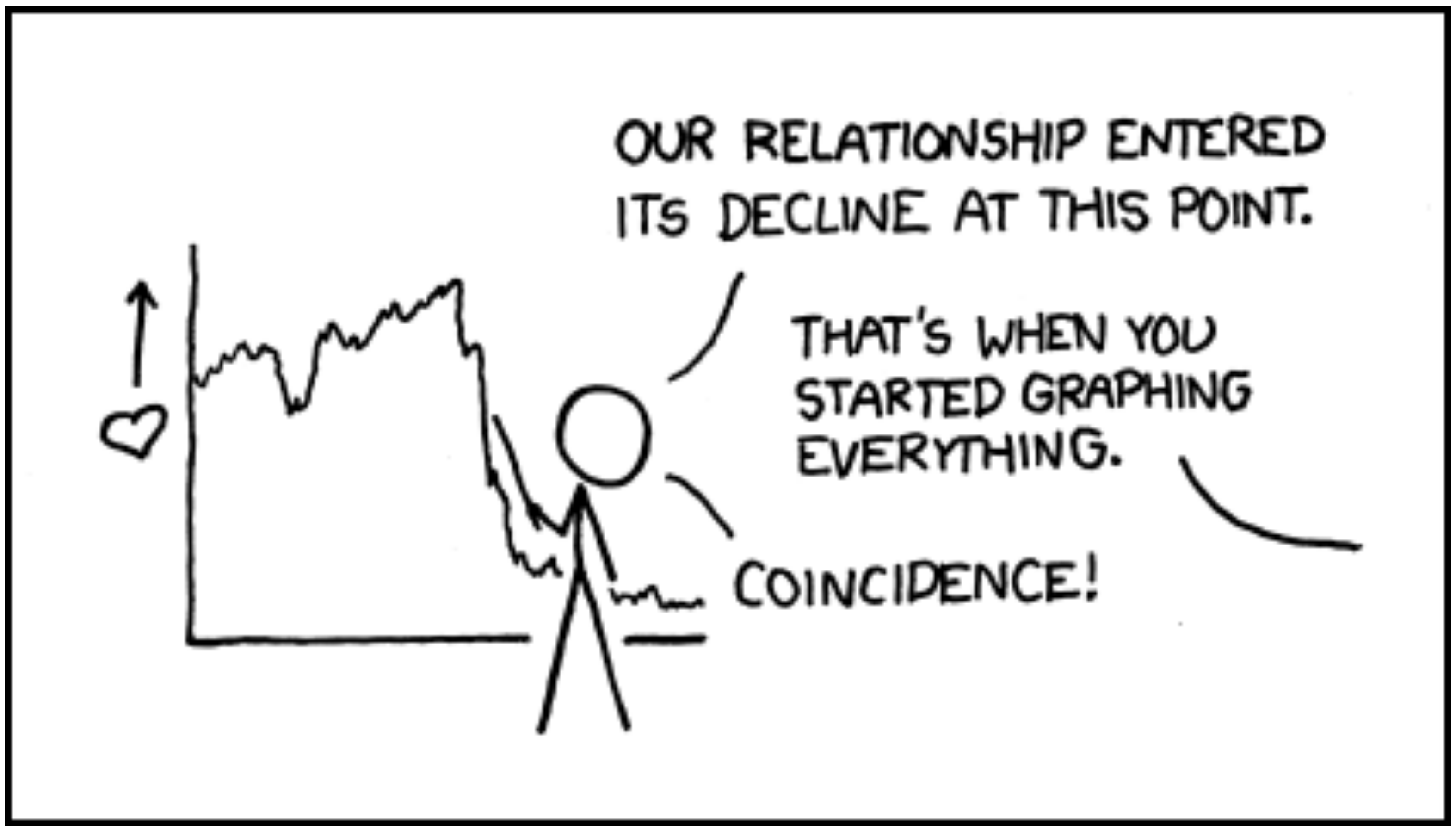


Visual

Clarity:

data-to-ink ratio

Graph all the things?



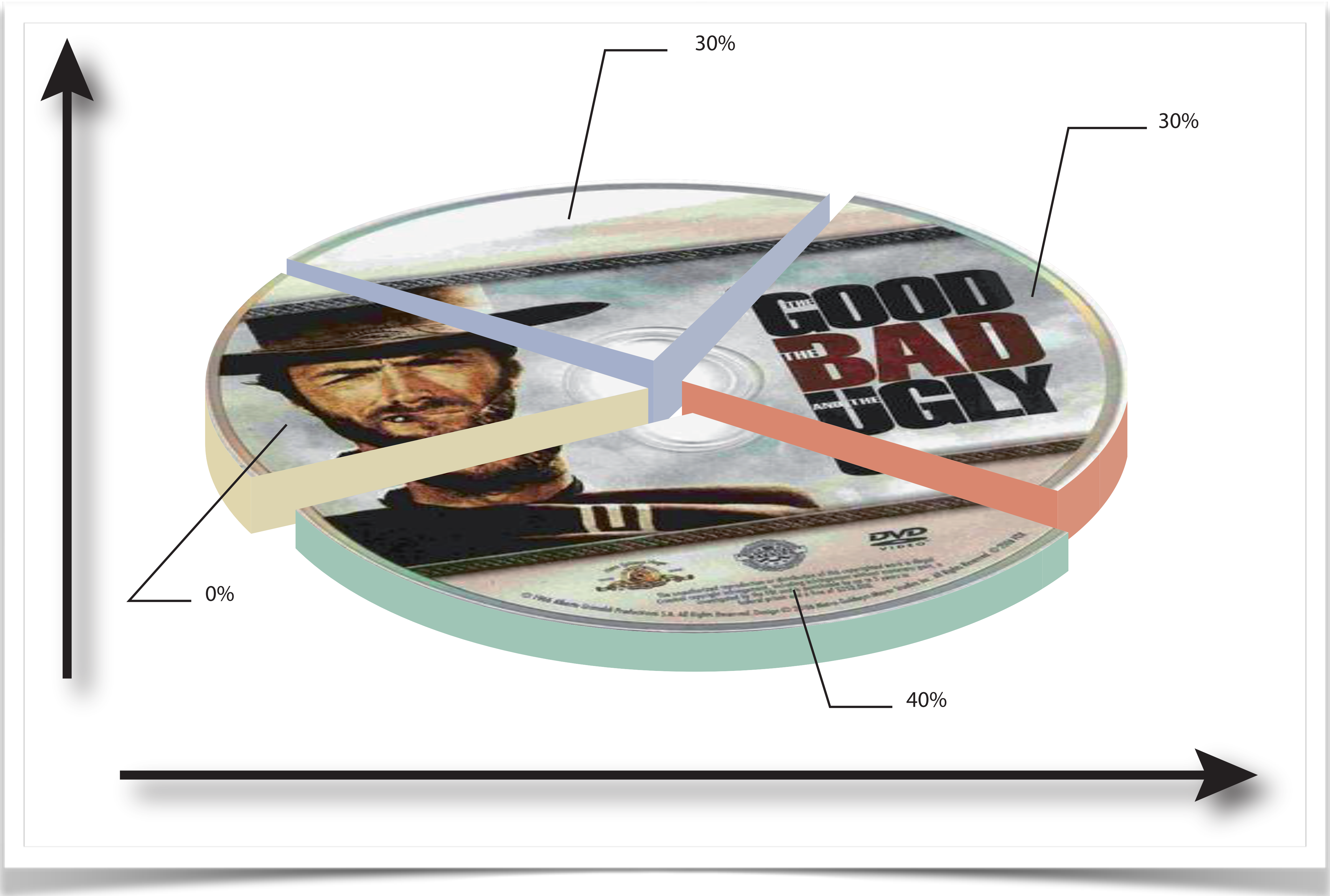
xkcd.com

Consider a table

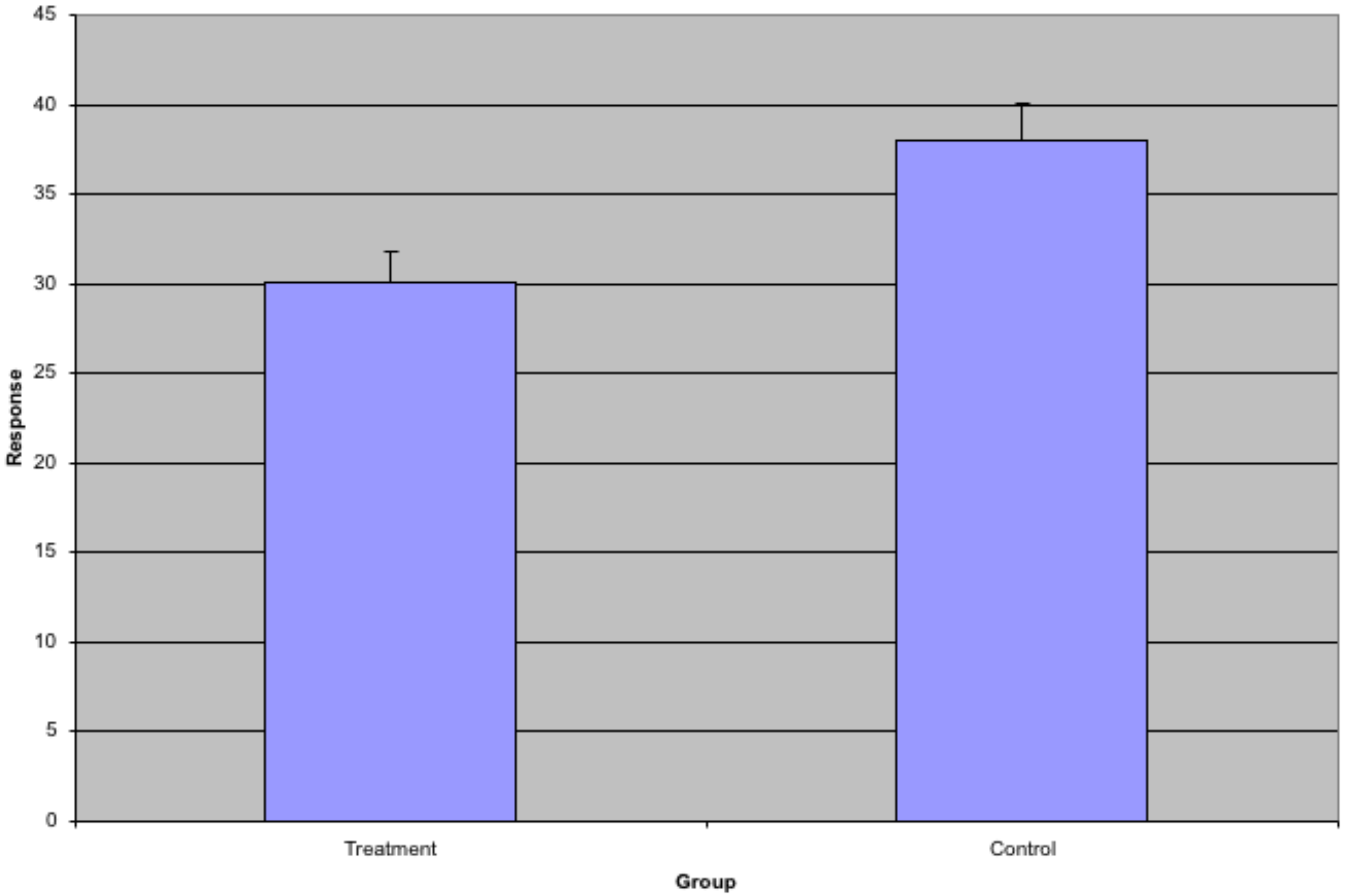
n	Arbitrary precision	Double precision
1	$(1.351522998772148 + 0.002682327826796i)$	$(1.351522998772154 + 0.002682327826791i)$
2	$(0.09475820788633184 + 0.006563919284008 84i)$	$(0.09475820788633782 + 0.006563919284008 89i)$
3	$(3.267511781081814 + 0.354044762711458i) \times 10^{-3}$	$(3.267511780908656 + 0.354044762723604i) \times 10^{-3}$
4	$(8.234338861126748 + 1.361708455386841i) \times 10^{-5}$	$(8.234338230741085 + 1.361708446137377i) \times 10^{-5}$
5	$(15.30077682100172 + 3.20759658015824i) \times 10^{-7}$	$(15.30004712362165 + 3.2074636639992i) \times 10^{-7}$
6	$(23.34600724021963 + 6.186419274080092i) \times 10^{-9}$	$(25.42872582340277 + 5.90596678628629i) \times 10^{-9}$
7	$(29.40892160067281 + 9.22544630049269i) \times 10^{-11}$	$(24.3107199444863 - 1.13271331394081i) \times 10^{-8}$
8	$(3.204531139340317 + 1.186184482330857i) \times 10^{-12}$	$(177.439991438448 - 2.0214735003898i) \times 10^{-7}$
9	$(3.038290261597983 + 1.287101819776947i) \times 10^{-14}$	$(67.0727643316326 + 1.57033685336724i) \times 10^{-5}$
10	$(2.5674093425467 + 1.240871523988642i) \times 10^{-16}$	$-0.03959069252015016 + 0.0007187691660 2068i$
11	$(1.94474203713492 + 1.055179886196251i) \times 10^{-18}$	$-10.11371972337842 - 0.1392559656 7256i$
12	$(13.38699265450917 + 8.13464528498008i) \times 10^{-21}$	$-1132.655389072814 + 0.299642890755i$
13	$(8.417729528036757 + 5.677389217679542i) \times 10^{-23}$	$(-86.48807724977711 + 1.50271433683522i) \times 10^{3}$
14	$(4.876046808254036 + 3.644961564953527i) \times 10^{-25}$	$(-29.88742021522111 + 6.65835422187729i) \times 10^{5}$
15	$(2.613375843631903 + 2.154801883308382i) \times 10^{-27}$	$(34.54711402938201 + 8.19472138834448i) \times 10^{7}$
16	$(1.303141351977849 + 1.184738044986223i) \times 10^{-29}$	$(45.78317881557951 + 9.731545021815603i) \times 10^{9}$
17	$(6.067251546625191 + 6.069699524562945i) \times 10^{-32}$	$(-3.816711620949946 + 1.082670199384622i) \times 10^{12}$
18	$(2.647391356803932 + 2.916878553003213i) \times 10^{-34}$	$(-154.3422495126499 + 7.8521375375244i) \times 10^{13}$
19	$(1.085651390657799 + 1.317672507647534i) \times 10^{-36}$	$(-166.490936601337536 - 1.779710476225576i) \times 10^{15}$
20	$(4.194570626830792 + 5.621507702515121i) \times 10^{-39}$	$(21.346348083272847360 - 1.199678065337379840i) \times 10^{18}$
21	$(1.530005420781641 + 2.269669591435182i) \times 10^{-41}$	$(100.285925474474 - 3.244785438691i) \times 10^{20}$

h:	$x_{\max}$:	0.01	0.1	1	2	3	4	5	6	7	8	10	12	15	20	25	30	40	50	60	70	80
	N	5	5	7	9	11	11	13	15	17	17	21	23	27	35	41	47	63	77	95	127	111
1.1	N_θ	6	6	6	7	7	8	8	9	9	10	15	15	15	20	25	35	40	40	80	80	1200
	error	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	10^{-12}	10^{-11}	10^{-9}	10^{-7}	10^{-4}
	N	5	5	9	11	11	13	15	15	19	19	23	27	31	37	45	53	69	93	115		
1.3	N_θ	9	9	9	9	9	10	15	15	15	15	15	20	20	25	45	30	50	45	500		
	error	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	10^{-12}	10^{-9}	10^{-7}	10^{-3}		
	N	5	7	11	13	15	15	19	19	21	23	25	27	33	41	49	61	75	103			
2	N_θ	20	20	20	20	20	20	20	20	25	25	25	25	30	35	45	35	50	45			
	error	–	–	–	–	–	–	–	–	–	–	–	–	–	–	10^{-12}	10^{-11}	10^{-7}	10^{-4}			
	N	5	7	11	15	17	19	21	23	23	25	29	31	35	45	51	57	59				
4	N_θ	40	40	40	40	40	7	40	45	45	45	50	50	60	70	70	90	90				
	error	–	–	–	–	–	10^{-3}	–	–	–	–	–	–	–	10^{-13}	10^{-11}	10^{-9}	10^{-4}				
	N	5	7	11	15	19	19	19	23	25	27	31	35	37	41	47	47					
7	N_θ	70	70	70	70	70	70	80	80	80	80	90	90	100	200	130	130					
	error	–	–	–	–	–	–	–	–	–	–	–	–	–	10^{-11}	10^{-10}	10^{-6}					
	N	5	7	13	15	19	19	21	25	27	27	31	33	41	45	43	47					
10	N_θ	100	100	90	100	100	100	110	110	110	120	120	130	140	180	180	200					
	error	–	–	–	–	–	–	–	–	–	–	–	–	–	10^{-11}	10^{-8}	10^{-6}					
	N	5	7	13	15	19	21	23	23	27	29	33	37	43	43	49	41					
20	N_θ	200	200	200	200	200	200	200	220	220	240	260	260	280	300	550	400					
	error	–	–	–	–	–	–	–	–	–	–	–	–	–	10^{-12}	10^{-8}	10^{-4}					
	N	5	7	13	17	19	21	23	25	27	29	33	35	39	45	47	45					
50	N_θ	500	500	500	500	500	500	550	550	550	600	650	800	700	1100	900	1200					
	error	–	–	–	–	–	–	–	–	–	–	–	–	10^{-13}	10^{-12}	10^{-9}	10^{-6}					
	N	5	7	13	17	19	21	23	25	27	27	33	35	47	53	47						
100	N_θ	1000	1100	1000	1100	1000	1100	1100	1100	1100	1100	1300	1500	1400	1600	2000						
	error	–	–	–	–	–	–	–	–	–	–	–	–	–	–	10^{-9}						

The good, the bad, and the ugly

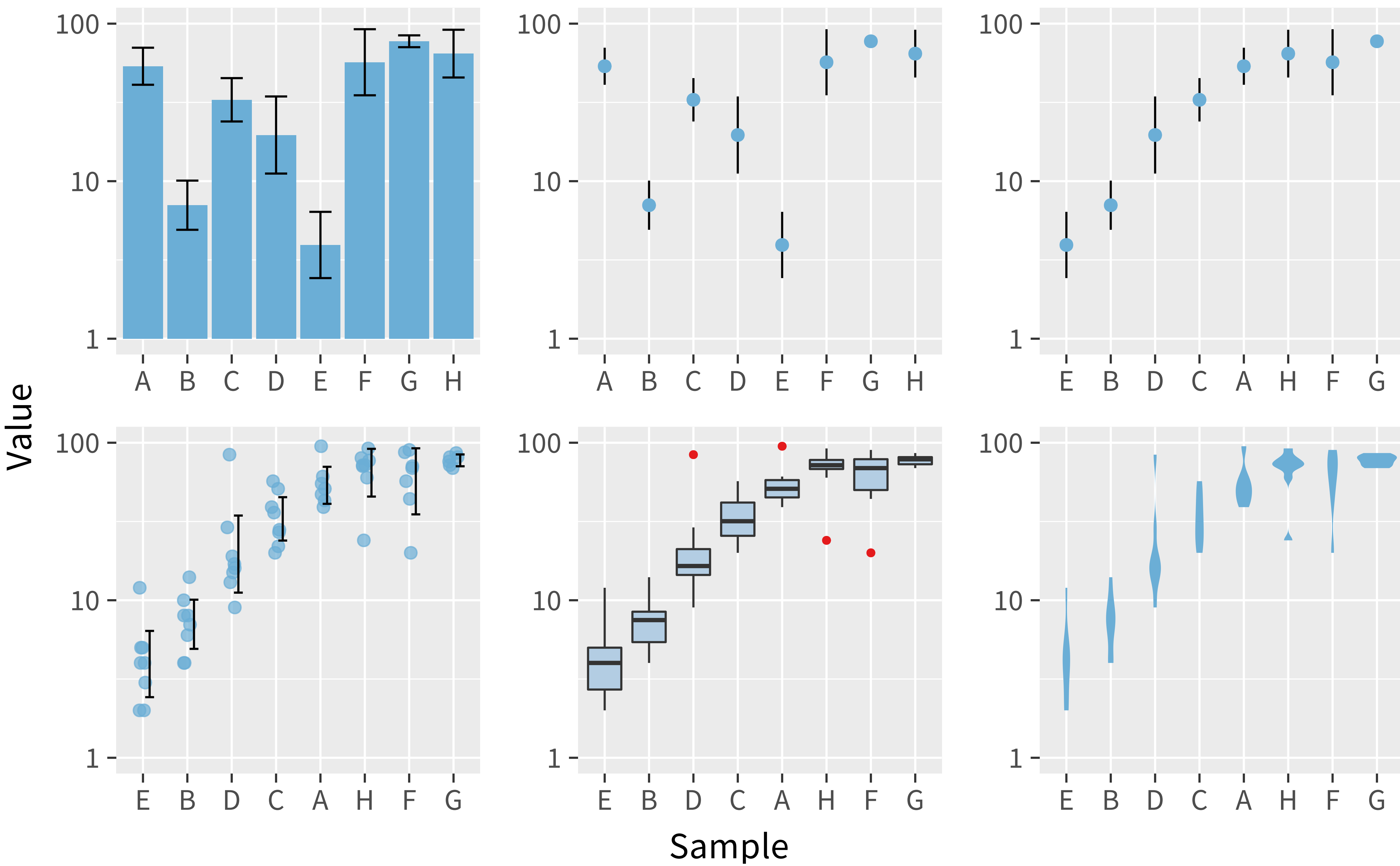


Dynamite plot

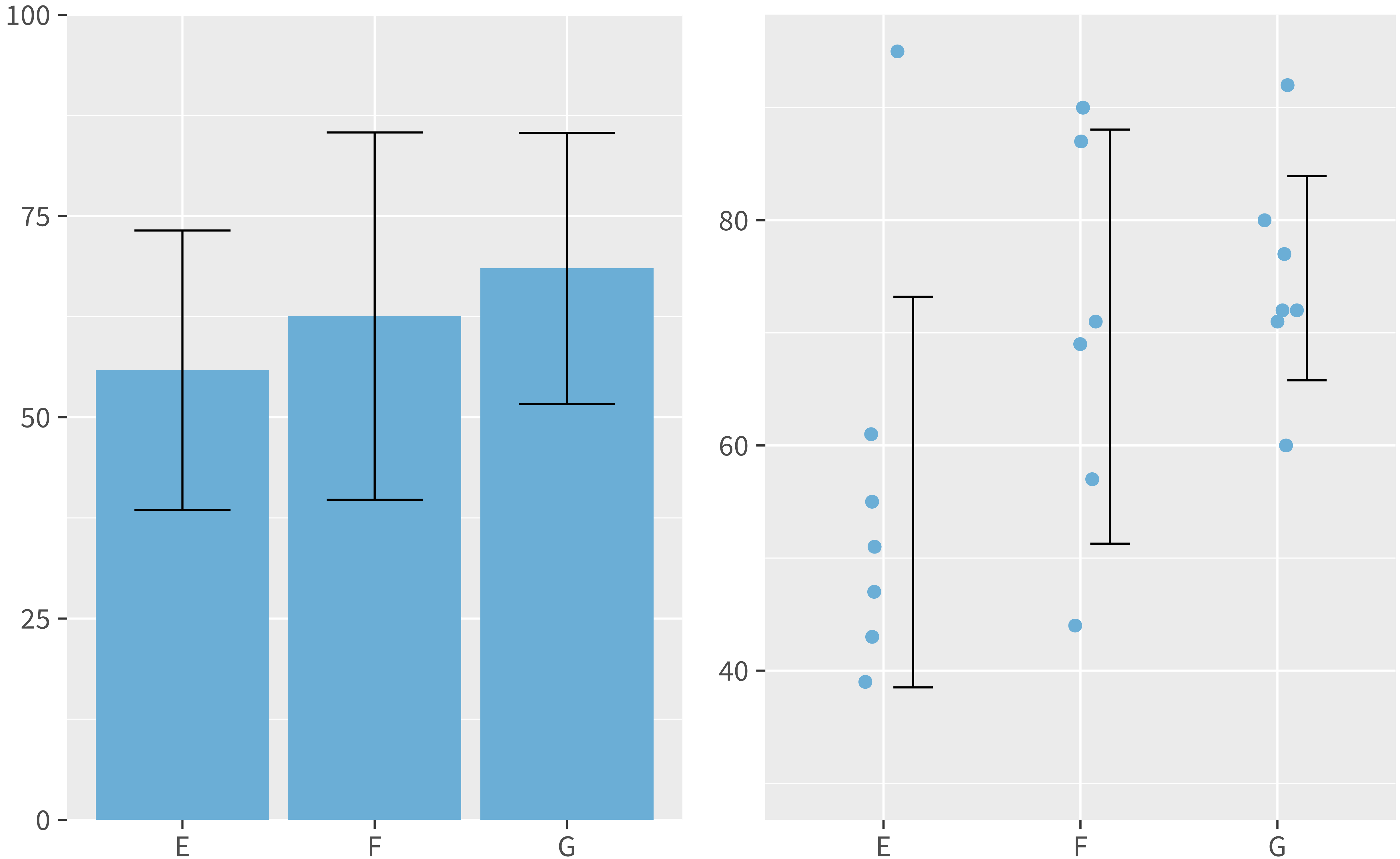


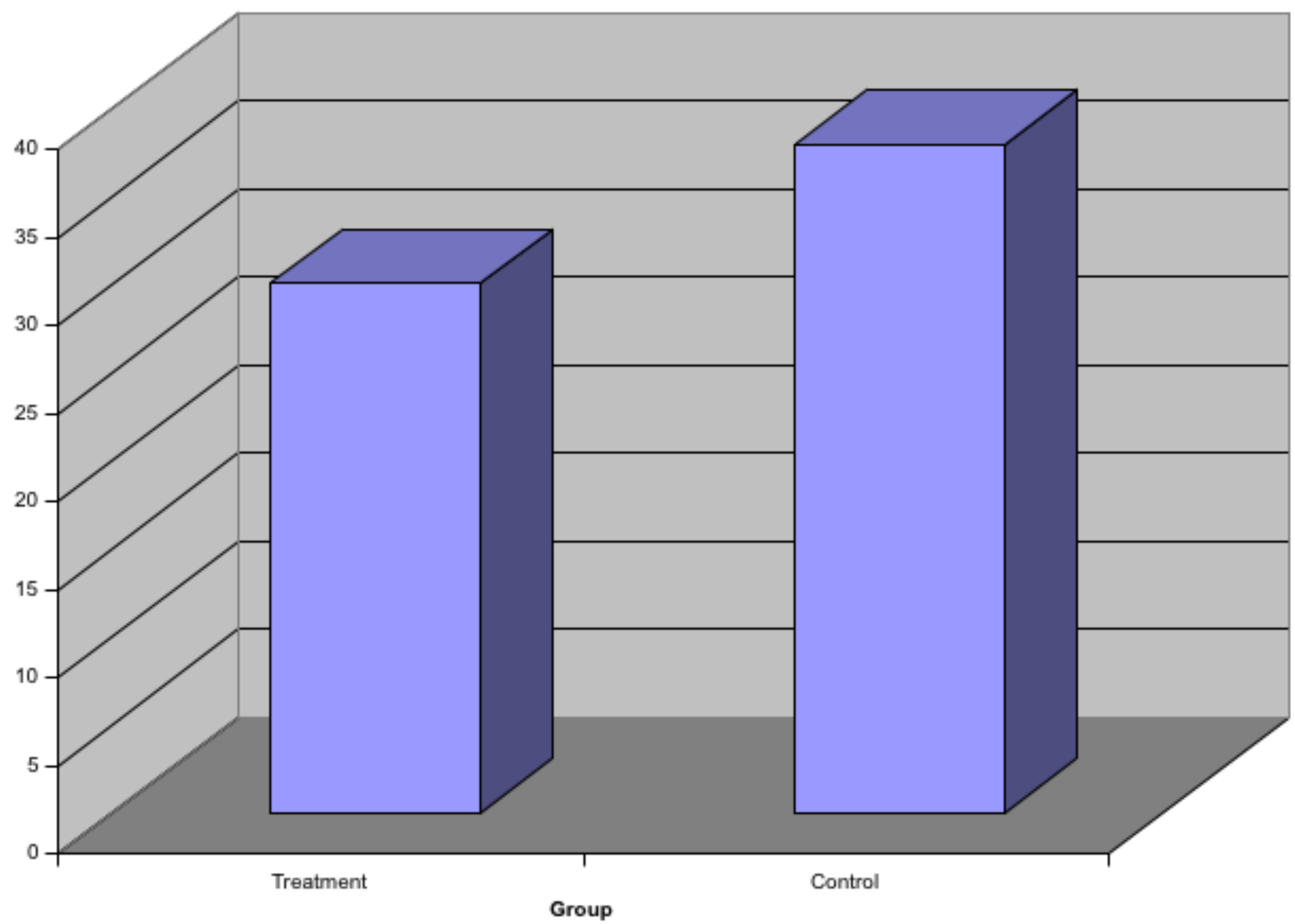
emdbolker.wikidot.com/blog:dynamite

Barplot alternatives: dot plot, boxplot



Always include 0?




40
35
30
25
20
15
10
5
0
Treatment
Control
Group

NATURE PHOTONICS DOI: 10.1038/NPHOTON.2012.300

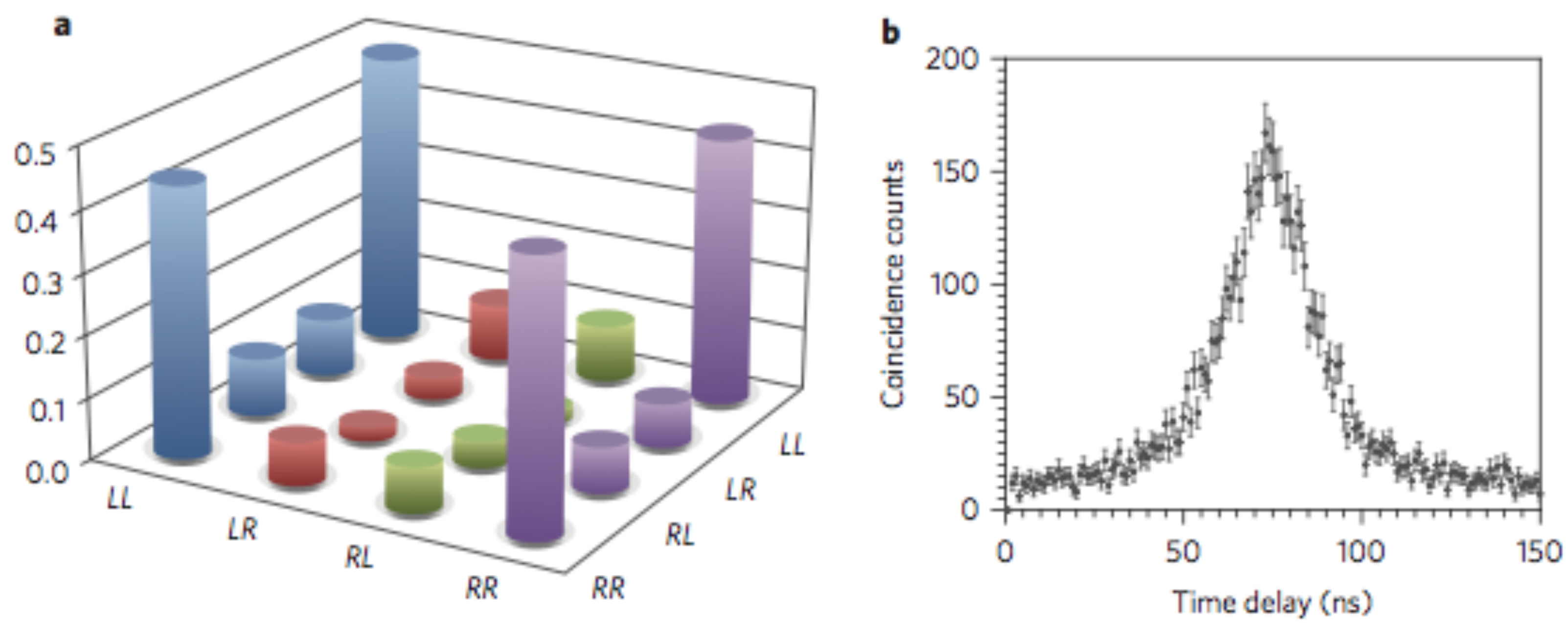
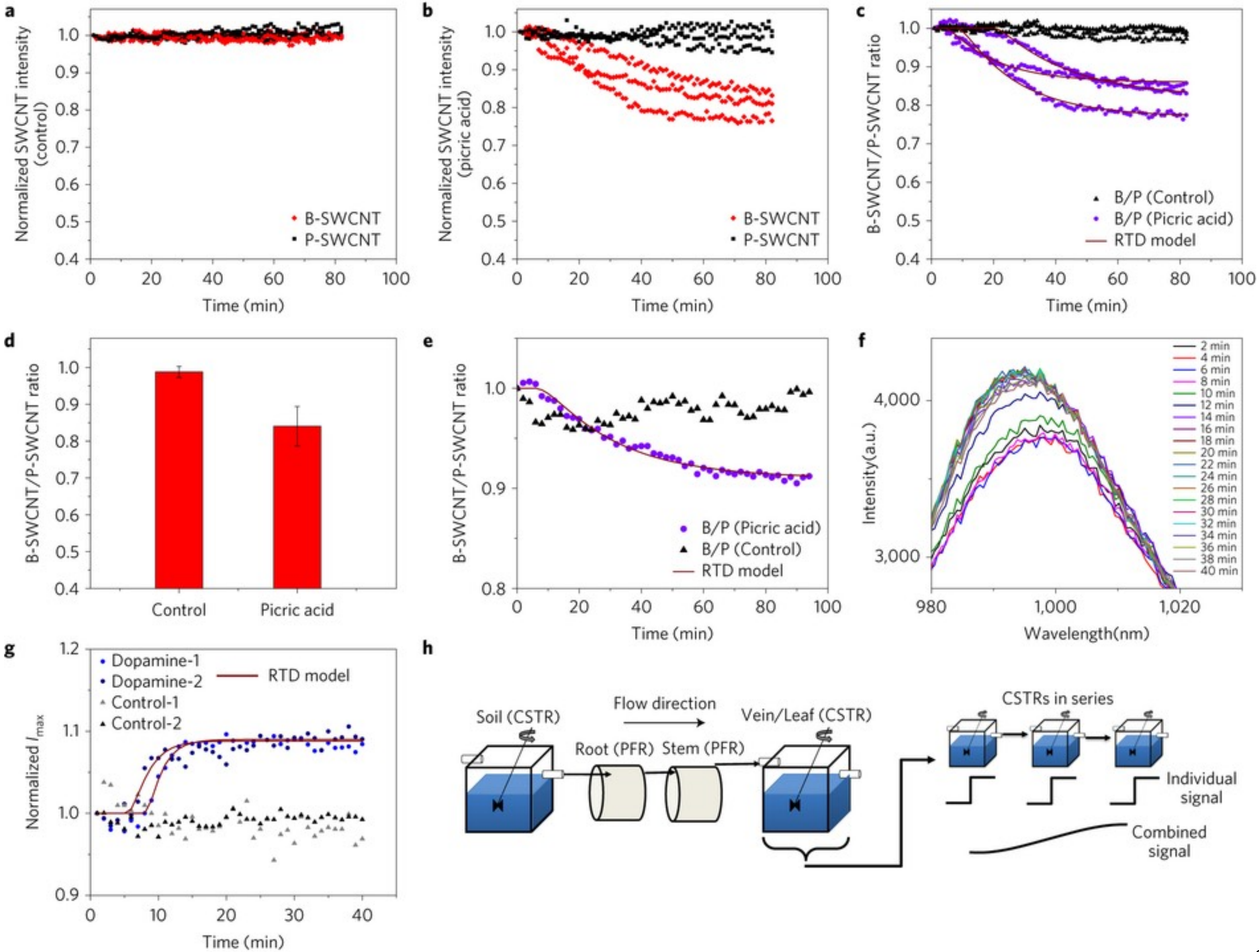
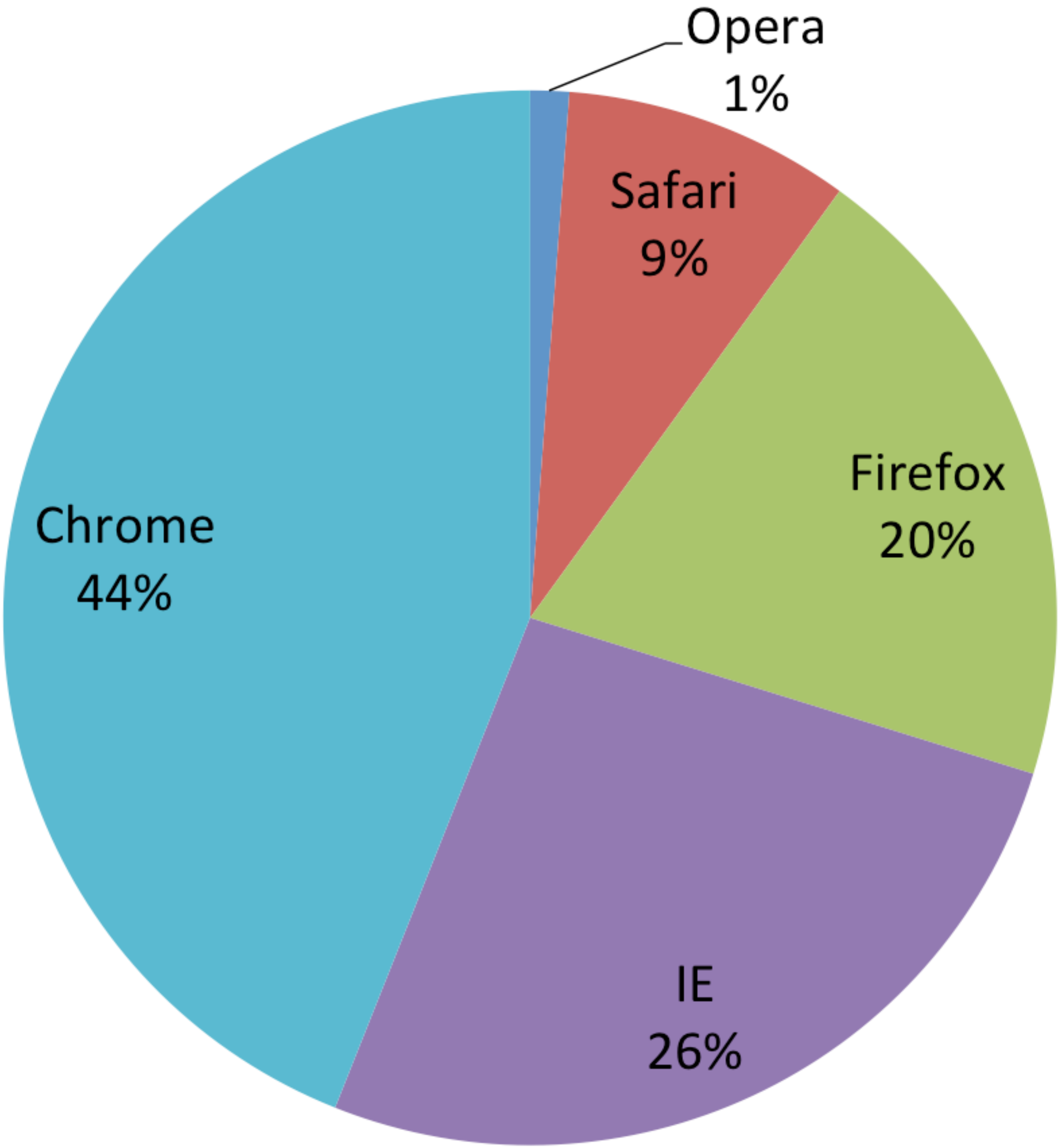


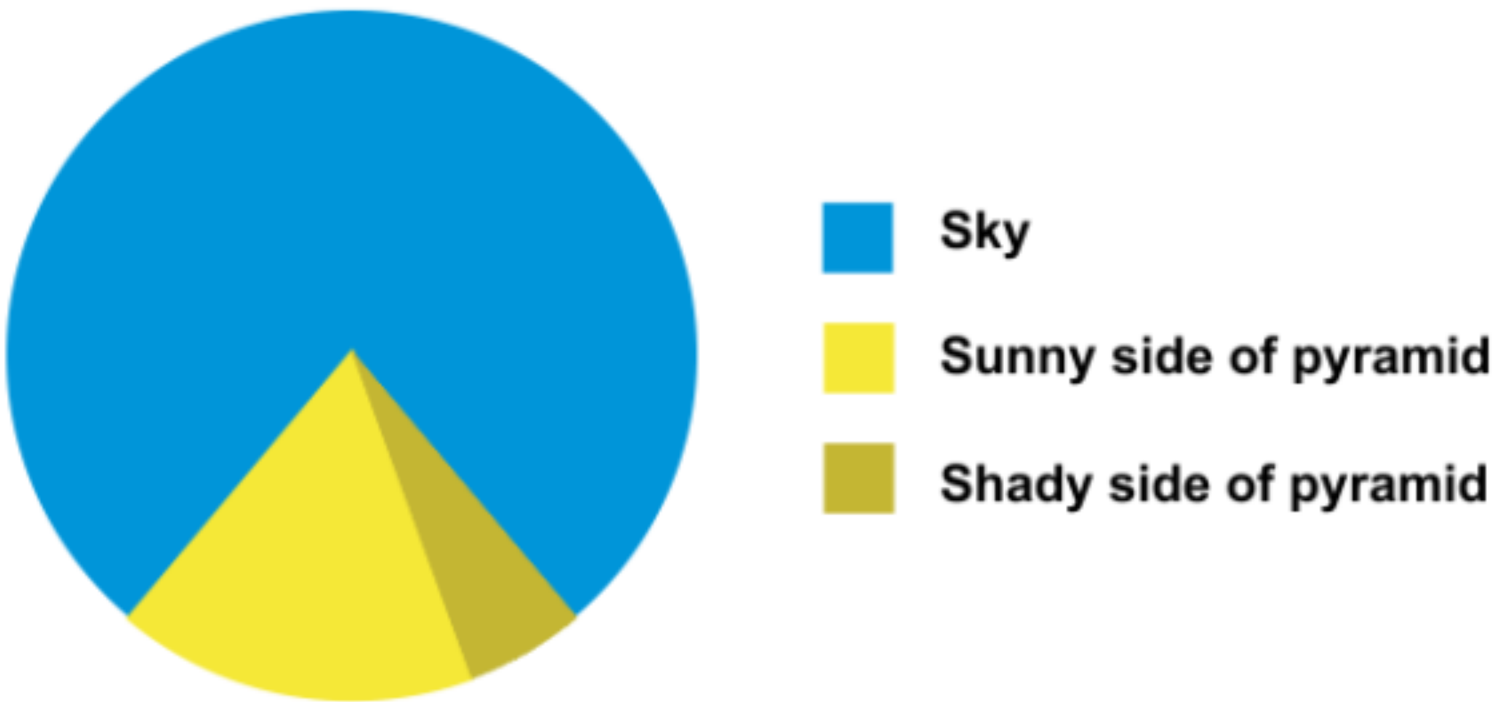
Figure 3 | NOON state characterization. a, Density matrix ρ (magnitudes only) from quantum state tomography, showing large coherence between $|LL\rangle$ and $|RR\rangle$ components. **b**, Measured correlation of the filtered CESPDC pairs (no background subtracted). The absence of modulation at the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

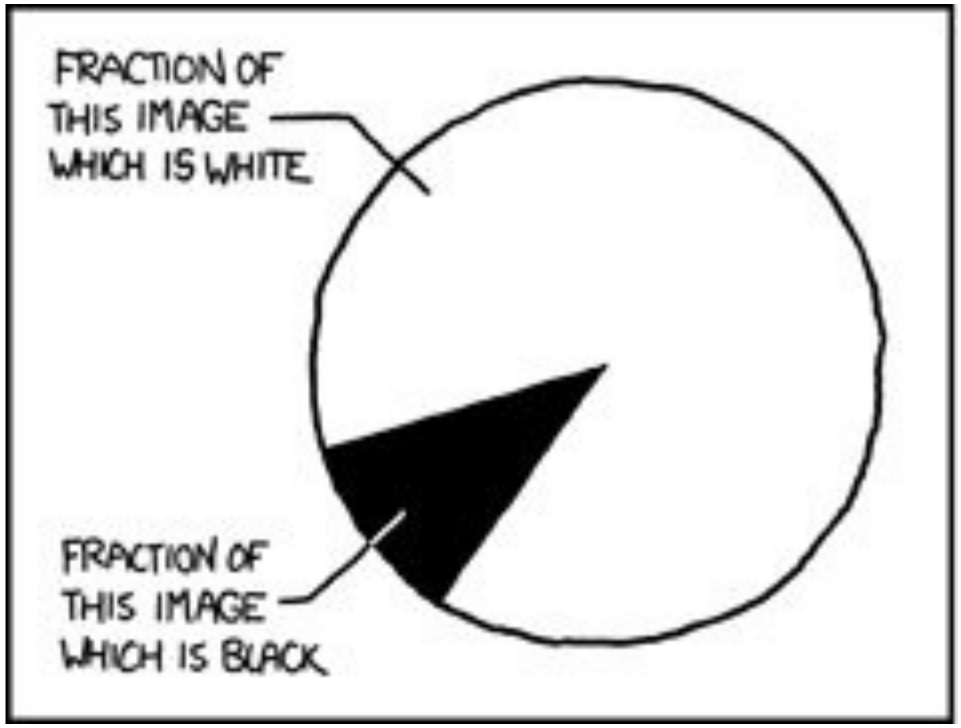


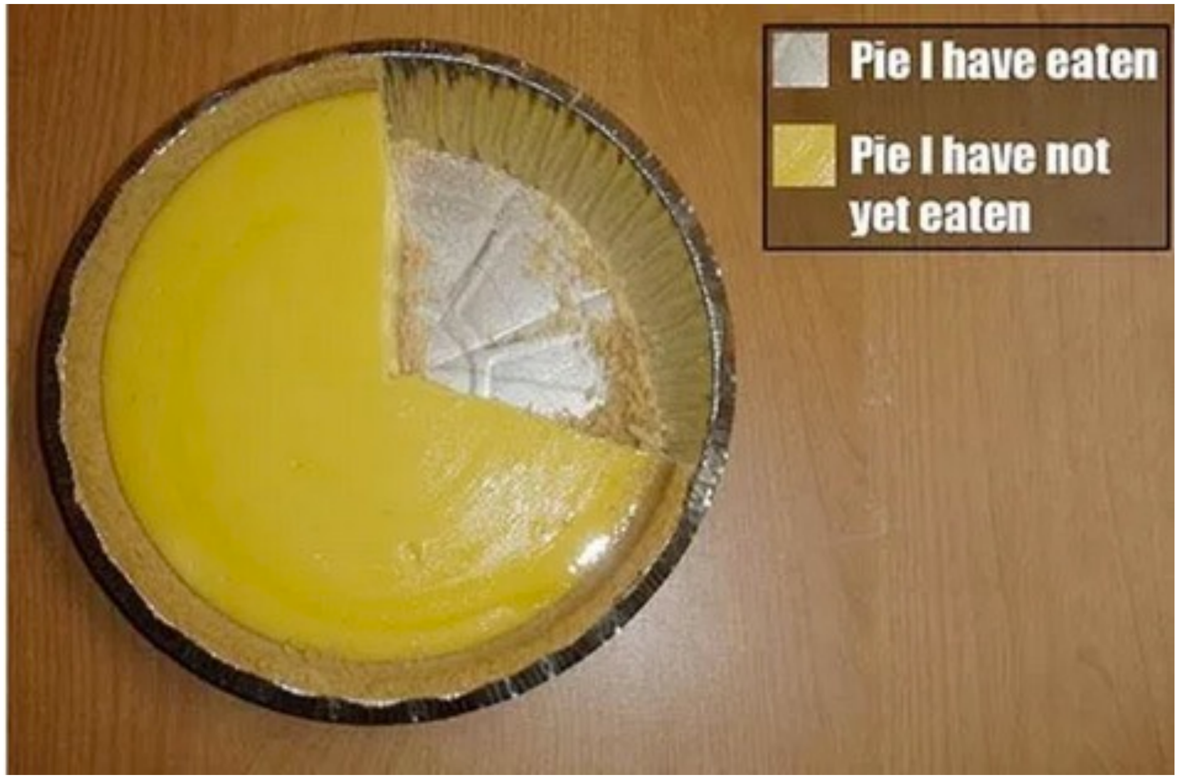
a
Normalized SWCNT intensity (control)
B-SWCNT
P-SWCNT
Time (min)
b
Normalized SWCNT intensity (picric acid)
B-SWCNT
P-SWCNT
Time (min)
c
B-SWCNT/P-SWCNT ratio
B/P (Control)
B/P (Picric acid)
RTD model
Time (min)
d
B-SWCNT/P-SWCNT ratio
Control
Picric acid
e
B-SWCNT/P-SWCNT ratio
B/P (Picric acid)
B/P (Control)
RTD model
Time (min)
f
Intensity(a.u.)
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}
Dopamine-1
Dopamine-2
Control-1
Control-2
RTD model
Time (min)
h
Soil (CSTR)
Flow direction
Root (PFR)
Stem (PFR)
Vein/Leaf (CSTR)
CSTRs in series
Individual signal
Combined signal

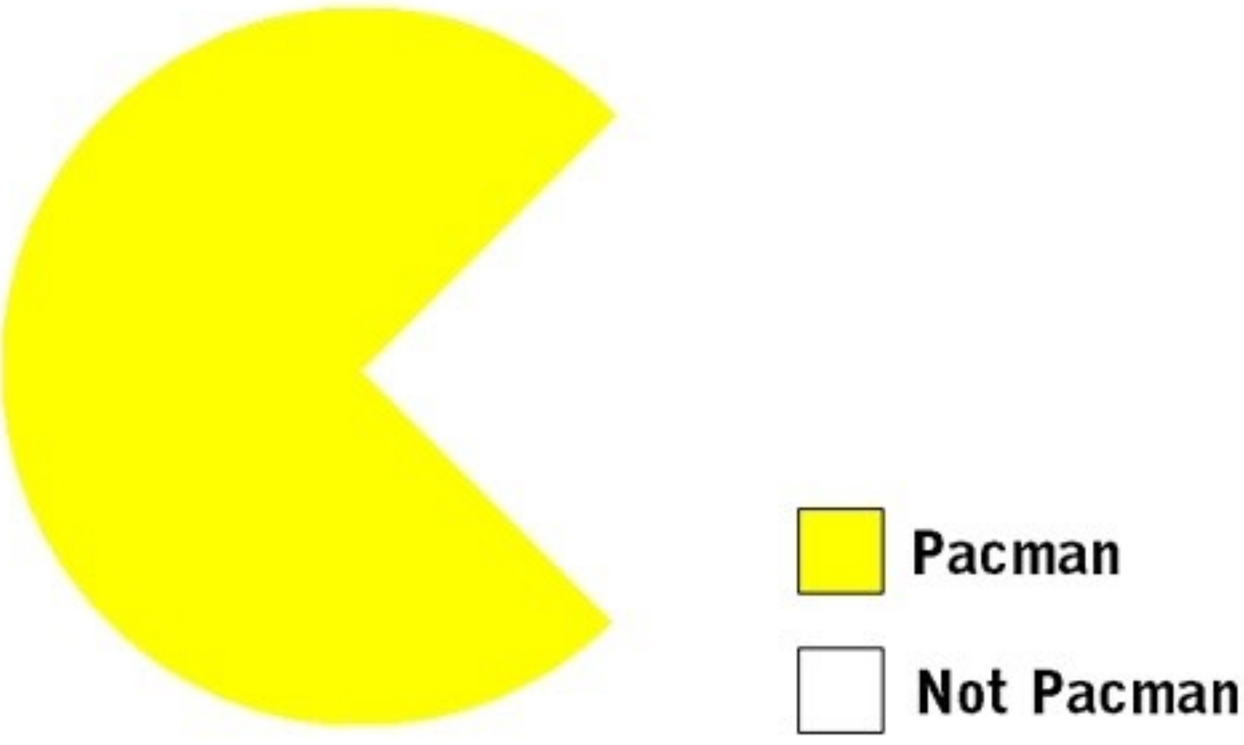

Opera
1%
Safari
9%
Firefox
20%
Chrome
44%
IE
26%

PIE CHARTS – LIMITED USE

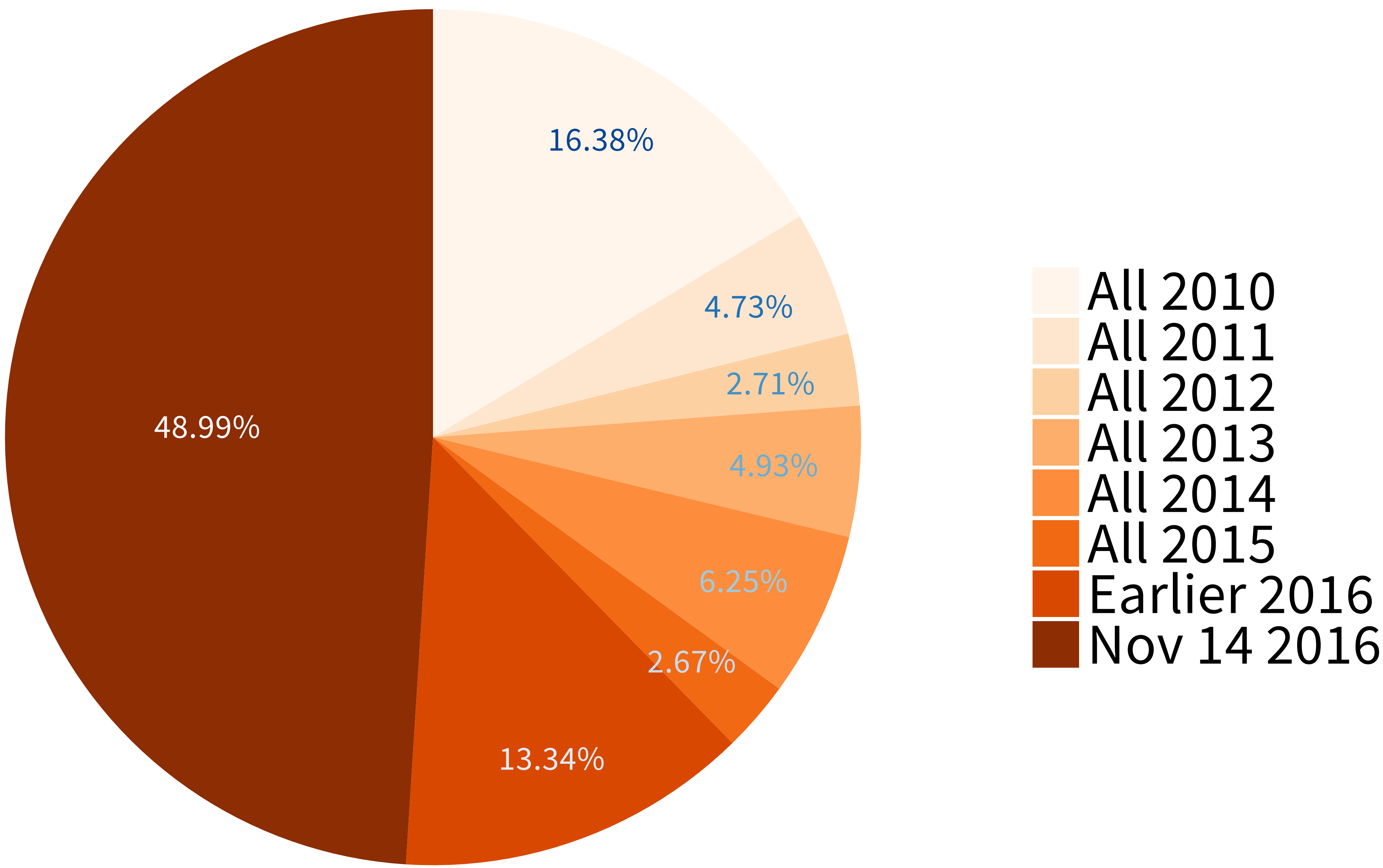




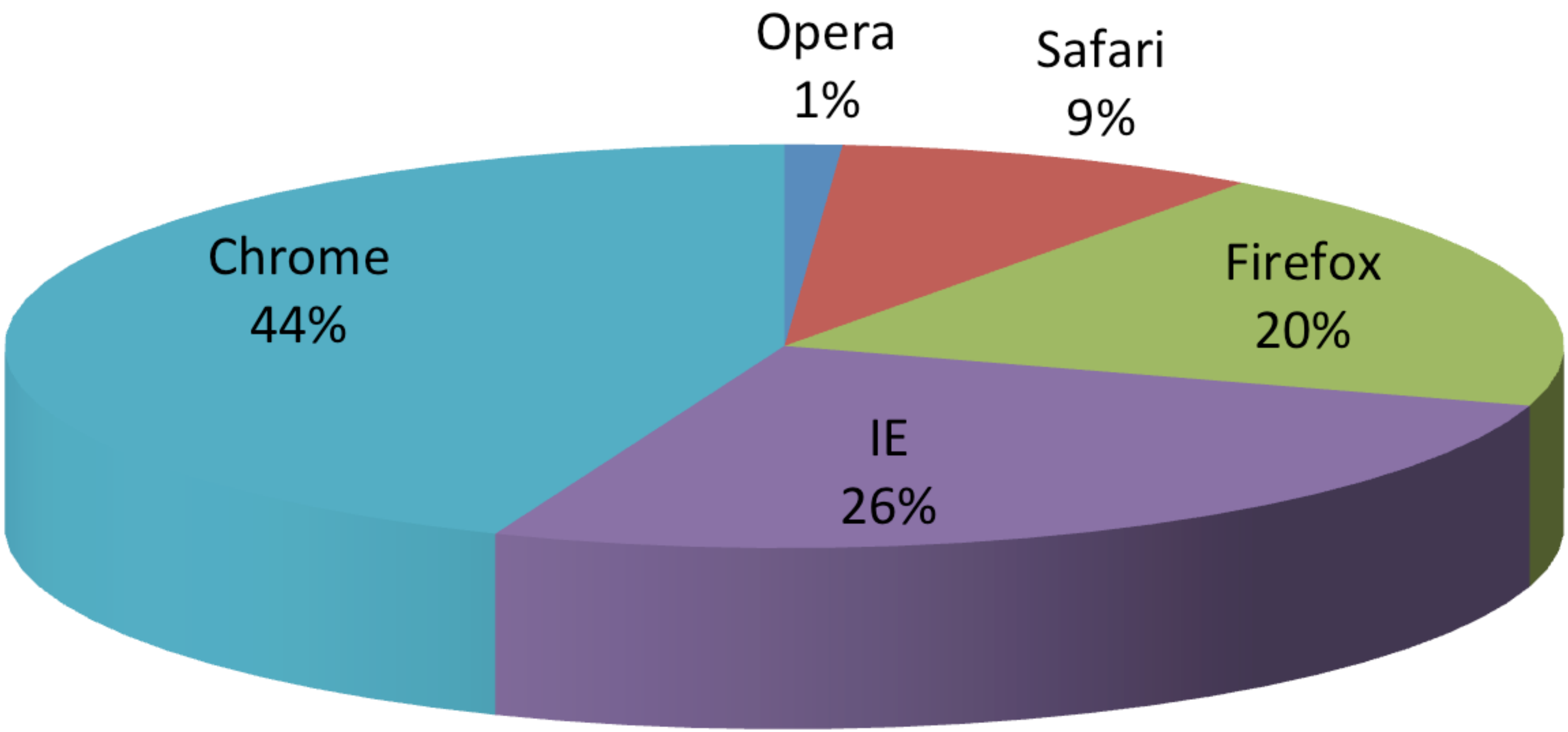


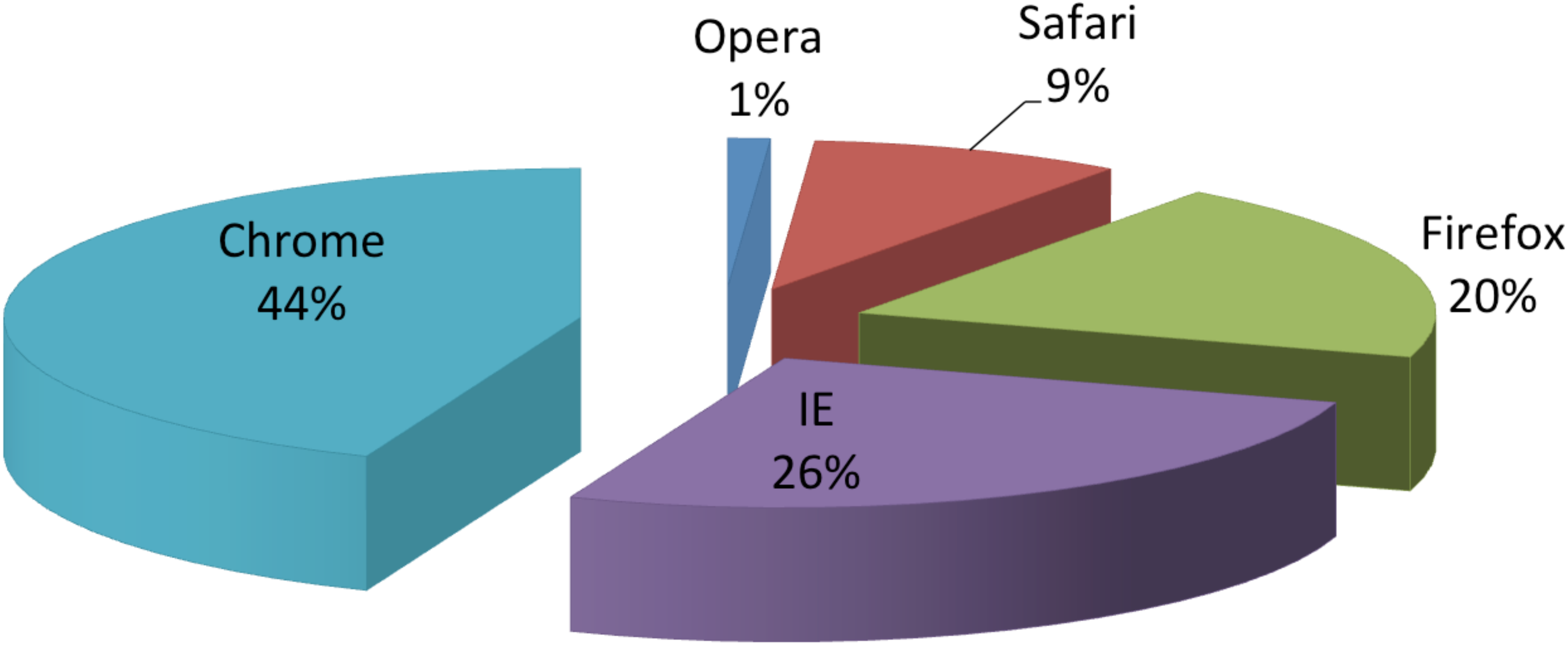


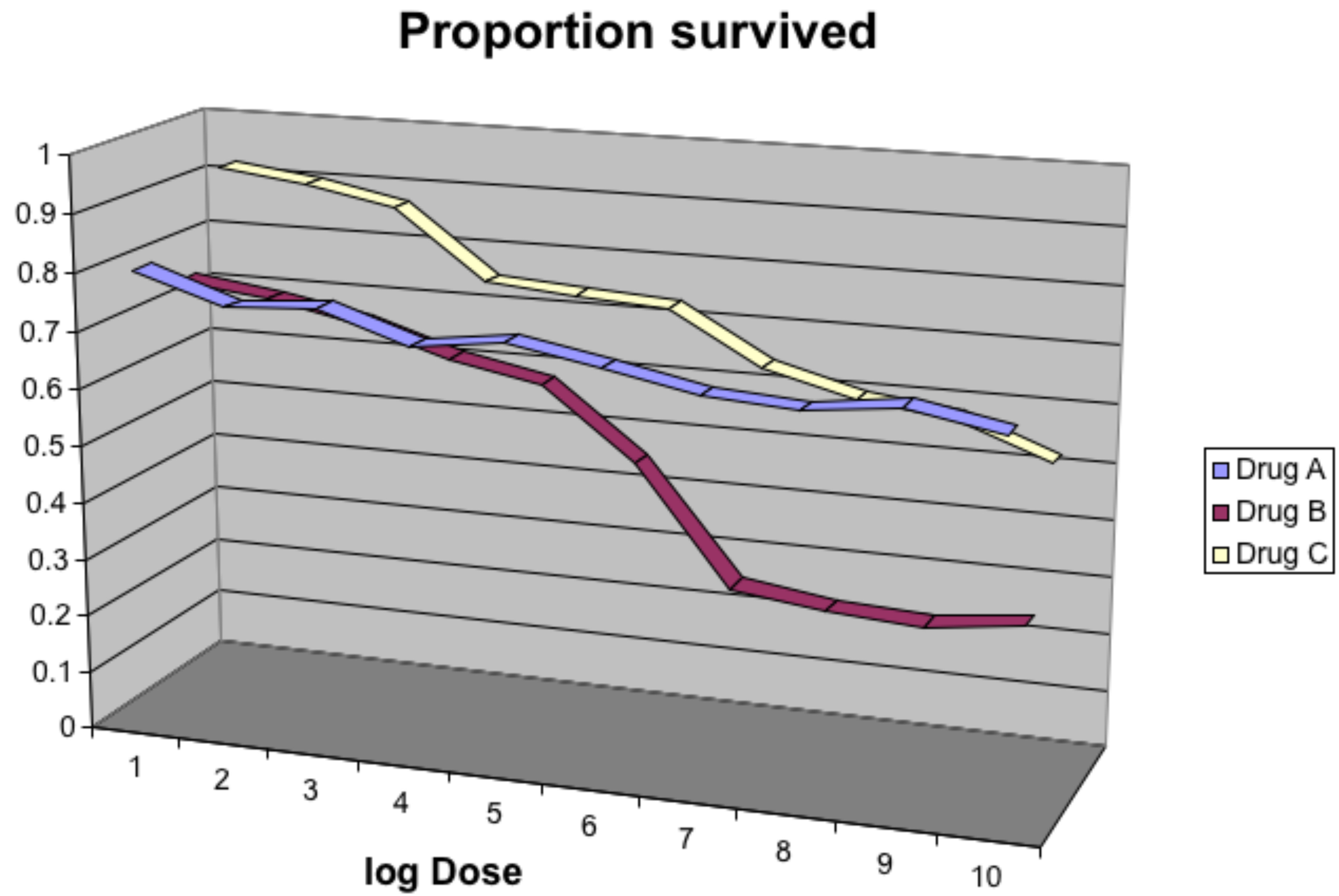
Energy released in earthquakes since 2010

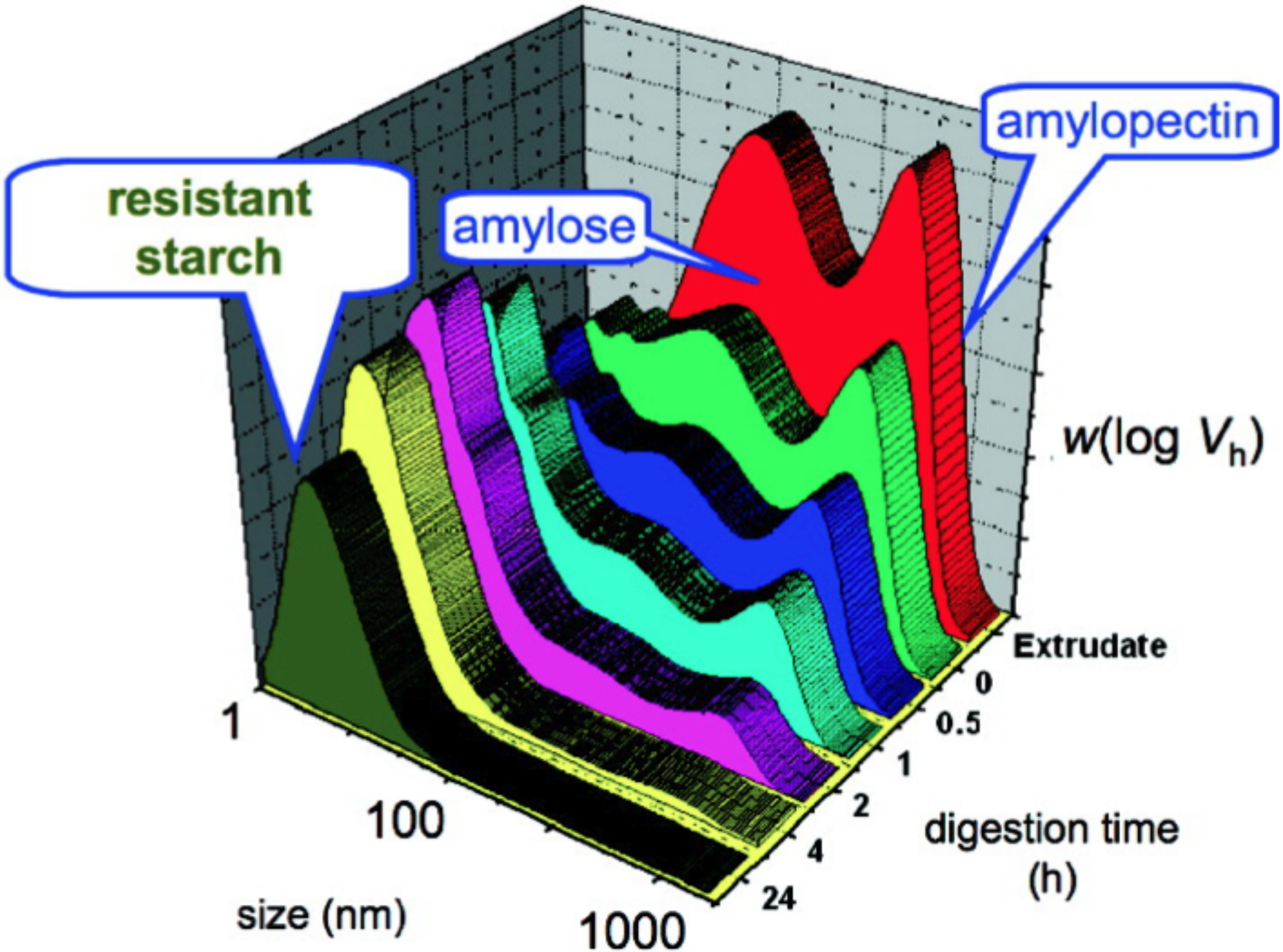


ellisp.github.io


Opera
1%
Safari
9%
Chrome
44%
Firefox
20%
IE
26%


Opera
1%
Safari
9%
Chrome
44%
Firefox
20%
IE
26%


Proportion survived
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1
2
3
4
5
6
7
8
9
10
log Dose
Drug A
Drug B
Drug C



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

Outline

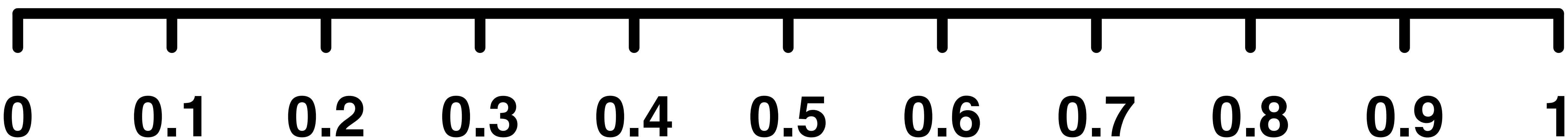
- **A philosophy of graphics**
  - *The good, the bad, and the ugly*
  - ***Tips and guidelines***
- **A grammar of graphics**
  - *Elements of theory*
  - *Glimpse of the future*
- **A vision for graphics**
  - *Aesthetics and impact*
  - *TOC figures, slides, posters*

Tip #1 • Graphic formats

- **Vector format**

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

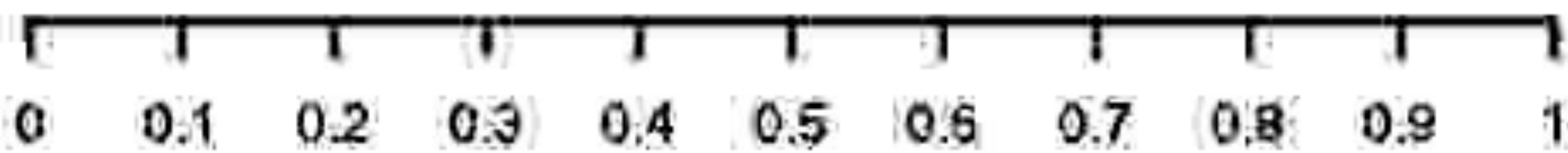
  graphs, schematics



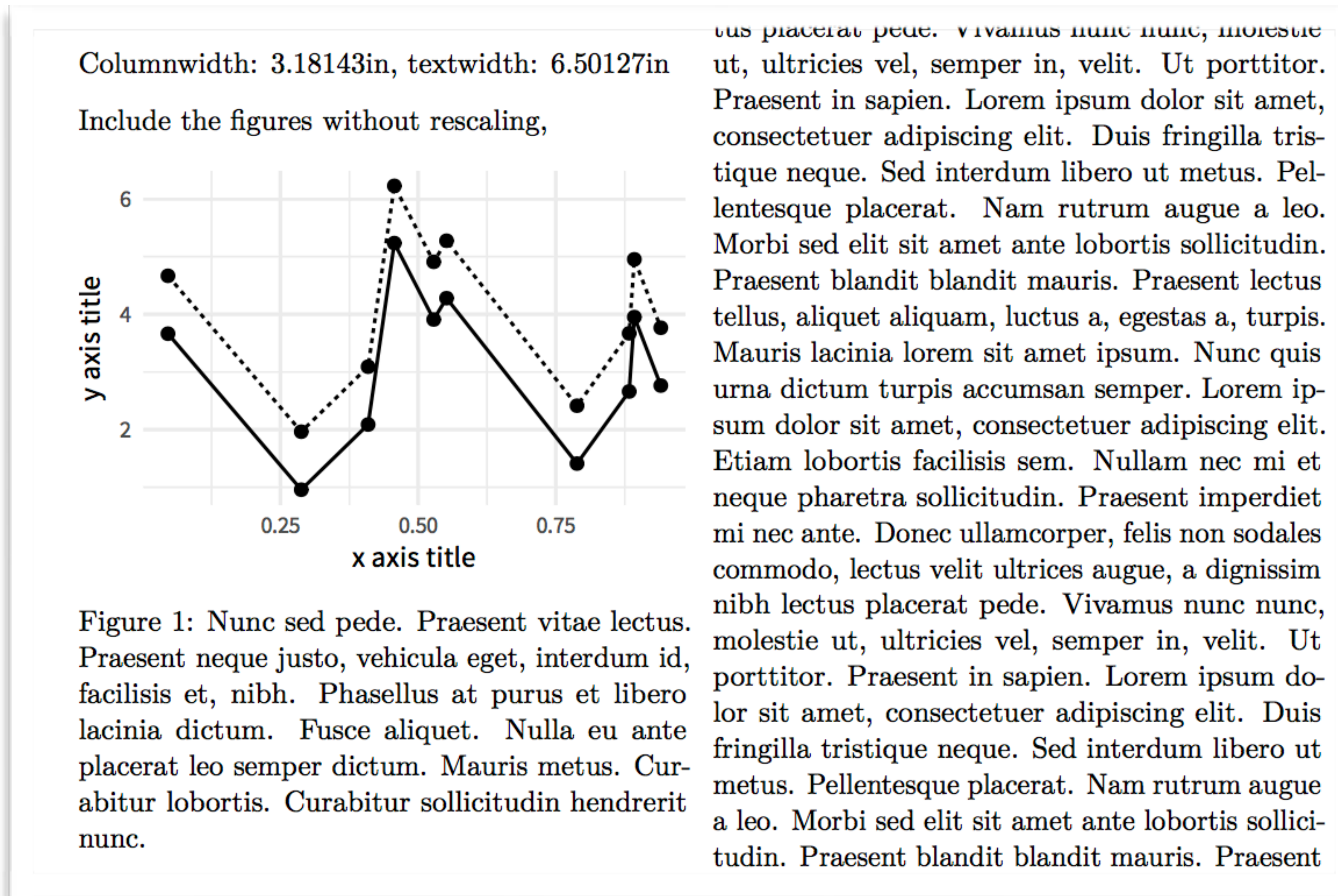
- **Raster format**

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

  photos, maps



Tip #2 • Image size: avoid rescaling



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. Mauris metus. Curabitur lobortis. Curabitur sollicitudin hendrerit nunc.

tus 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

LaTeX tip

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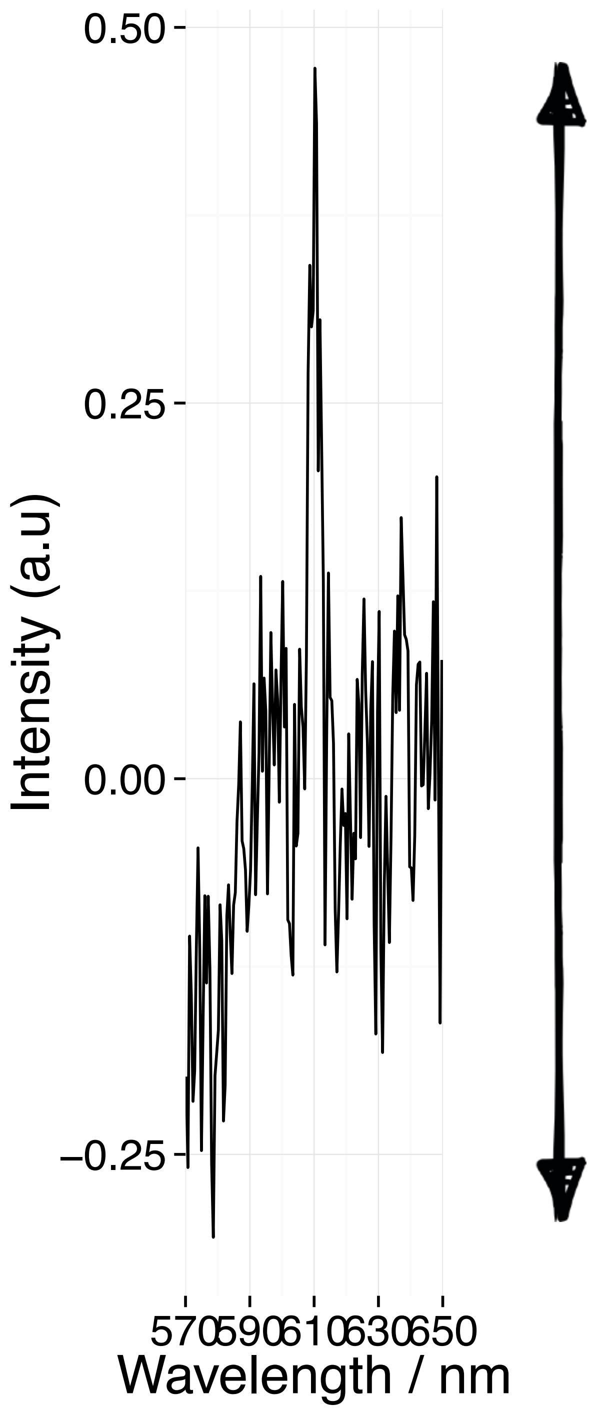
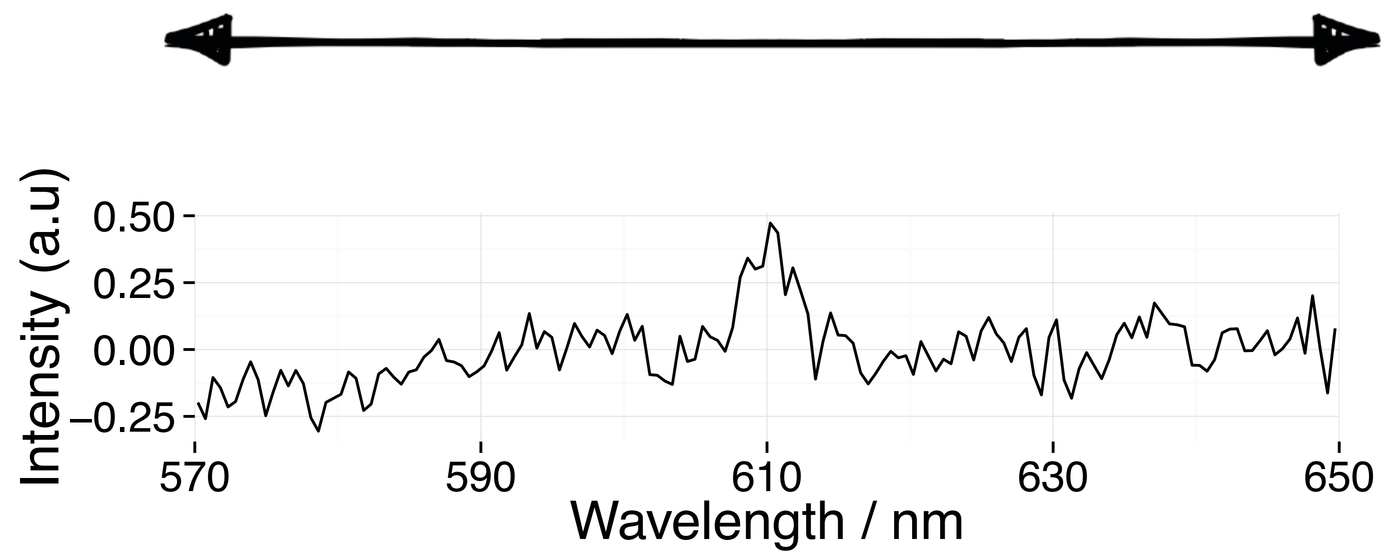
\usepackage{layouts}
\printinunitsof{in}\prntlen{\columnwidth}
\printinunitsof{in}\prntlen{\textwidth}
```

Tip #3 • Aspect ratio





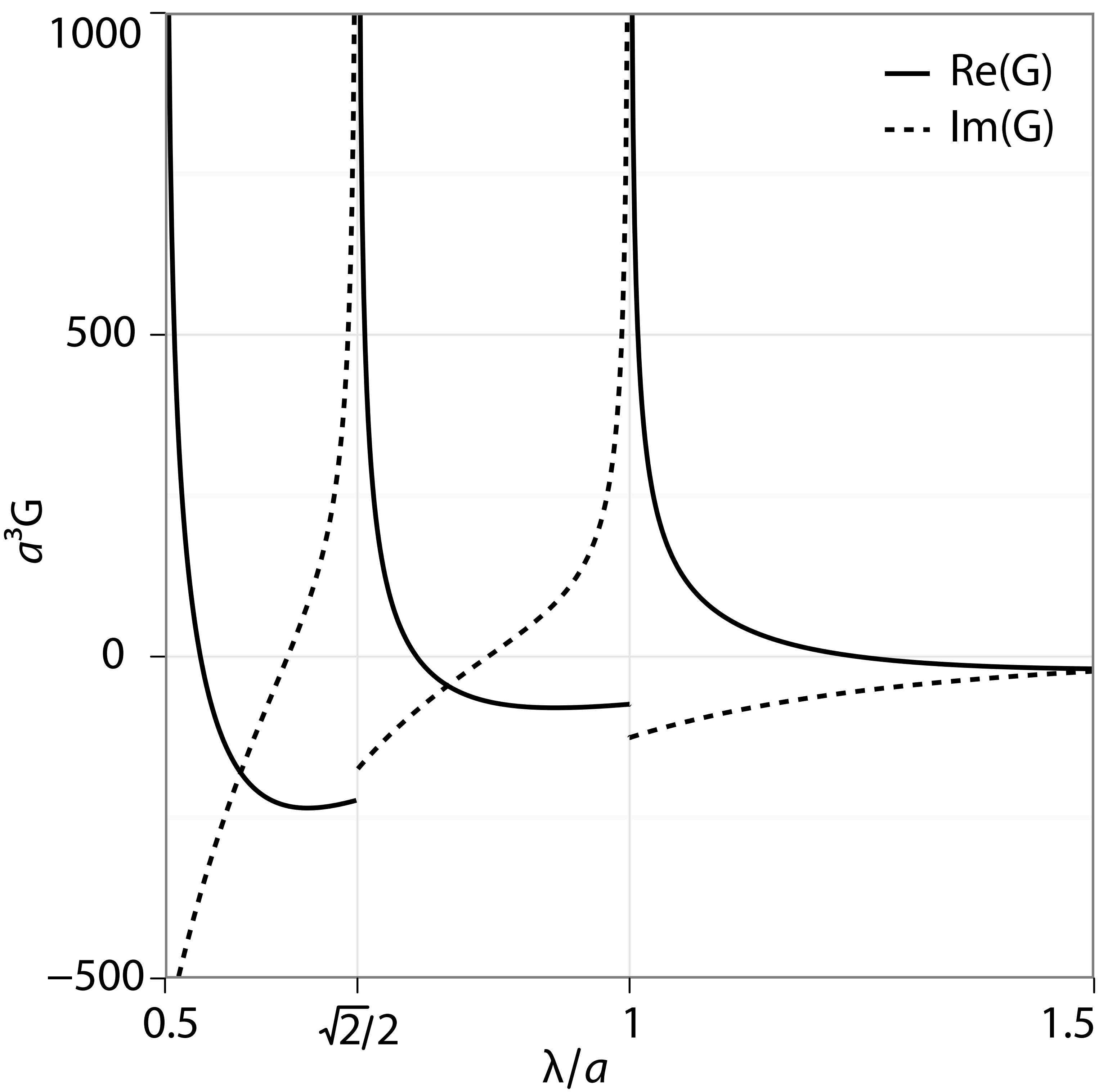
Try

- "banking" at 45°
- standard ratios

Tip #3 • Aspect ratio

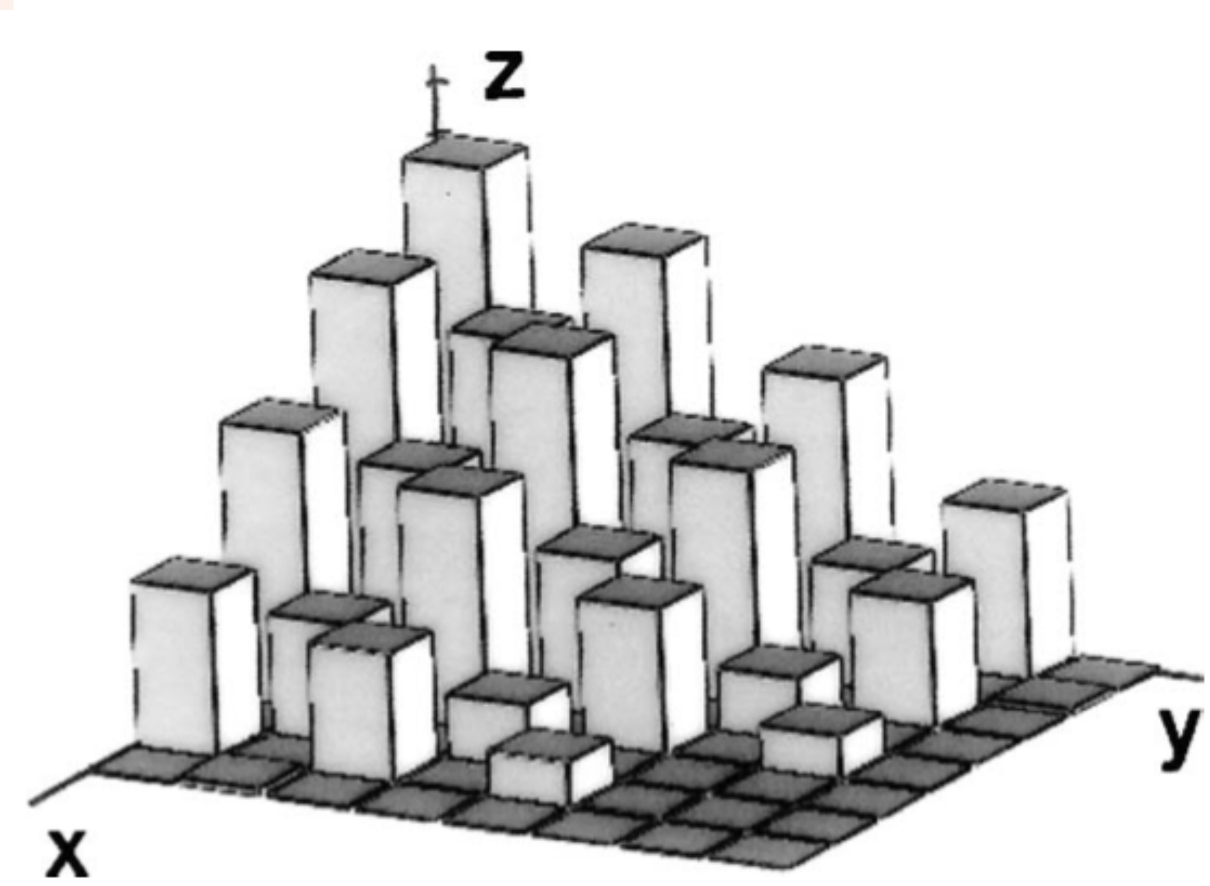
https://xkcd.com/1732/

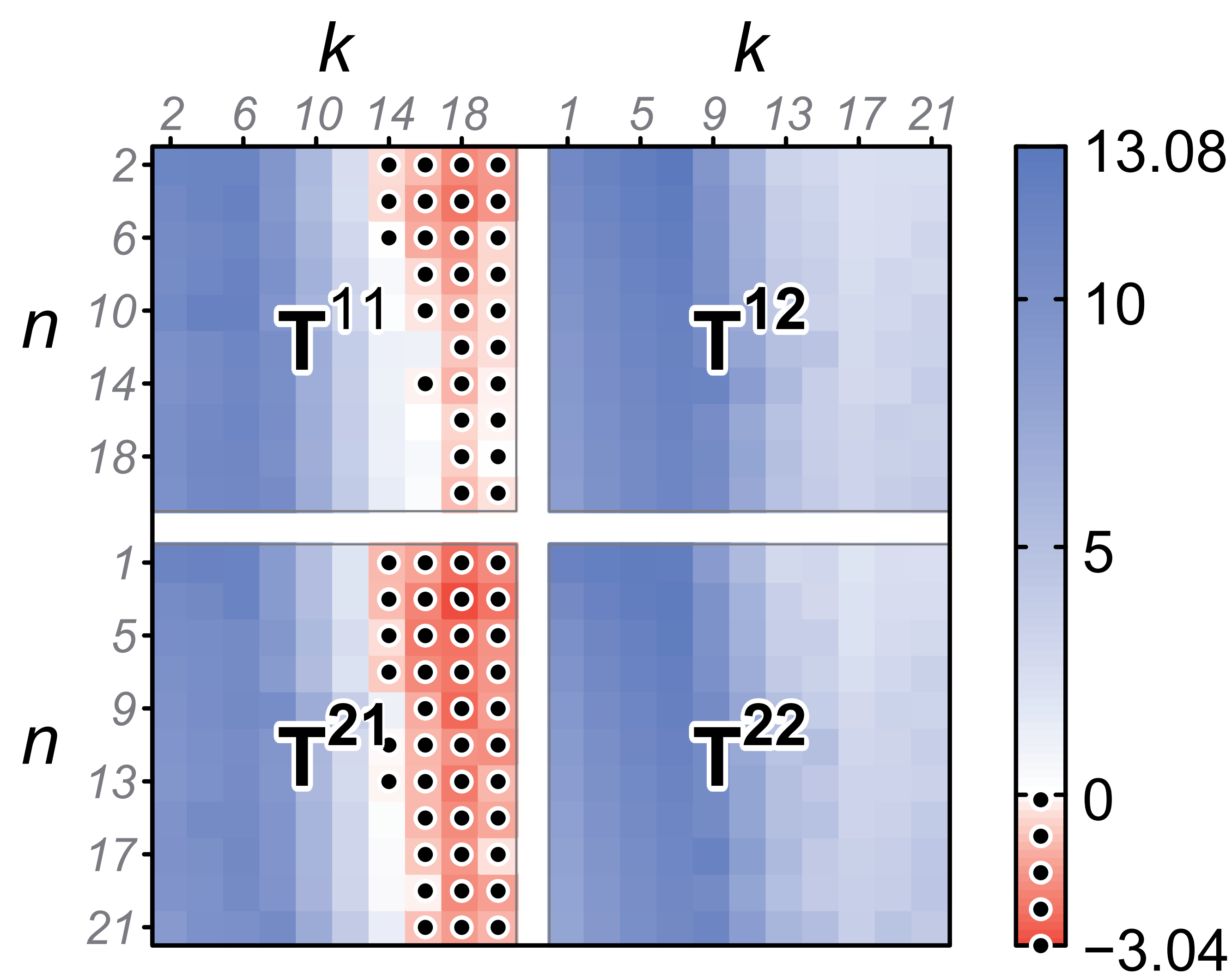
Tip #4 • Less is more



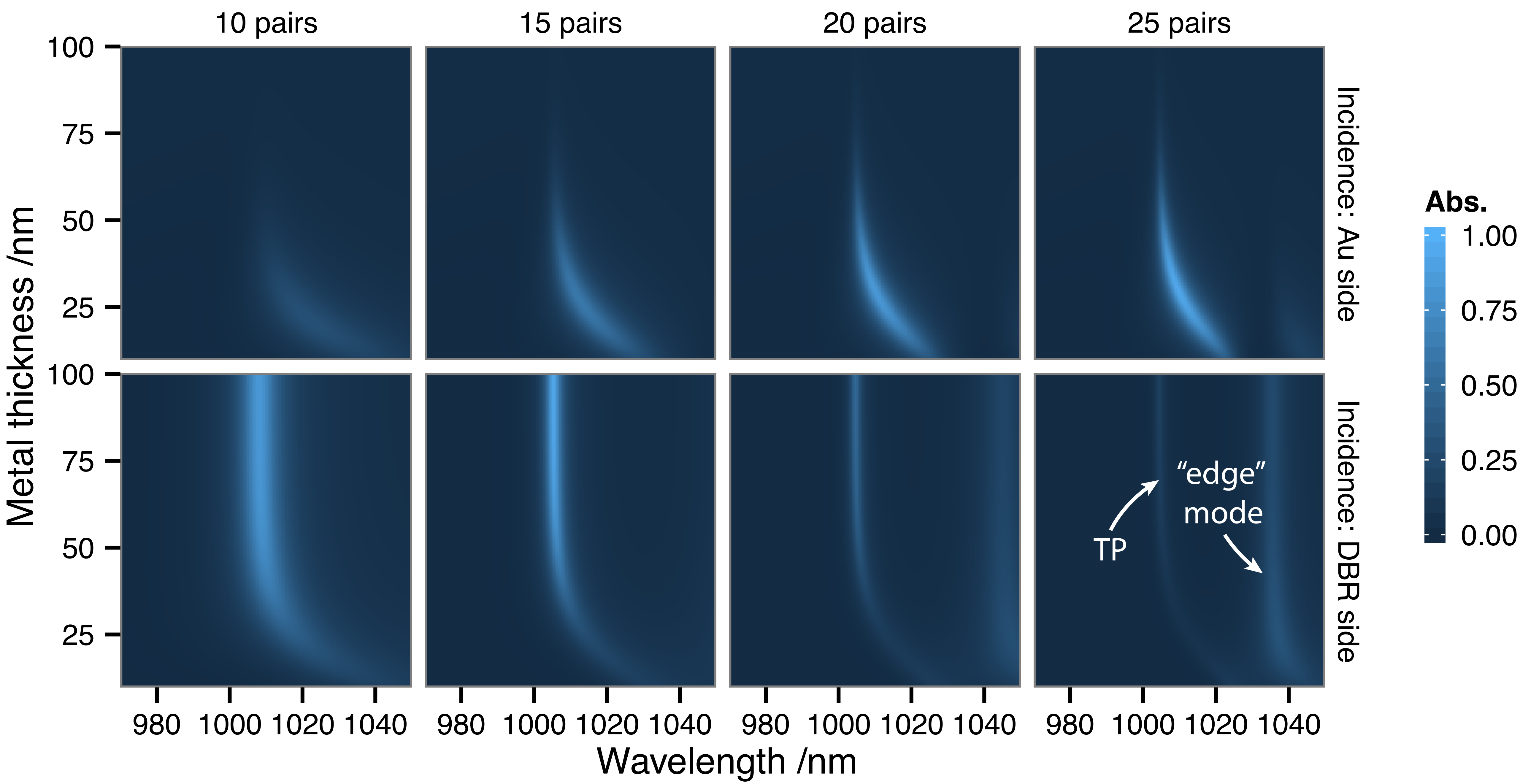
TIP #4 • LESS IS MORE

Fake 3D is often counterproductive

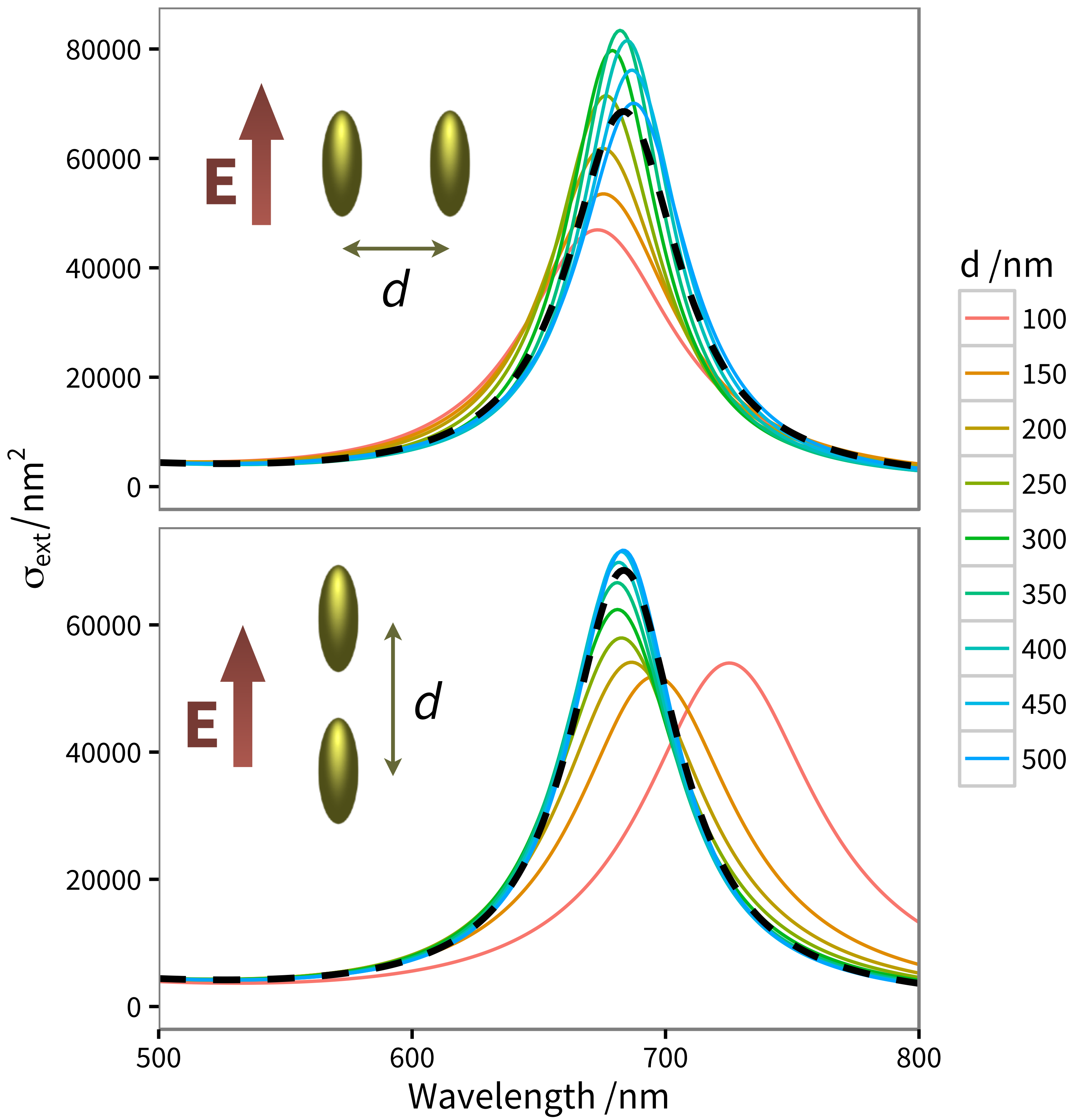


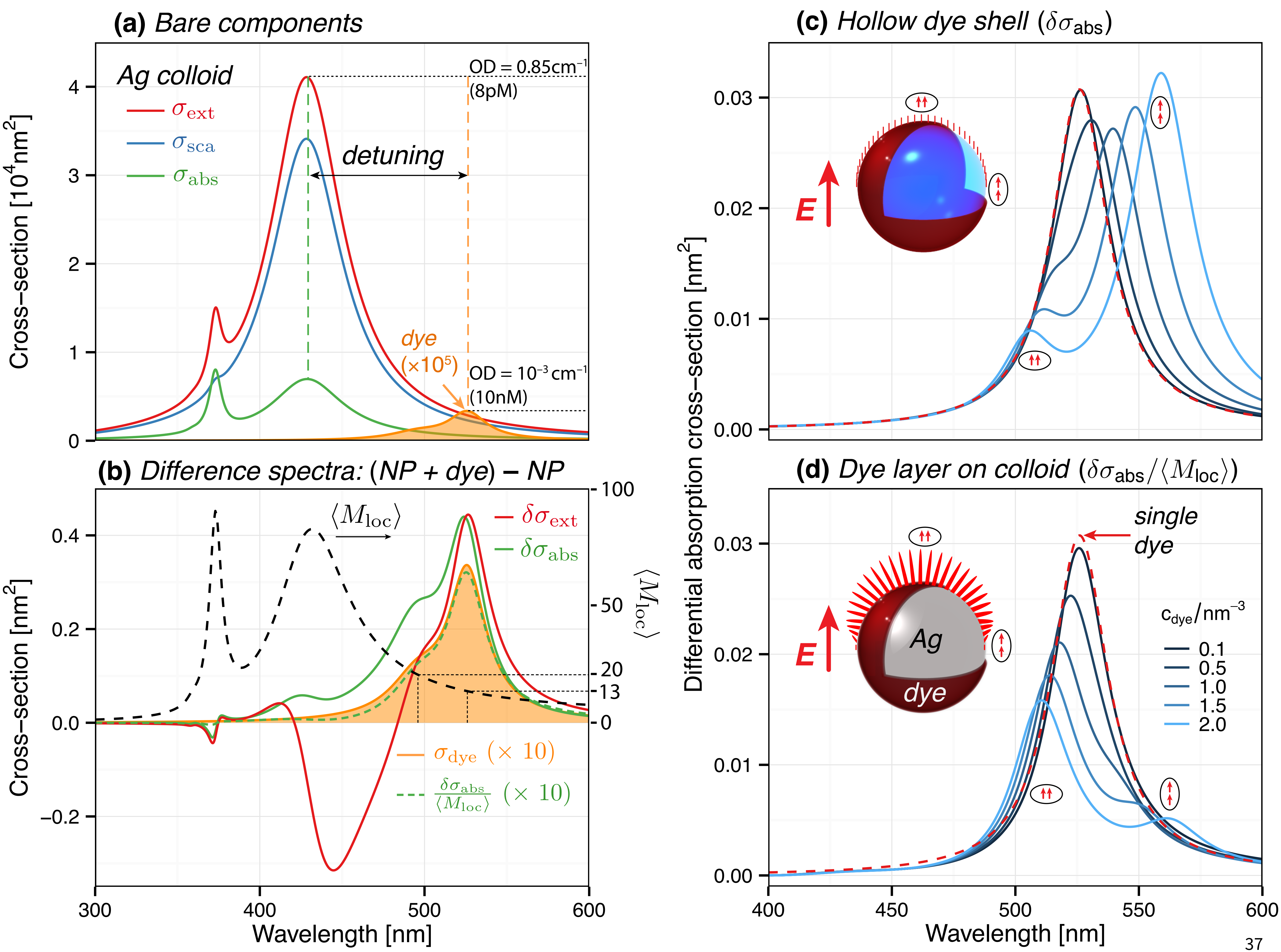


Tip #5 • Small multiples



Tip #6 • Contextual annotations





(a) Bare components
Ag colloid
σ_{ext}
σ_{sca}
σ_{abs}
detuning
OD = 0.85cm⁻¹
(8pM)
dye
(×10⁵)
OD = 10⁻³ cm⁻¹
(10nM)
Cross–section [10⁴nm²]
(b) Difference spectra: (NP + dye) − NP
$\langle M_{\text{loc}} \rangle$
$\delta\sigma_{\text{ext}}$
$\delta\sigma_{\text{abs}}$
σ_{dye} (× 10)
$\frac{\delta\sigma_{\text{abs}}}{\langle M_{\text{loc}} \rangle}$ (× 10)
Cross–section [nm²]
Wavelength [nm]
(c) Hollow dye shell ($\delta\sigma_{\text{abs}}$)
E
Differential absorption cross-section [nm²]
(d) Dye layer on colloid ($\delta\sigma_{\text{abs}}/\langle M_{\text{loc}} \rangle$)
single
dye
Ag
dye
c_{dye}/nm⁻³
0.1
0.5
1.0
1.5
2.0
Wavelength [nm]

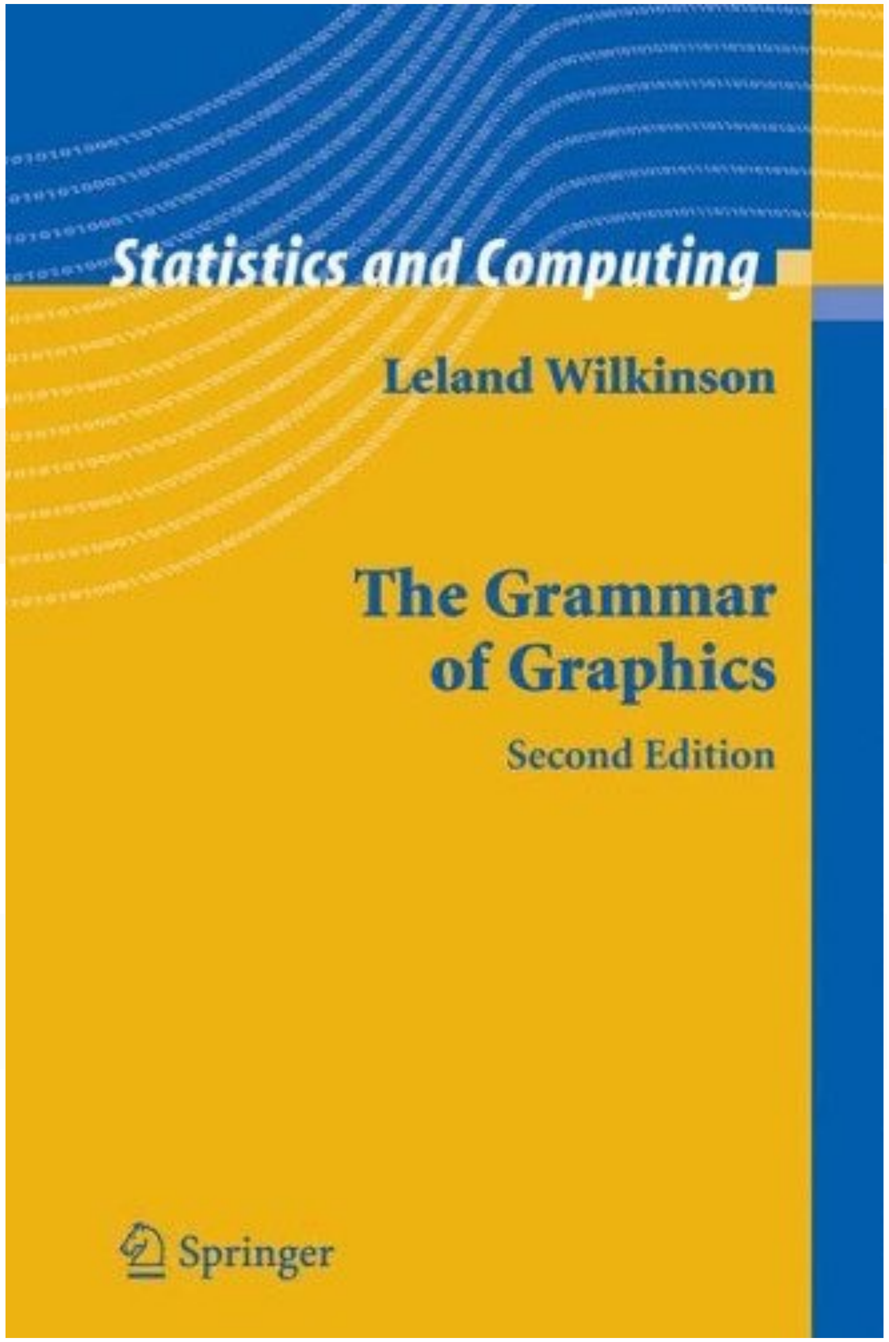
Summary • Key points

- **Show the data '*as nature intended*'**
  - Maximise data/ink (*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

Part II • A grammar of graphics

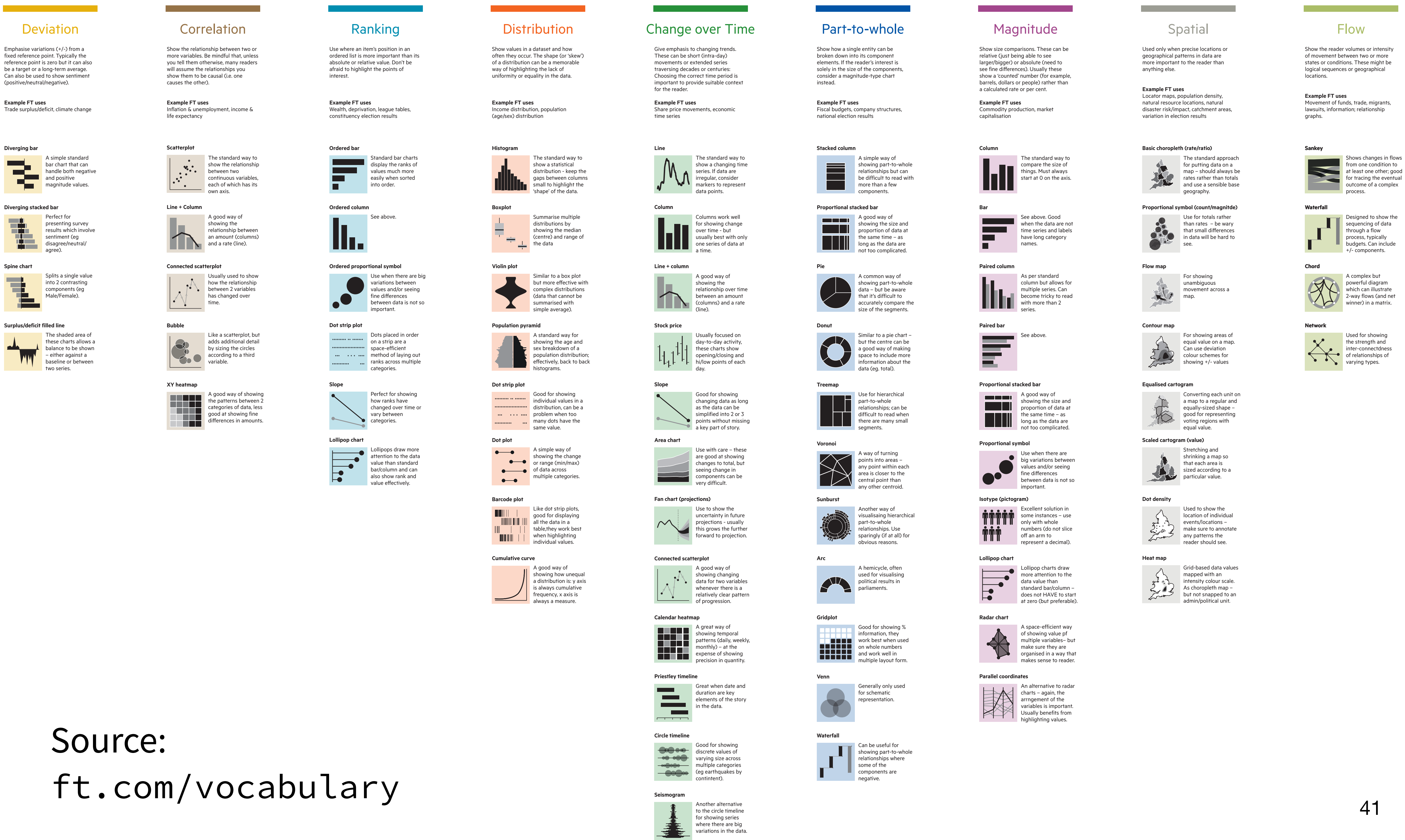
- A philosophy of graphics
  - *The good, the bad, and the ugly*
  - *Tips and guidelines*
- **A grammar of graphics**
  - *Elements of theory*
  - *Glimpse of the future*
- A vision for graphics
  - *Aesthetics and impact*
  - *TOC figures, slides, posters*



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

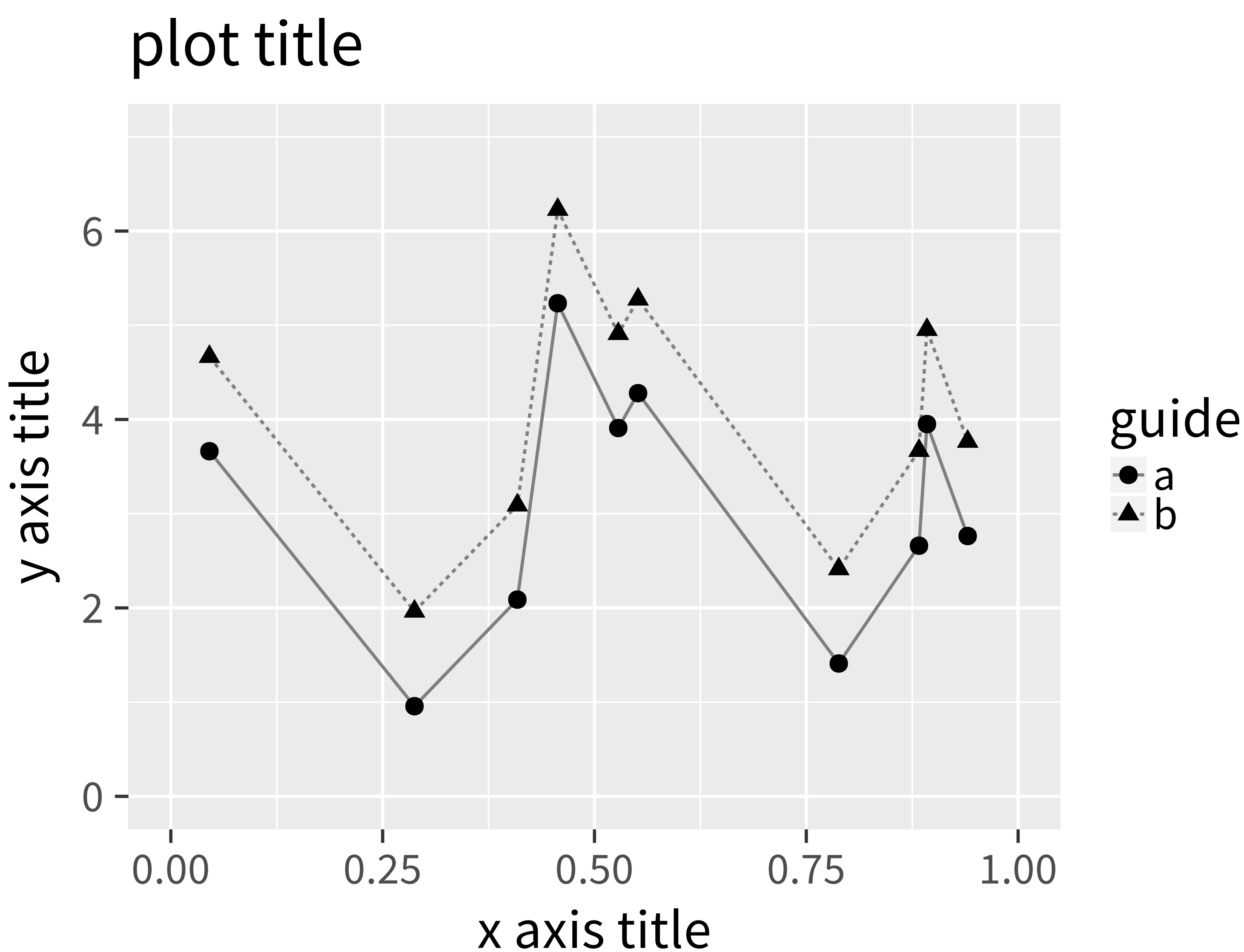
L. Wilkinson

TAXONOMY OF GRAPHICS

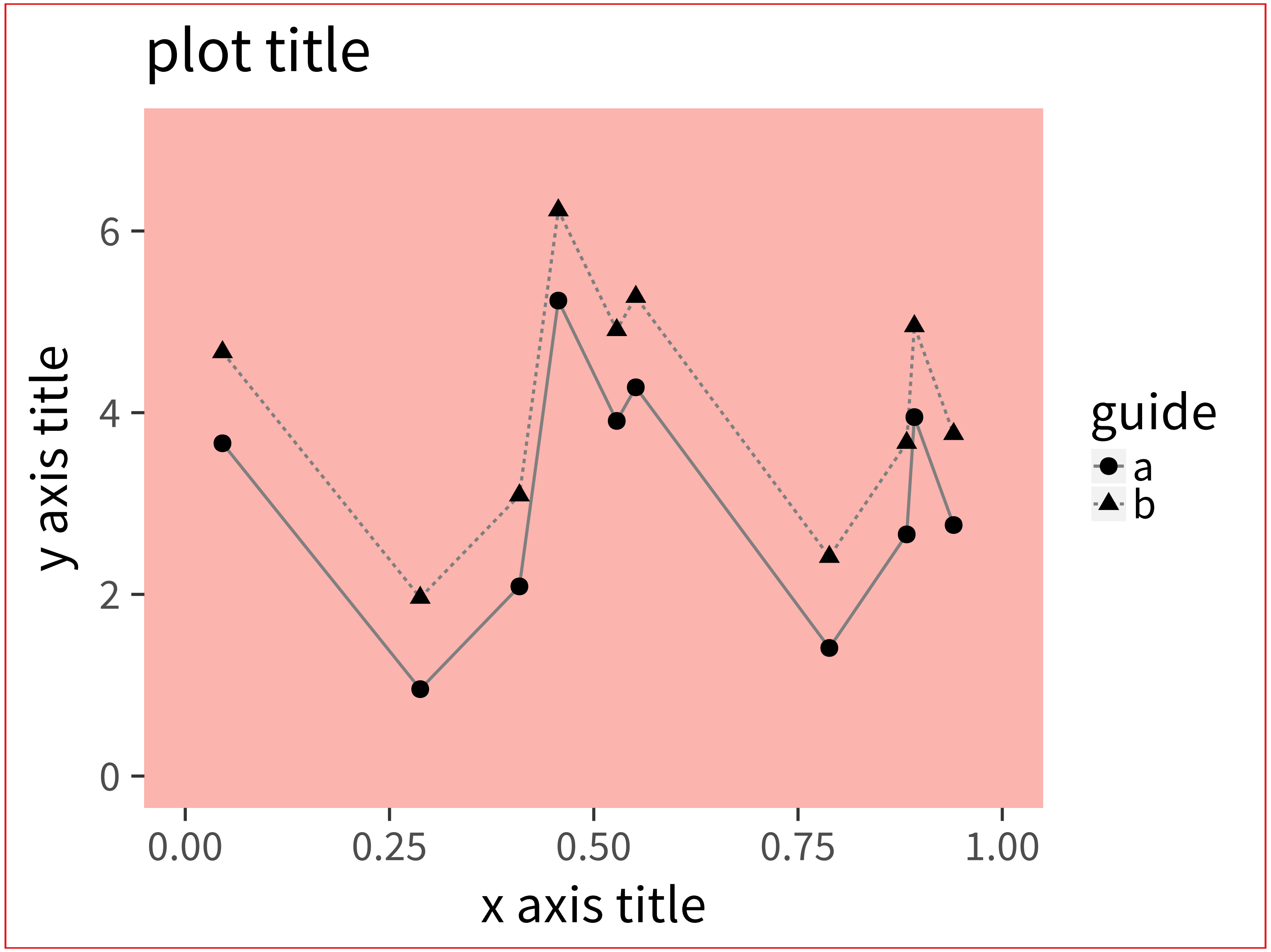


Source:
ft.com/vocabulary

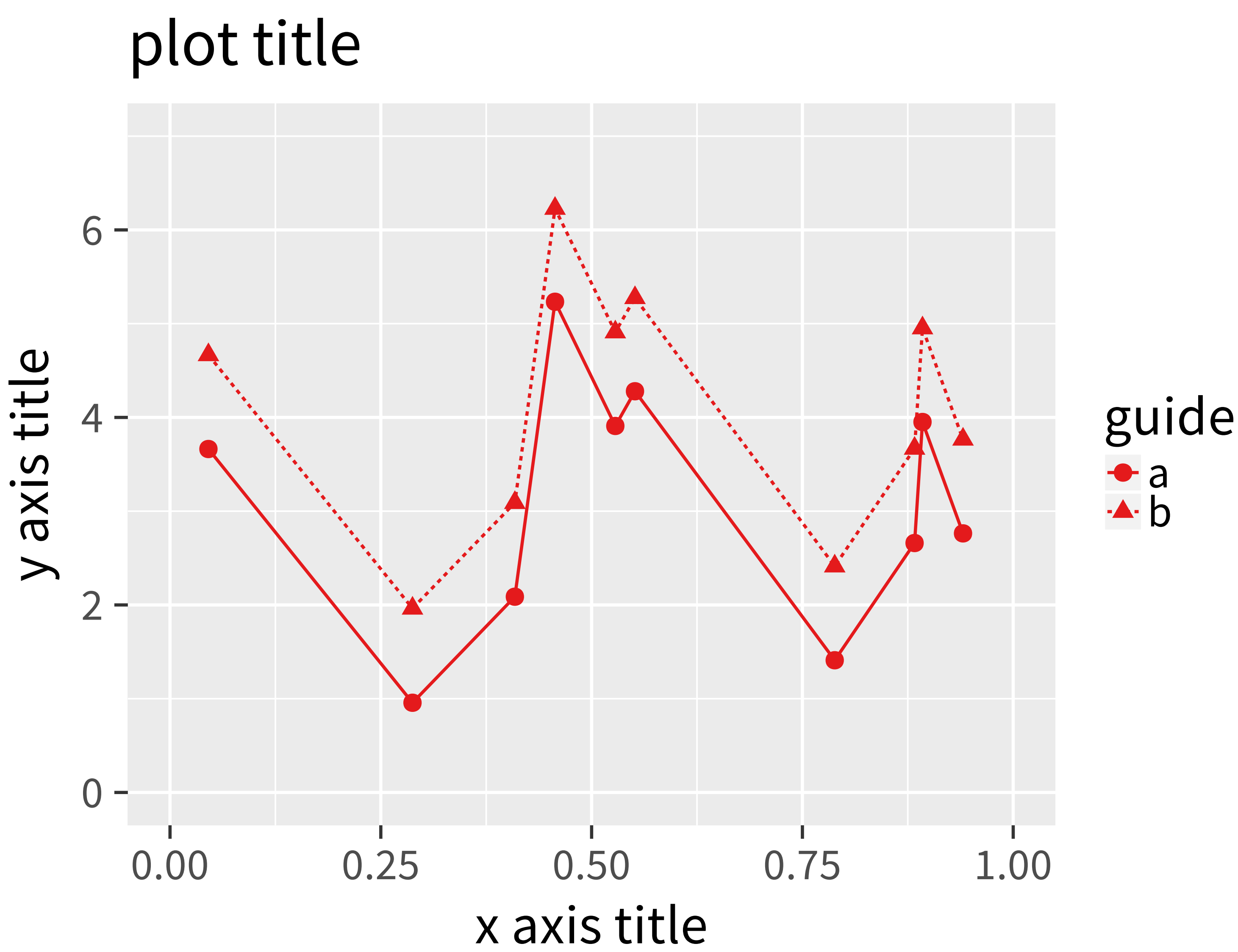
ANATOMY OF A PLOT



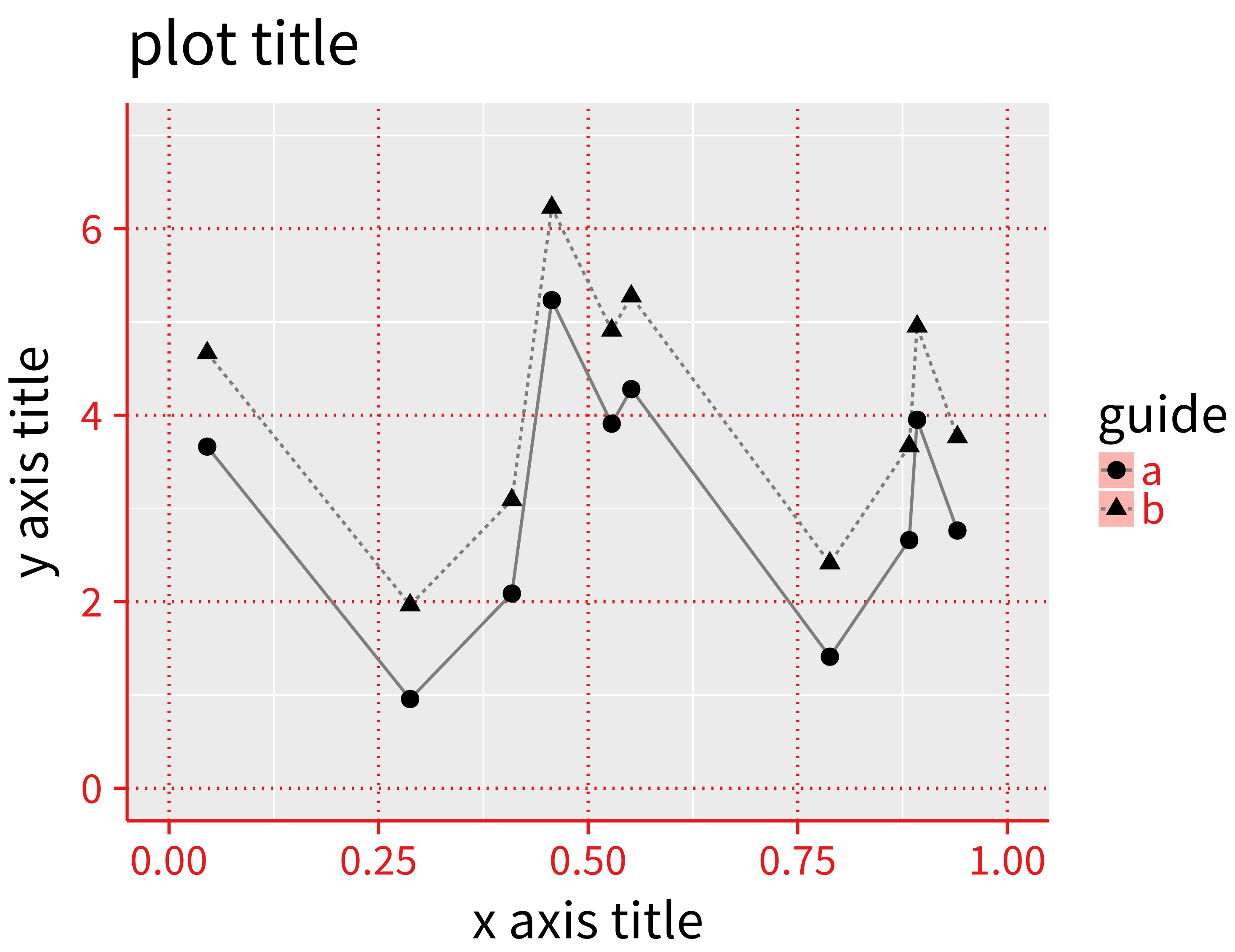
ANATOMY OF A PLOT • *PLOT PANEL*



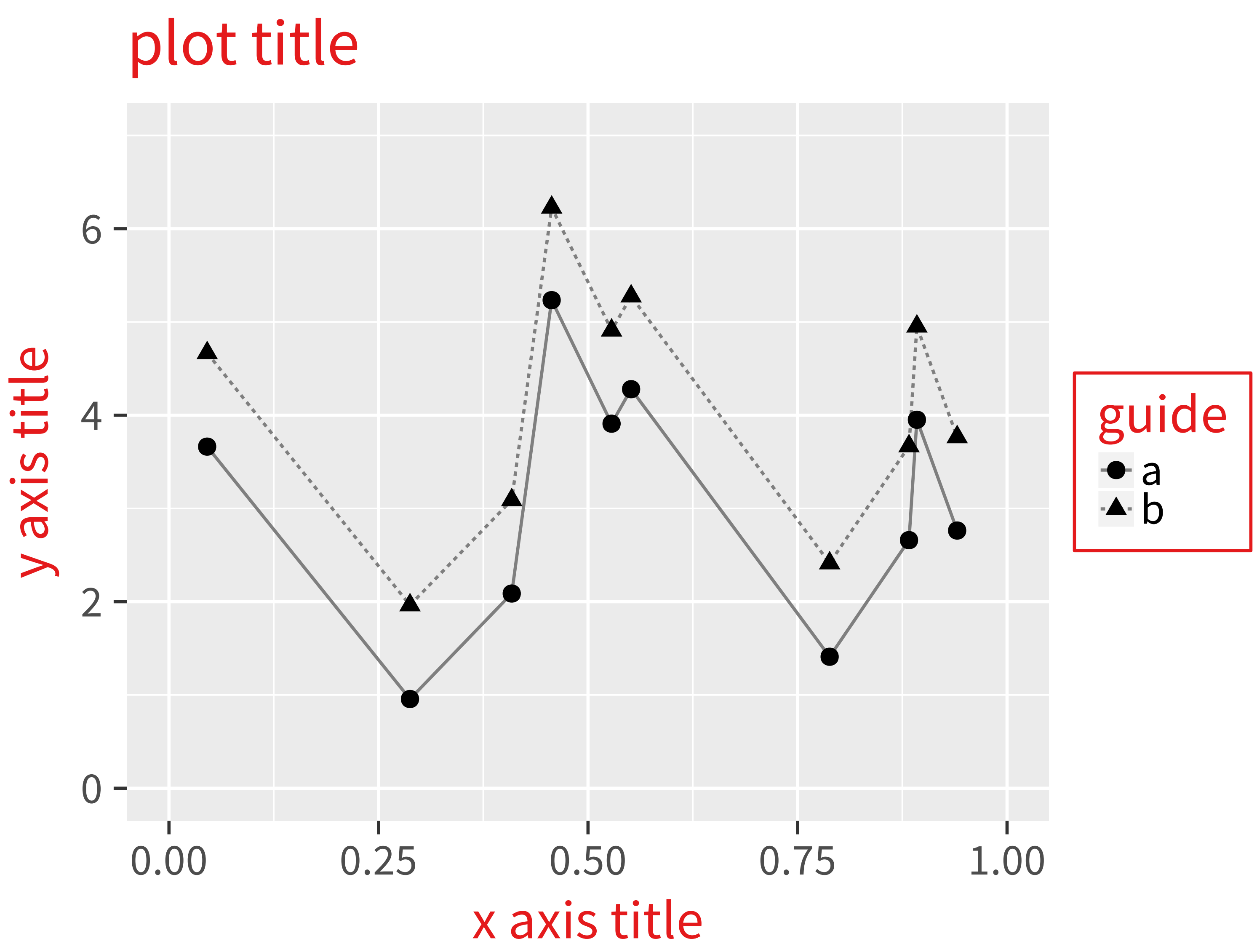
ANATOMY OF A PLOT • *THE DATA*



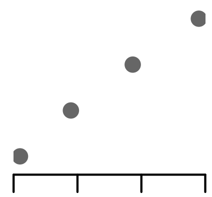
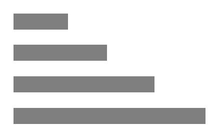
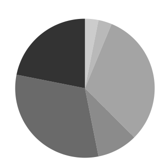
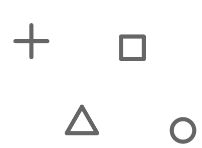
ANATOMY OF A PLOT • *GUIDES*

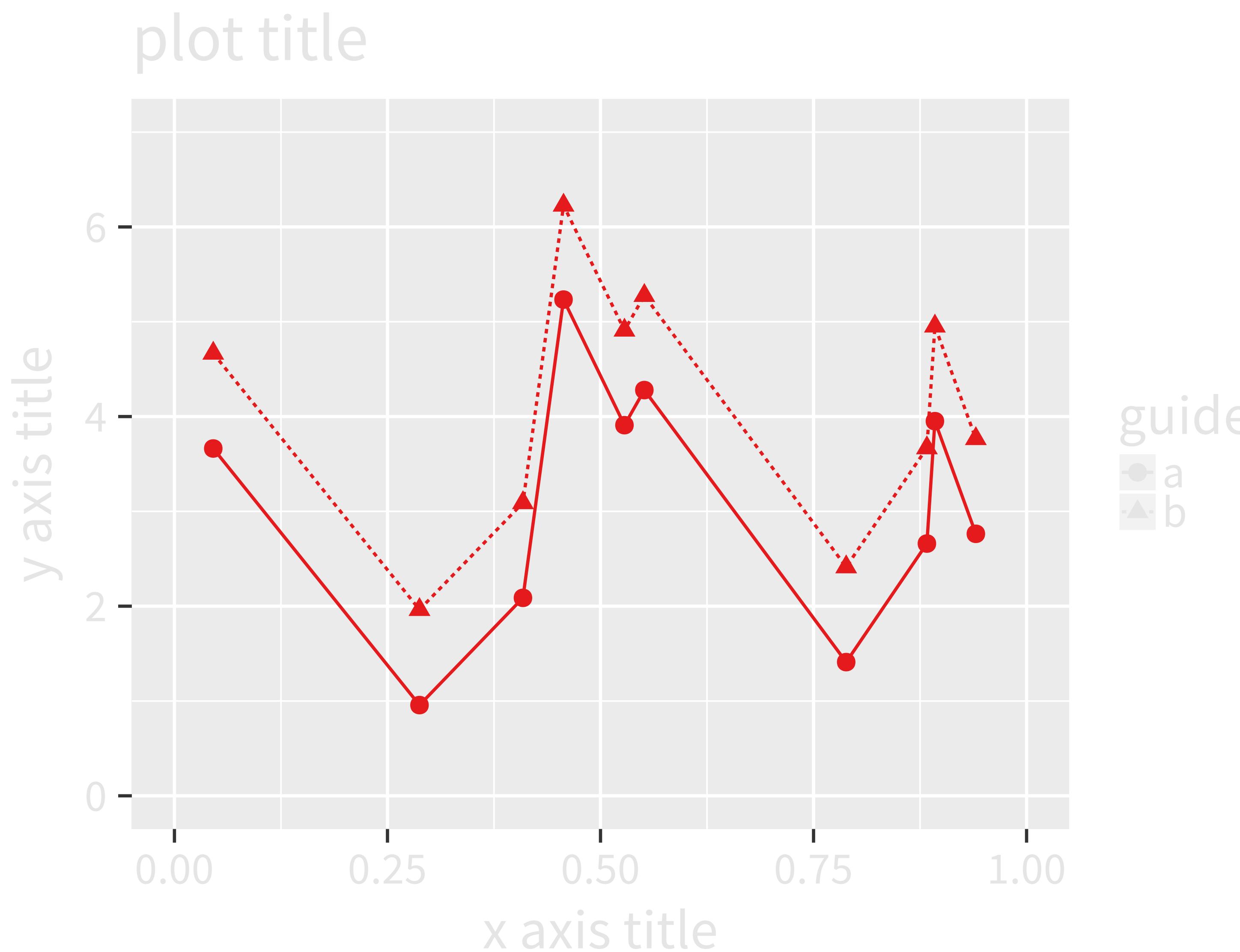


ANATOMY OF A PLOT • *ANNOTATIONS*



A GRAMMAR OF GRAPHICS – MAPPING DATA

- **POSITION** 
- **LENGTH** 
- ANGLE 
- AREA 
- **COLOUR**
- **SHAPE** 
- **LINE TYPE, SIZE,** TIME, **...**

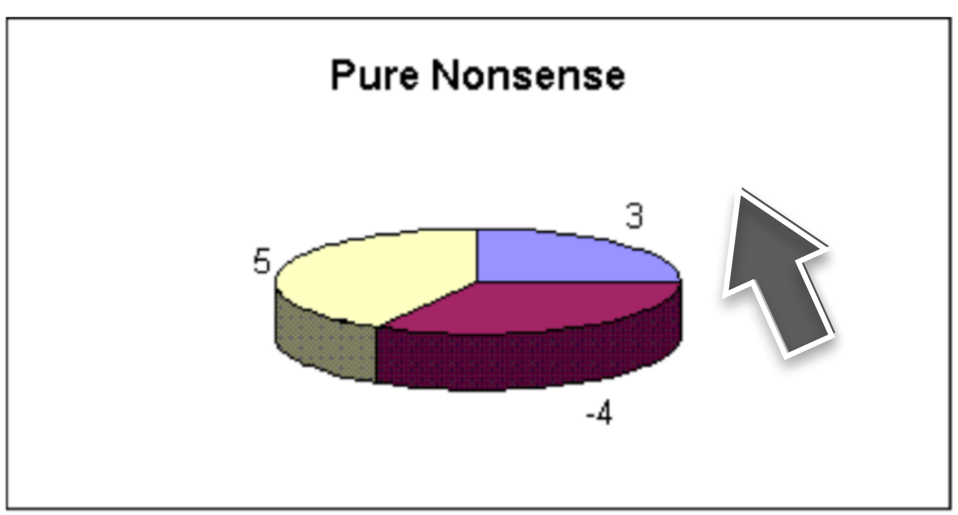


Expressivity and legibility

- **Point n' click**

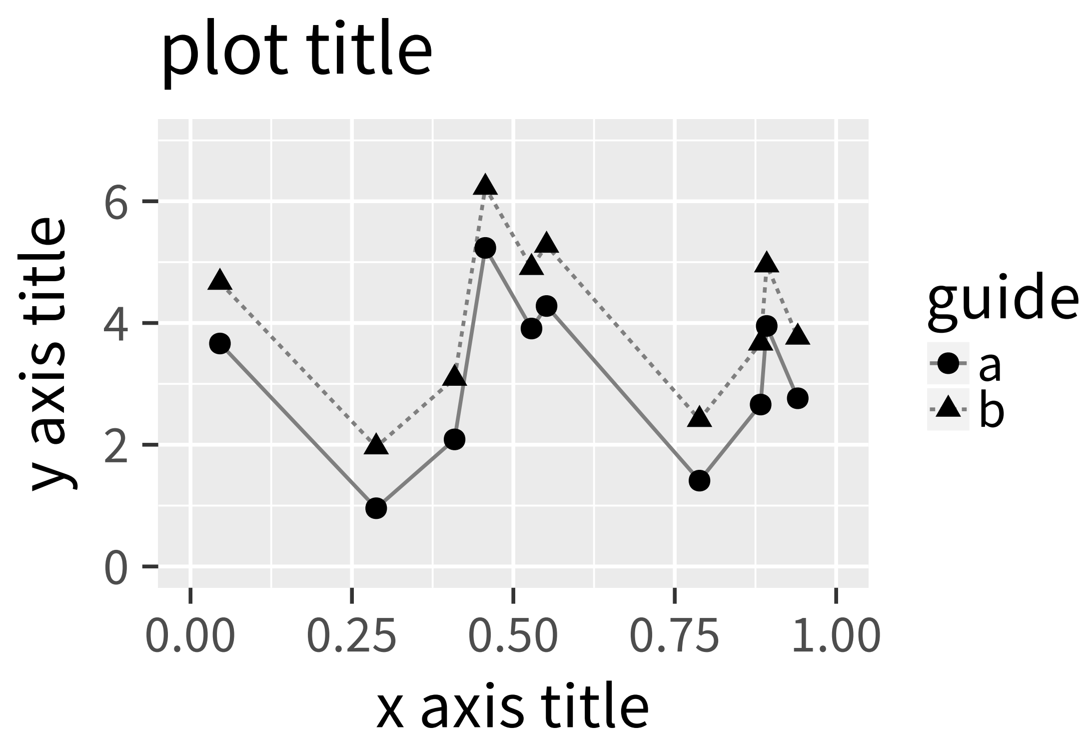
Yeah but, no but, yeah but, no but ! ! !
yeah but . . . I swear * * * * * * * ! ! ! ? ! ! !
. . . but yeah _(ツ)_/ **Computer Says No**

Ctrl-Z



- **Grammar of graphics**

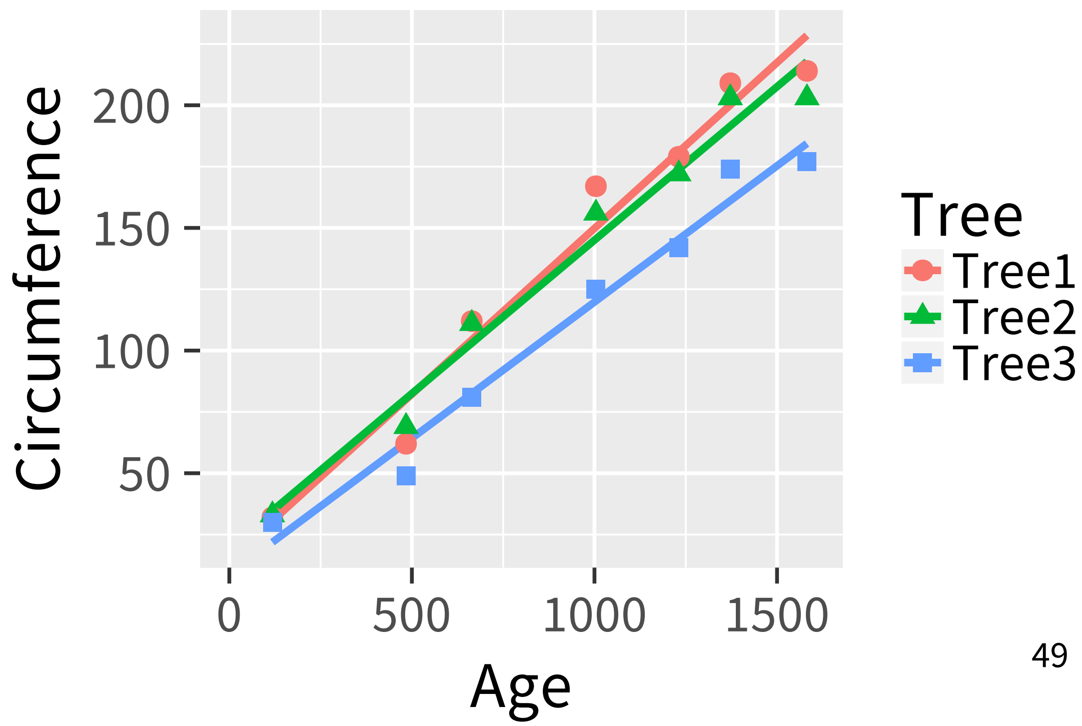
```
plot(data, map(x, y)) +
  layer(point, map(colour = z))   +
  layer(line,  map(linetype = t)) +
  theme(fontsize = 12)
```



Mapping data to glyphs

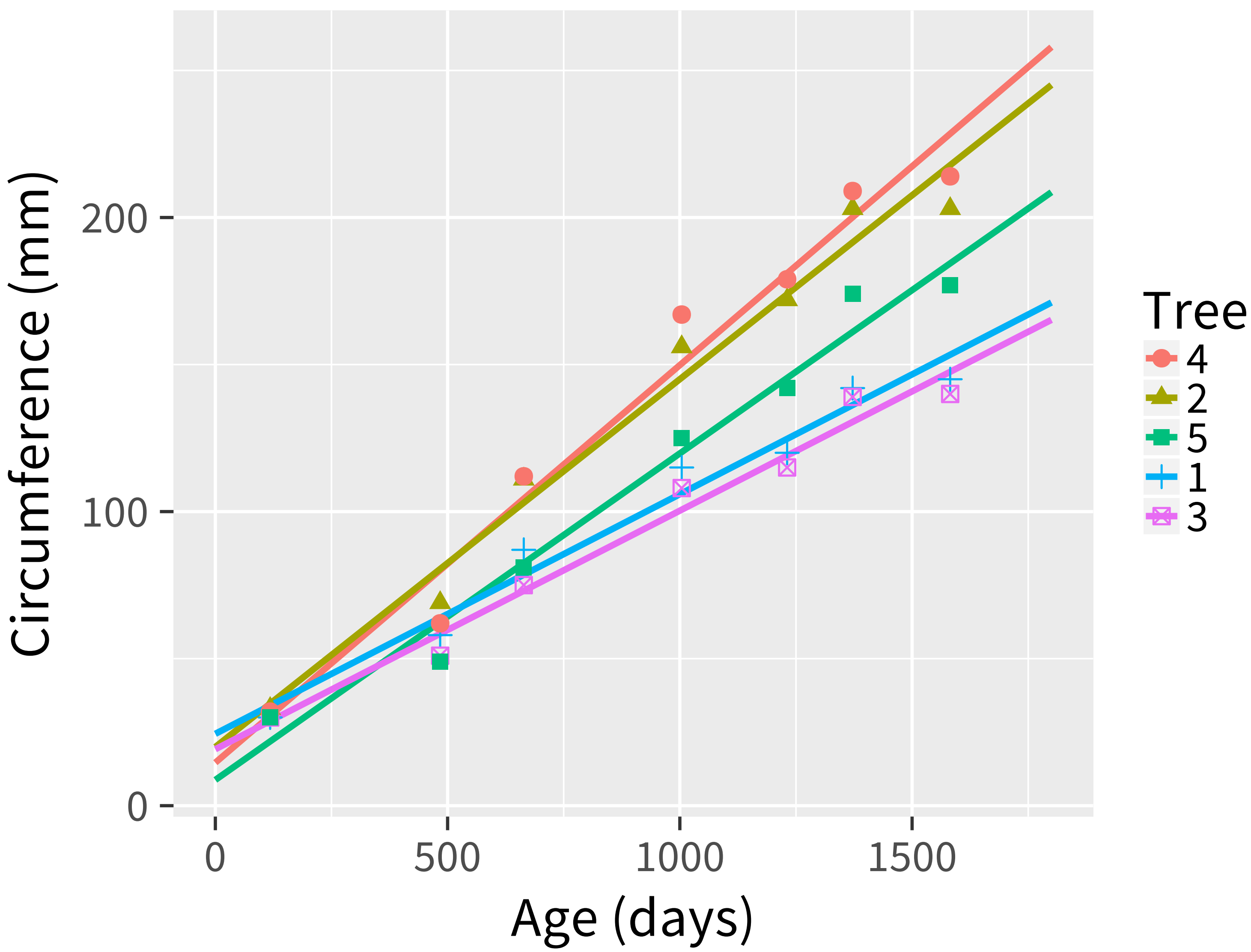
```
plot(data = d,
     mapping = map(x = age,
                   y = circumference)) +
  layer(type = "point",
        mapping = map(shape = Tree,
                      colour = Tree))  +
  layer(type = "line",
        mapping = map(colour = Tree))
```

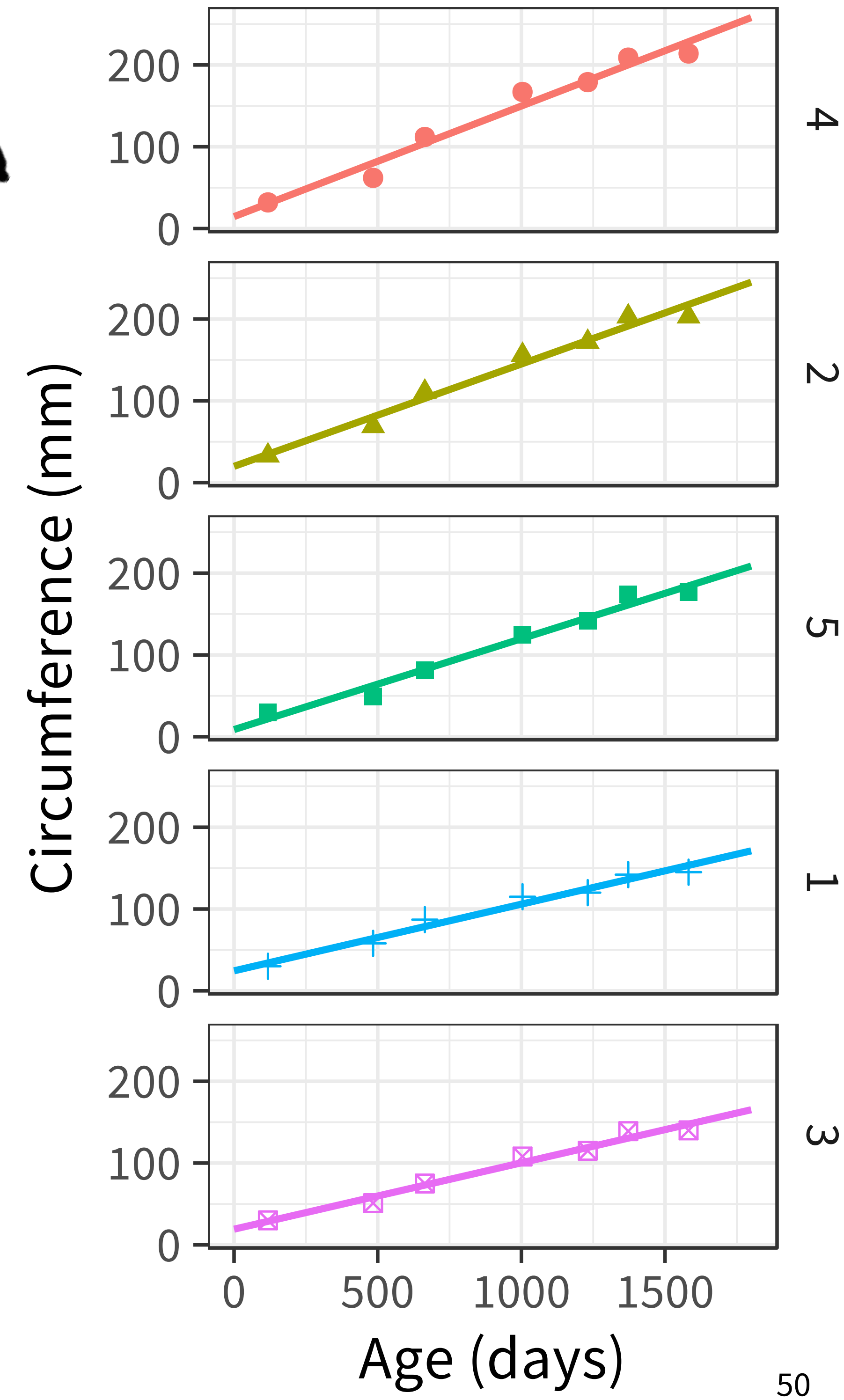
	Tree	age	circ.
1	Tree1	1582	214
2	Tree1	118	32
3	Tree2	118	33
4	Tree2	1372	203
5	Tree3	484	49
6	Tree3	1372	174
7	Tree3	1004	125



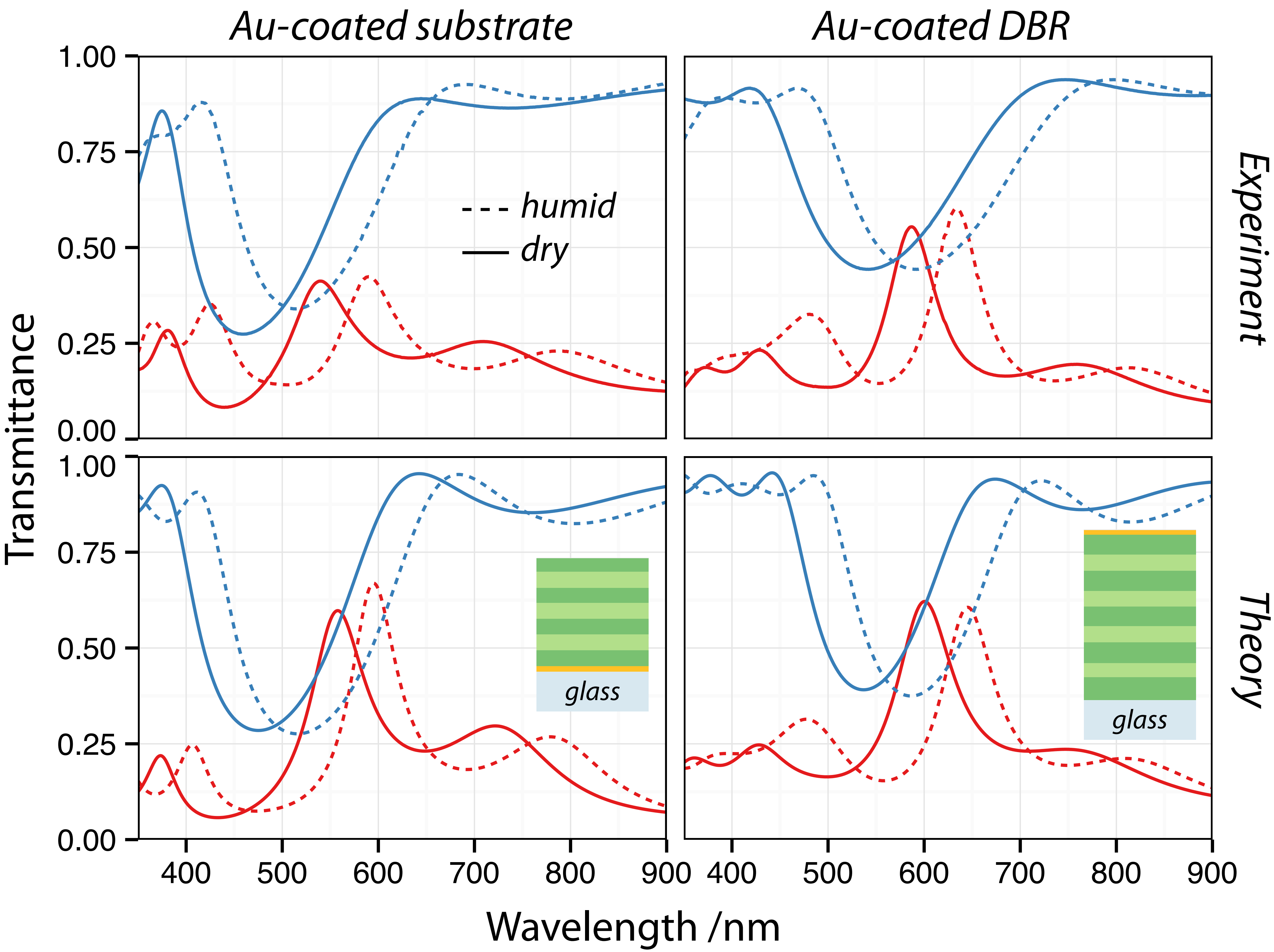
Graphical explorations

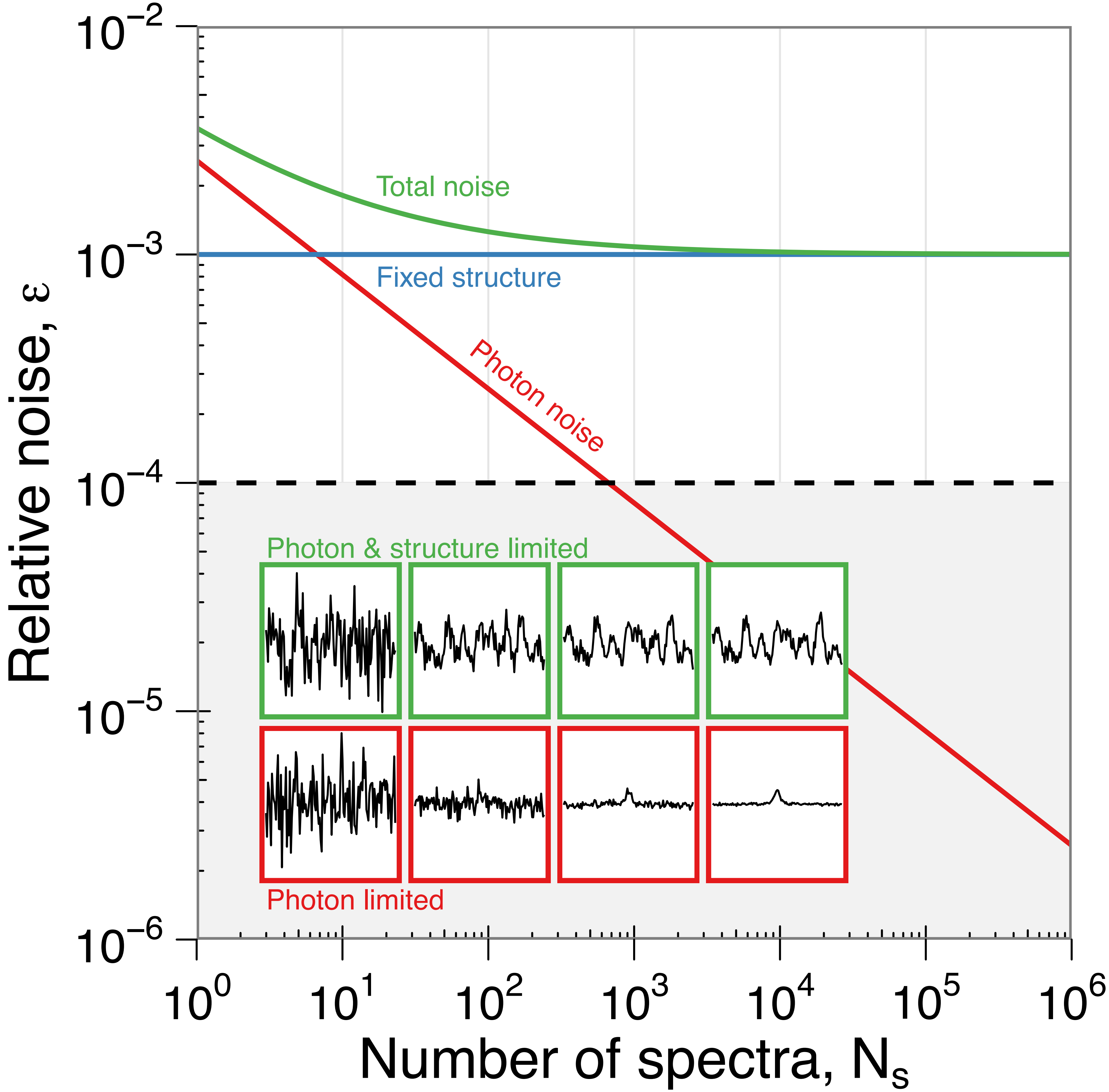
```
last_plot() +
  facet_grid(Tree ~ .) +
  theme_publication
```



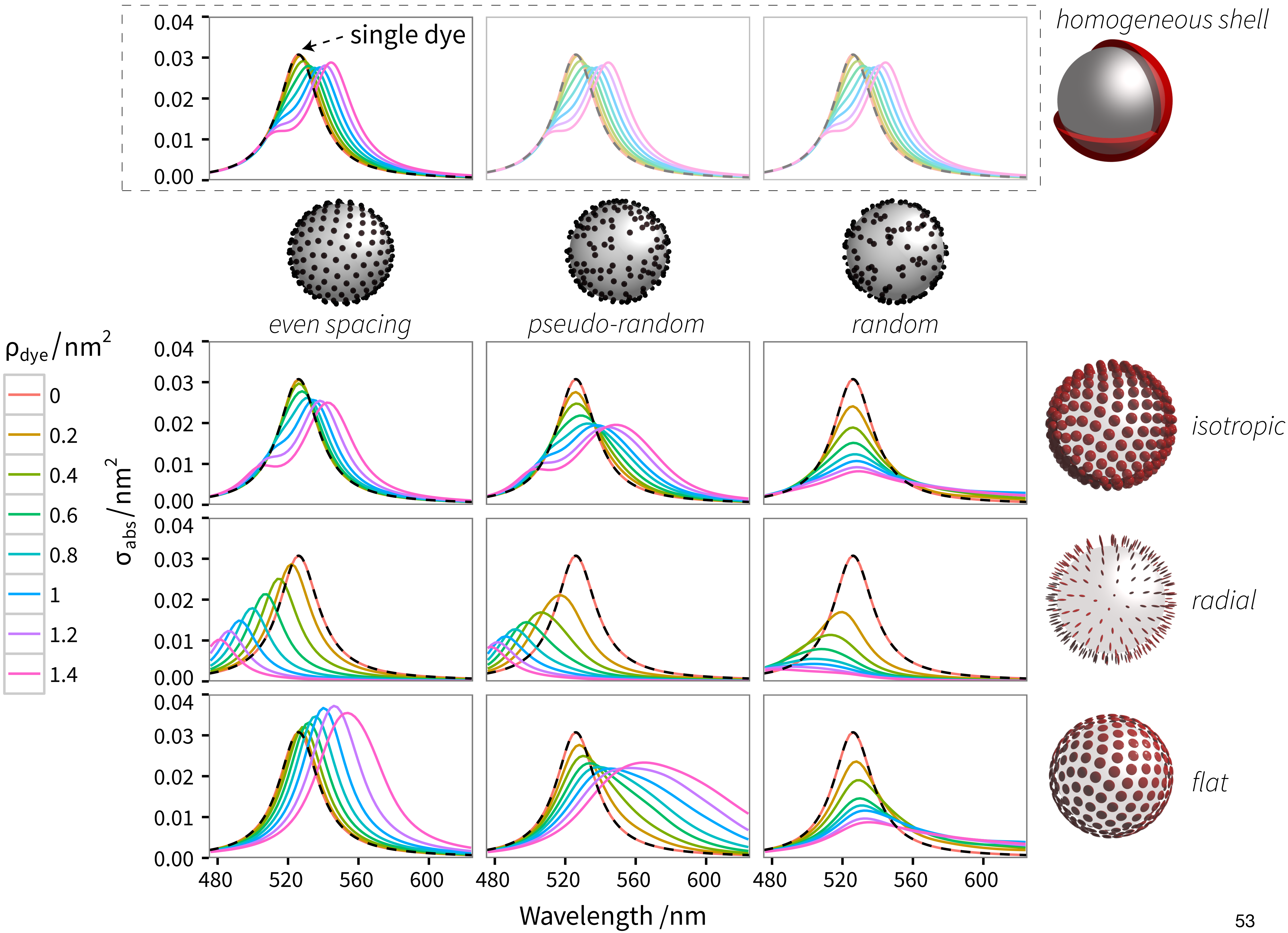


Small multiples revisited





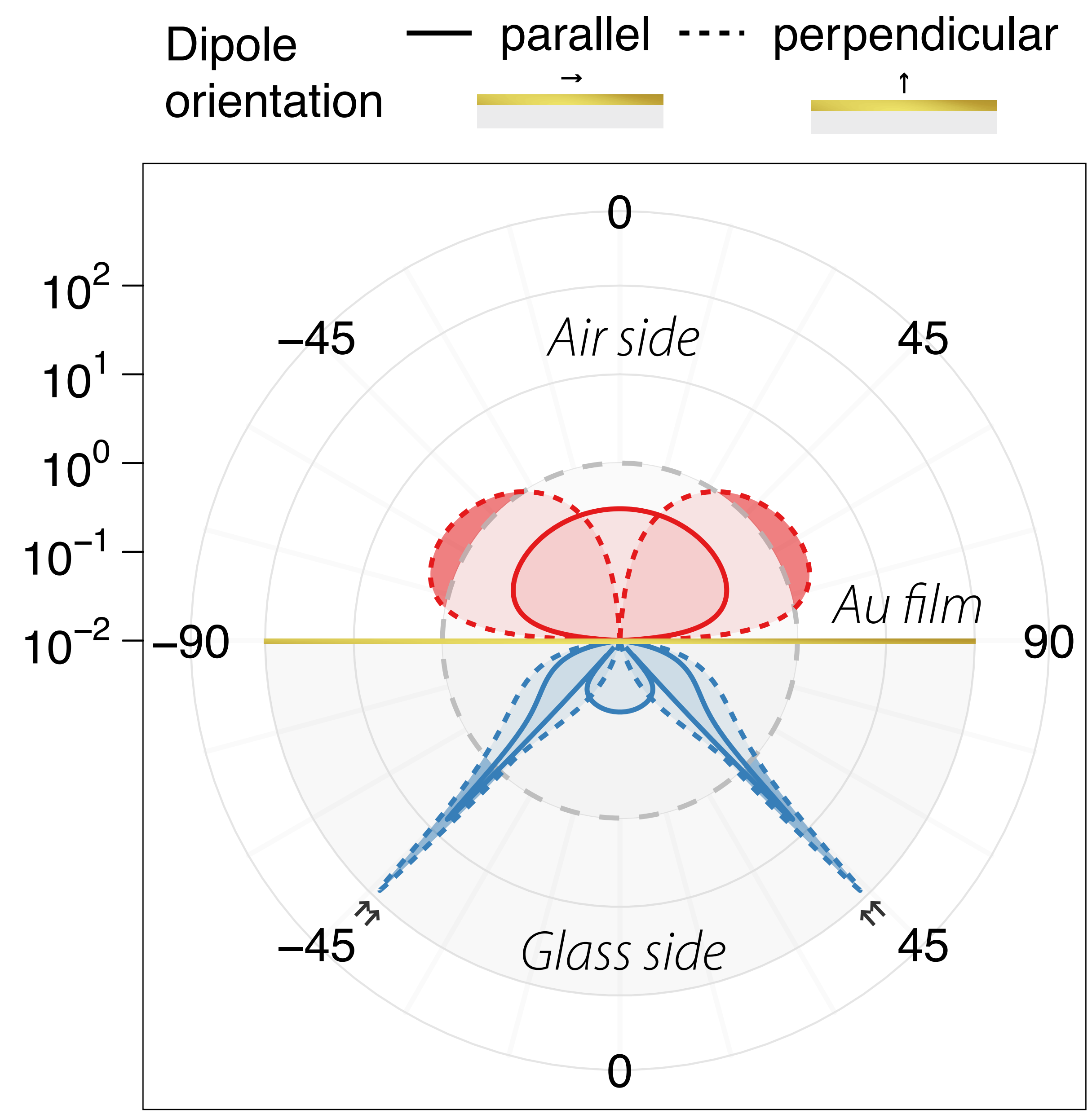
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
Relative noise, ε
Total noise
Fixed structure
Photon noise
Photon & structure limited
Photon limited
10^0
10^1
10^2
10^3
10^4
10^5
10^6
Number of spectra, N_s



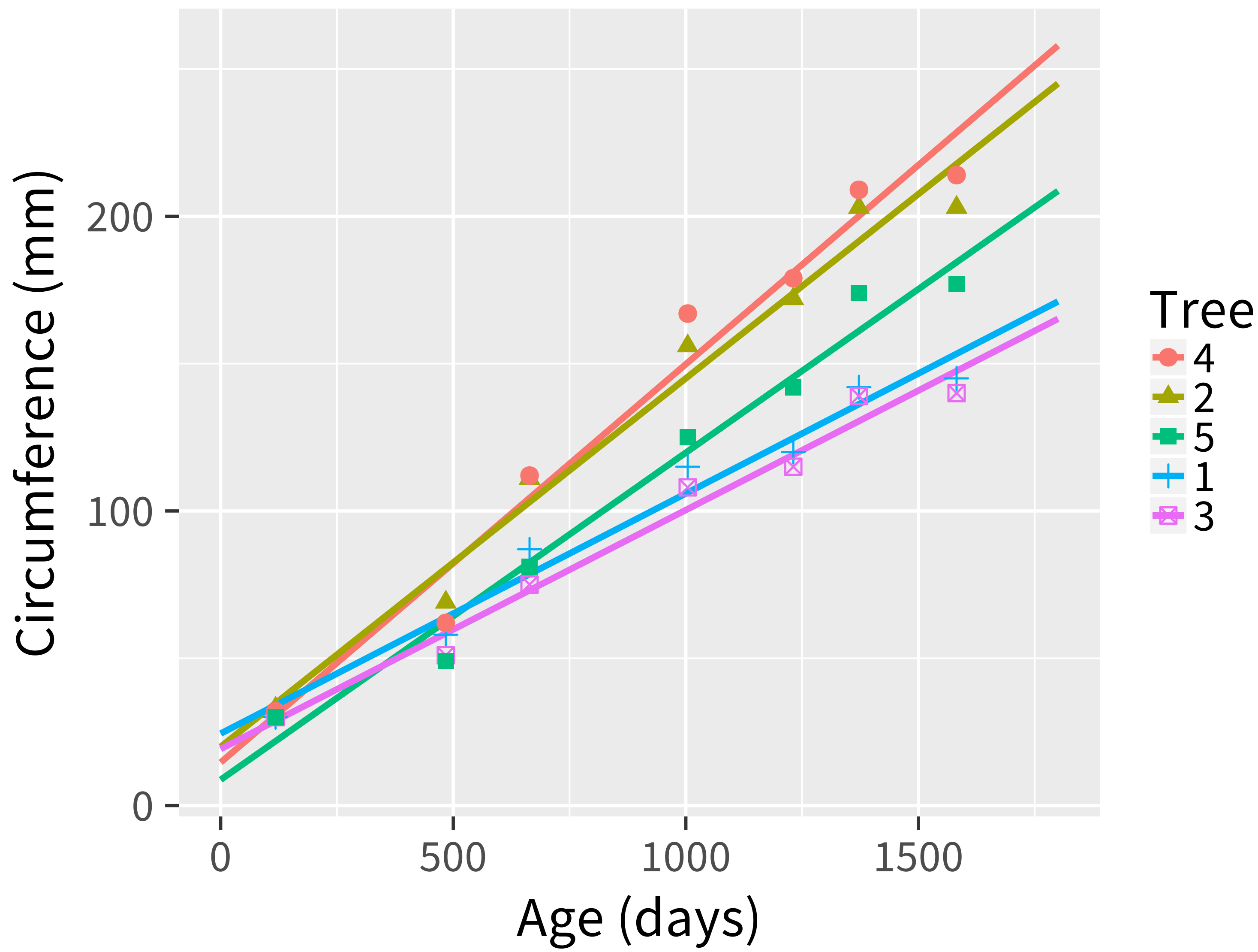
single dye
homogeneous shell
even spacing
pseudo-random
random
isotropic
radial
flat
ρ_{dye} / nm^2
0
0.2
0.4
0.6
0.8
1
1.2
1.4
σ_{abs} / nm^2
0.00
0.01
0.02
0.03
0.04
480
520
560
600
Wavelength / nm

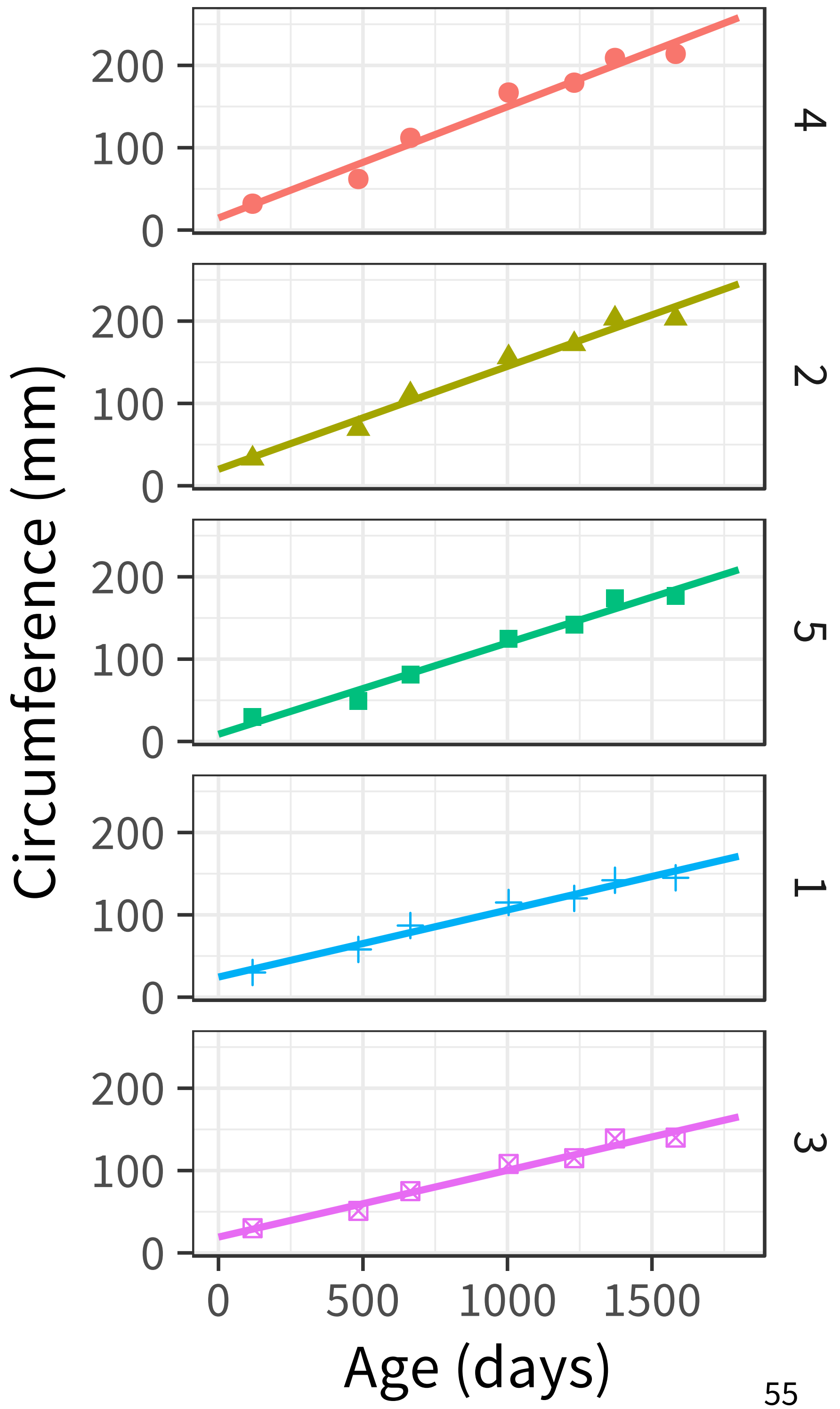
Coordinate transformations

```
plot(data, map(x, y)) +
  layer(line,  map(linetype = t)) +
  coord_polar(theta = x) +
  . . .
```



D.R.Y. PRINCIPLE





Benefits of scripting graphics

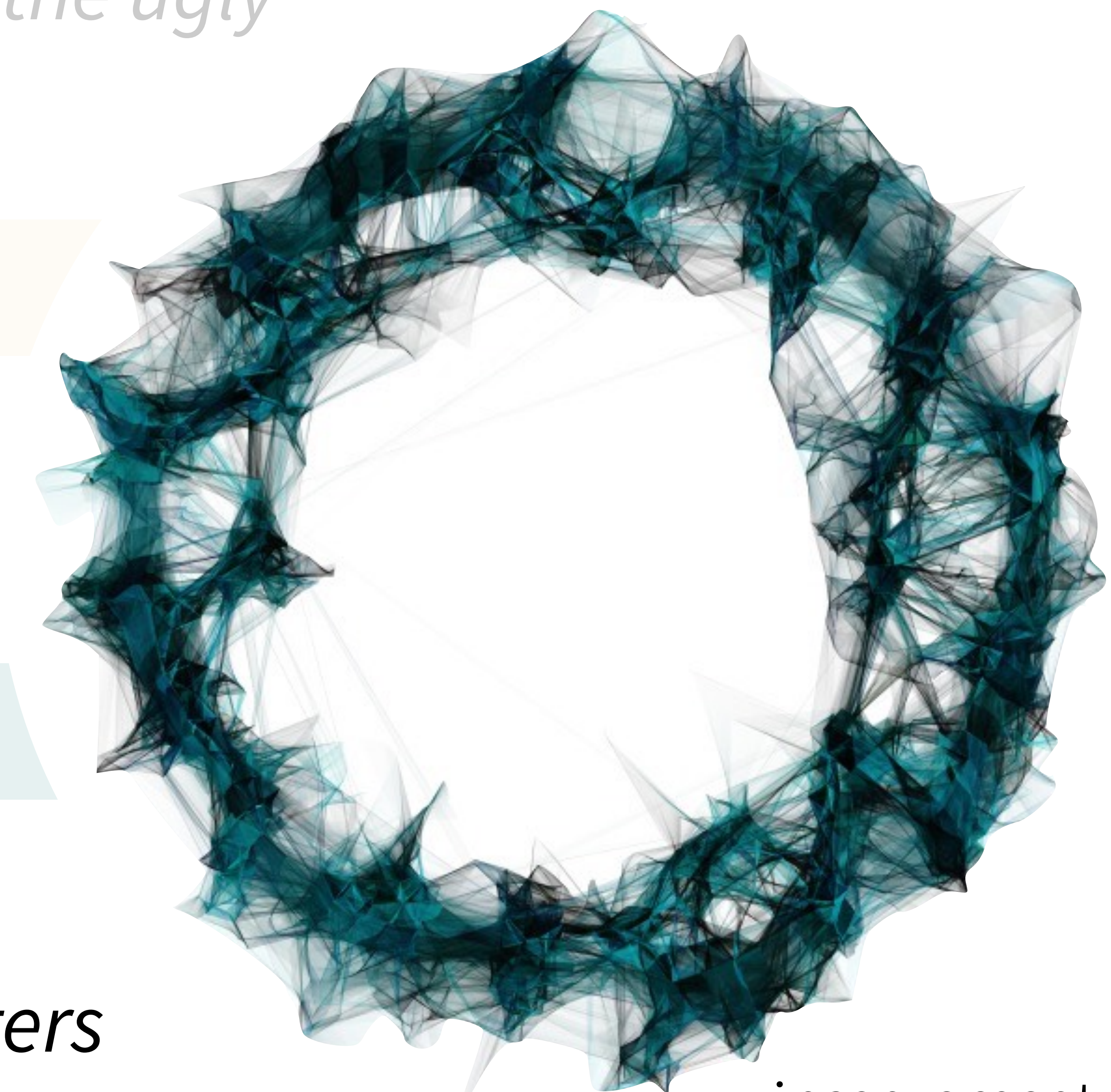
- **Explore more possibilities**
  - Save time
  - Try multiple variations
- **Consistency**
  - Reproducible code & aesthetics
  - Self-documenting analysis

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

R. Kosara

OUTLINE

- **A PHILOSOPHY OF GRAPHICS**
  - *The good, the bad, and the ugly*
  - *Tips and guidelines*
- **A GRAMMAR OF GRAPHICS**
  - *Elements of theory*
  - *Glimpse of the future*
- **A VISION FOR GRAPHICS**
  - *Aesthetics and impact*
  - *TOC figures, slides, posters*



inconvergent.net

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

The temptation of the available riches is irresistible

Jan White

Choosing colour palettes

wesandersonpalettes.tumblr.com

Why use colour?

- **Use colour to symbolise**

  Be logical & follow conventions

- **Use colour to prioritise information**

  Smaller areas brighter, larger areas lighter

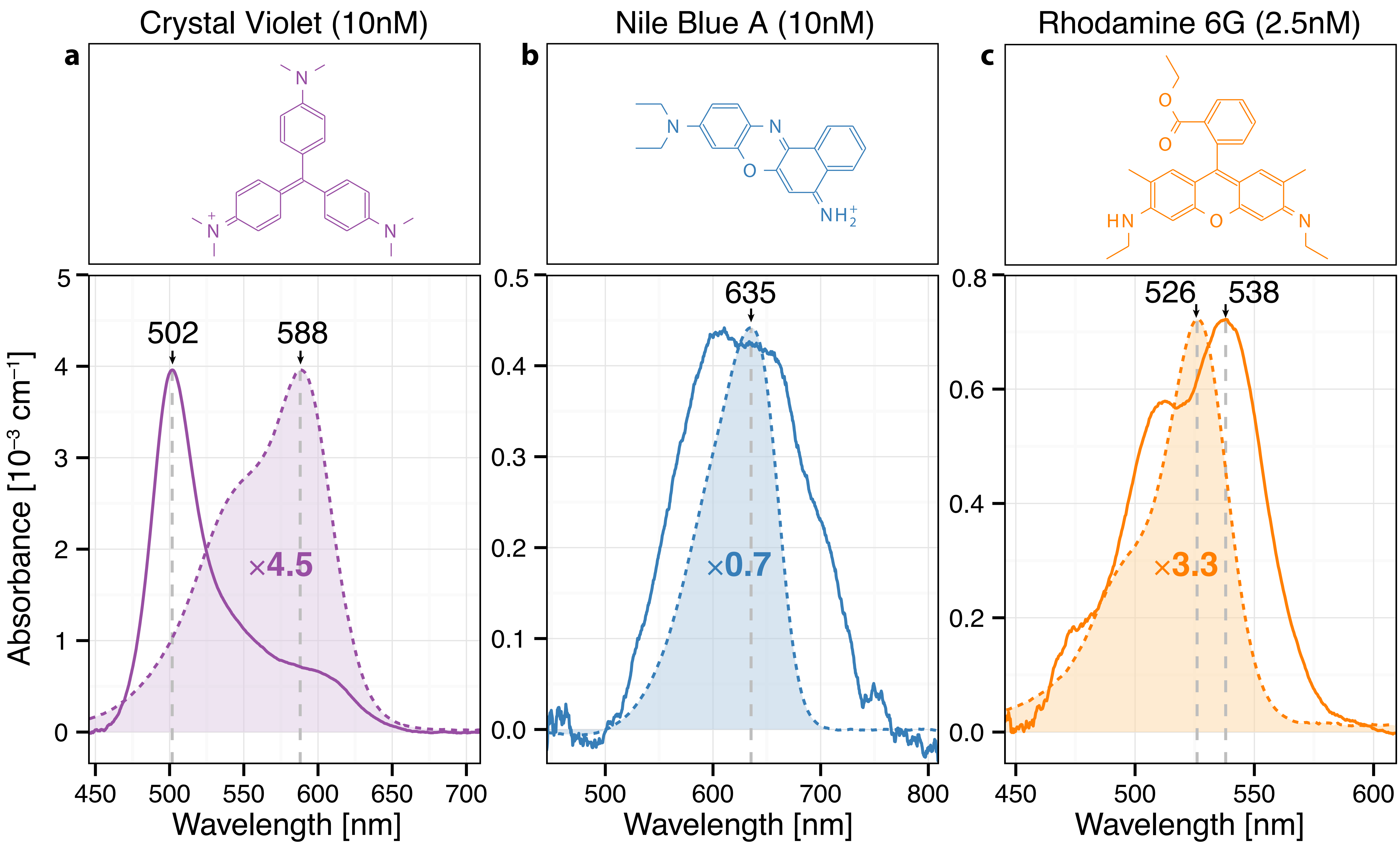
- **Use colour to identify a recurring theme**

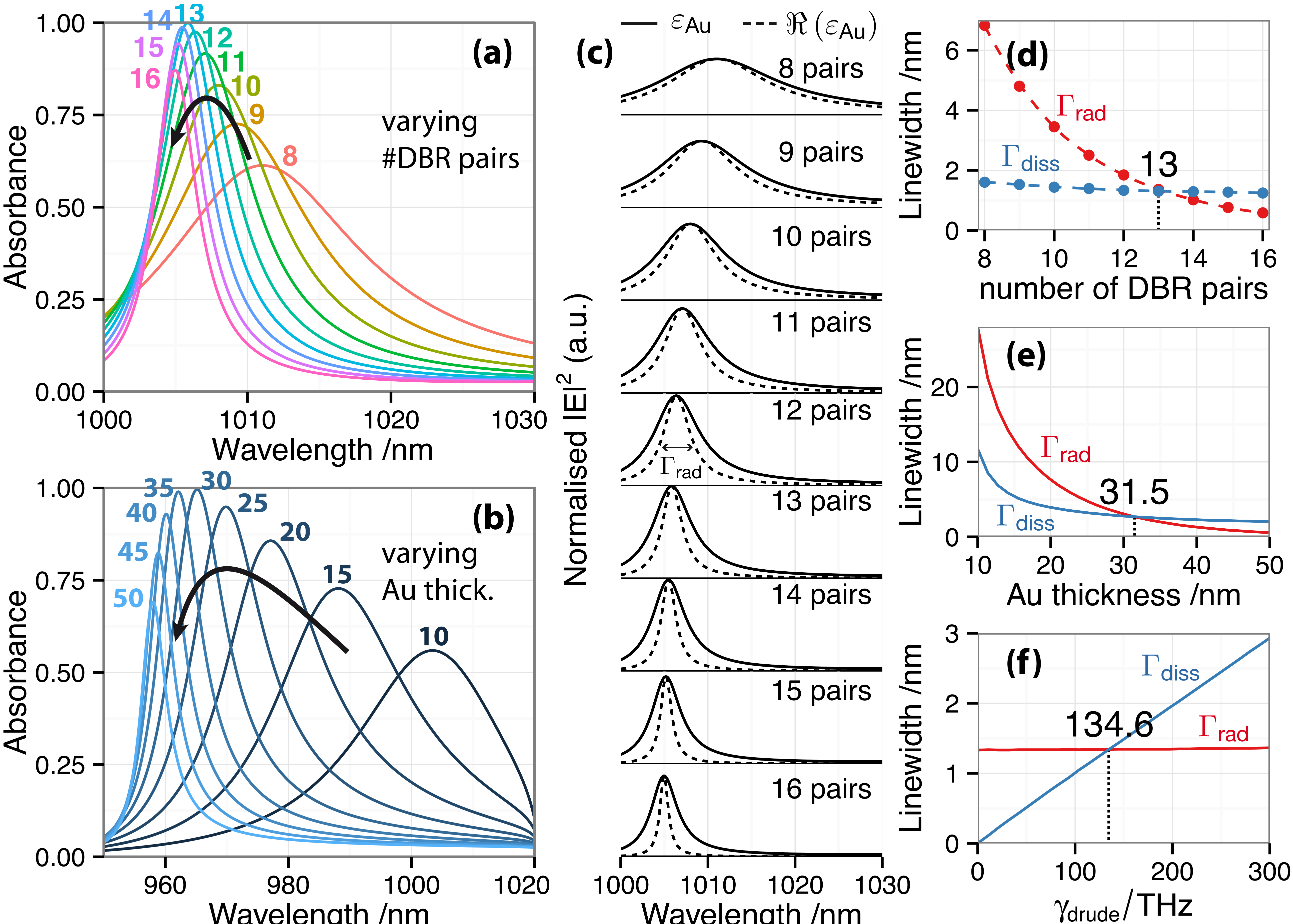
  Be consistent

CHOOSING COLOUR PALETTES

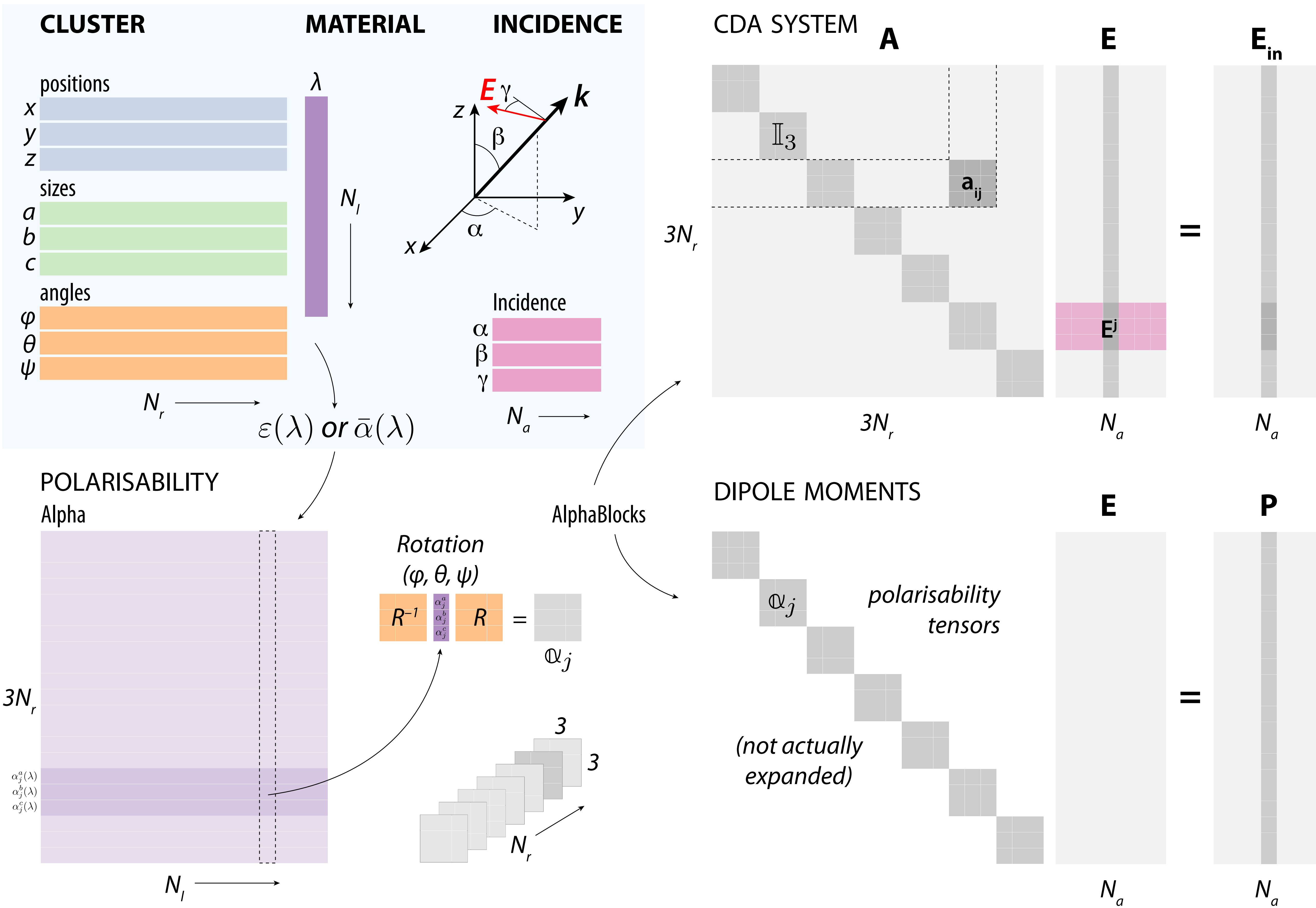
Note: ~**8%** of males, 0.5% of females, are **colour blind**

Colour and context



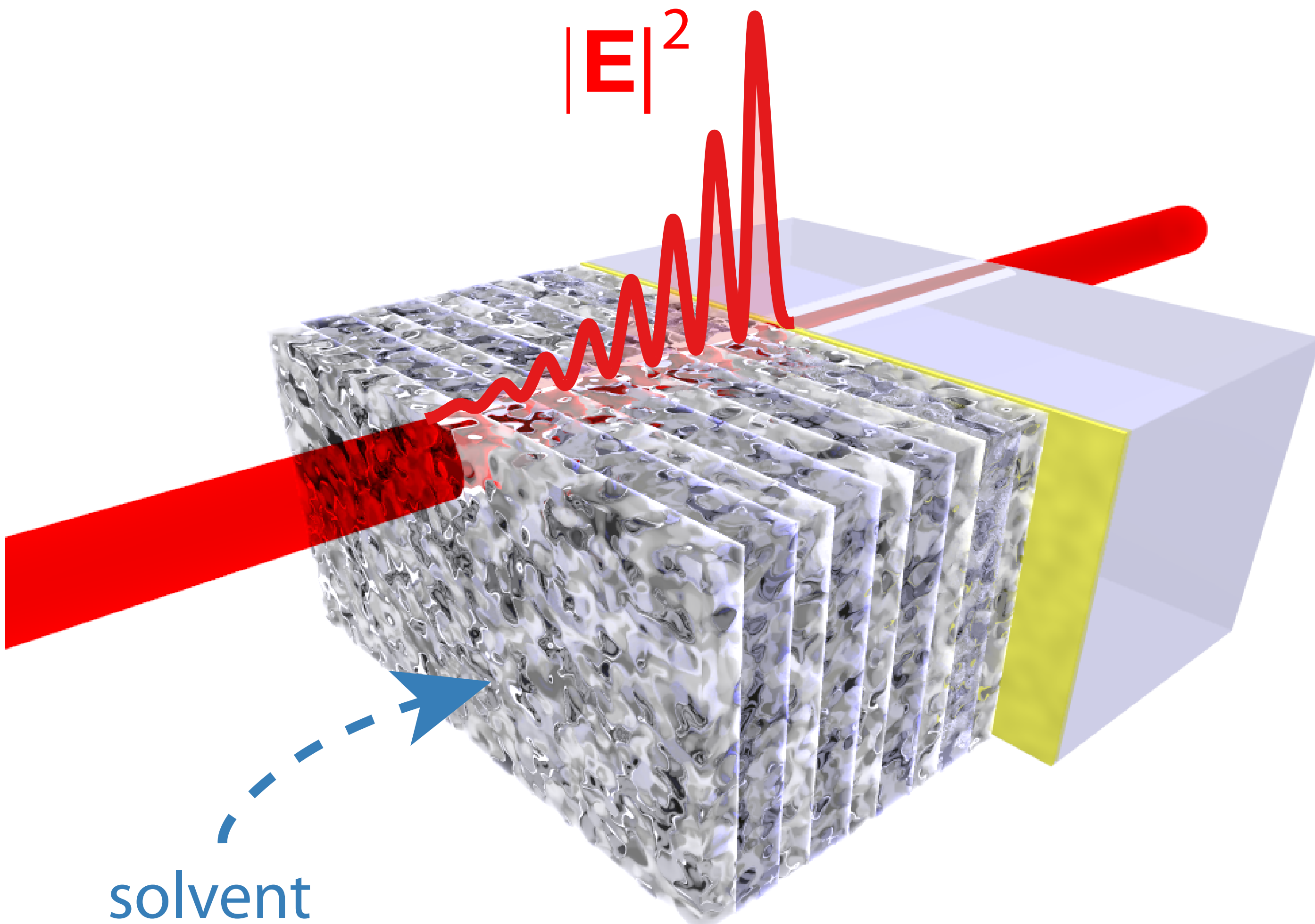


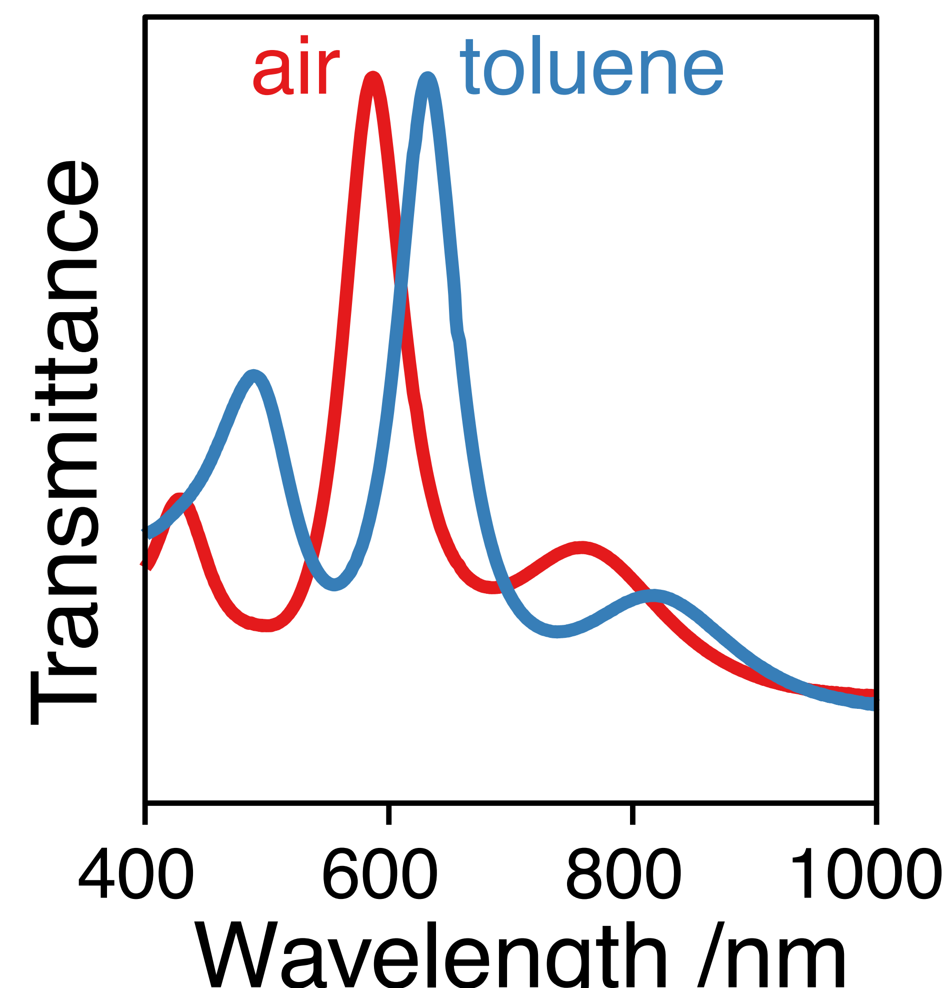
(a)
varying
#DBR pairs
Absorbance
Wavelength /nm
(b)
varying
Au thick.
(c)
8 pairs
9 pairs
10 pairs
11 pairs
12 pairs
13 pairs
14 pairs
15 pairs
16 pairs
Normalised |E|^2 (a.u.)
ε_{Au}
$\Re(\varepsilon_{Au})$
Γ_{rad}
(d)
Γ_{rad}
Γ_{diss}
13
Linewidth /nm
number of DBR pairs
(e)
31.5
Au thickness /nm
(f)
134.6
γ_{drude} / THz

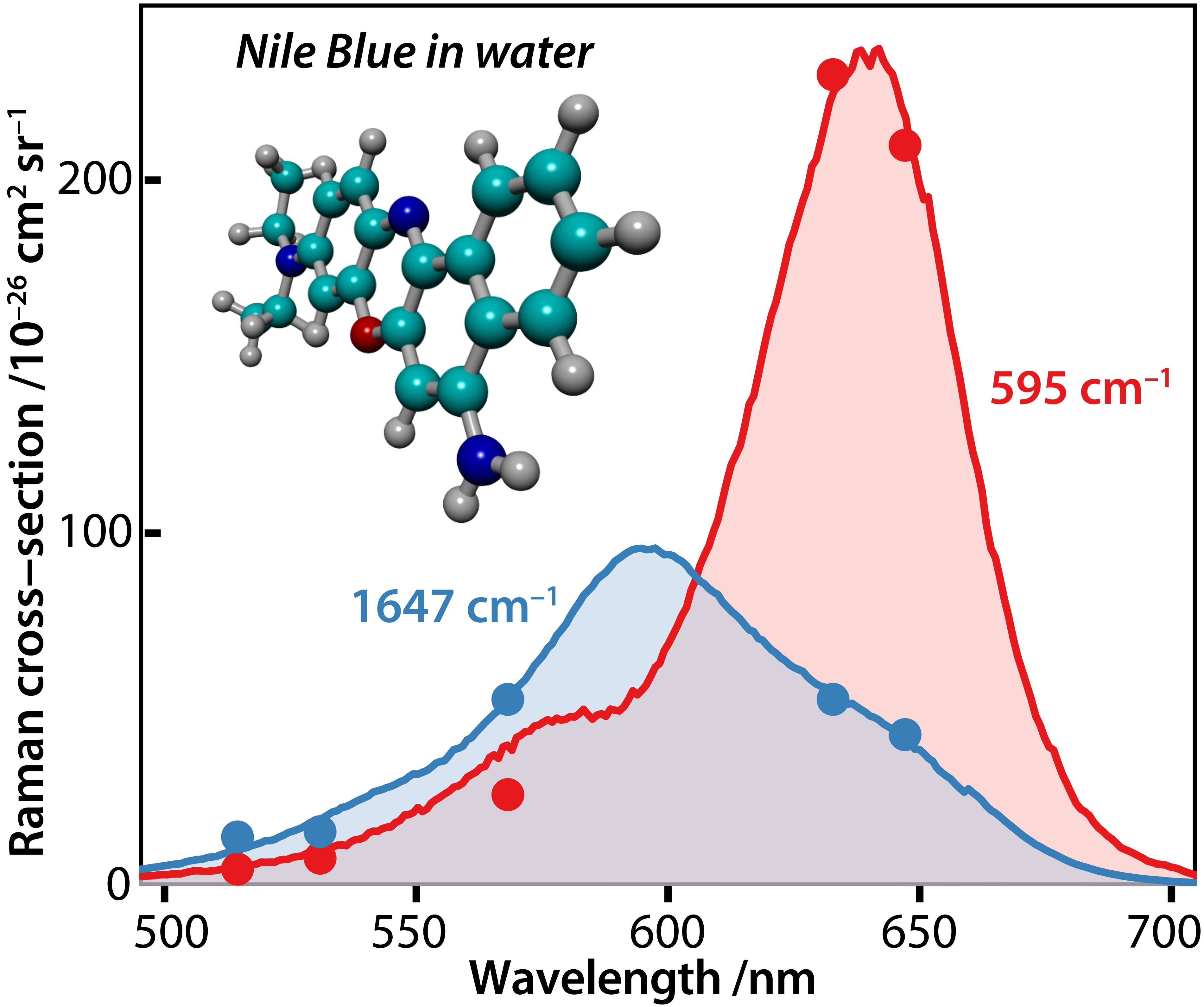


CLUSTER
MATERIAL
INCIDENCE
positions
x
y
z
sizes
a
b
c
angles
φ
θ
ψ
N_r
λ
N_l
E γ k
z
β
y
x
α
Incidence
α
β
γ
N_a
ε(λ) or ᾱ(λ)
CDA SYSTEM
A
E
E_in
I_3
a_ij
3N_r
E^j
=
3N_r
N_a
N_a
POLARISABILITY
Alpha
3N_r
N_l
Rotation
(φ, θ, ψ)
R^-1
R
=
α_j
3
3
N_r
AlphaBlocks
DIPOLE MOMENTS
E
P
α_j
polarisability
tensors
(not actually
expanded)
=
N_a
N_a

Table of contents artwork

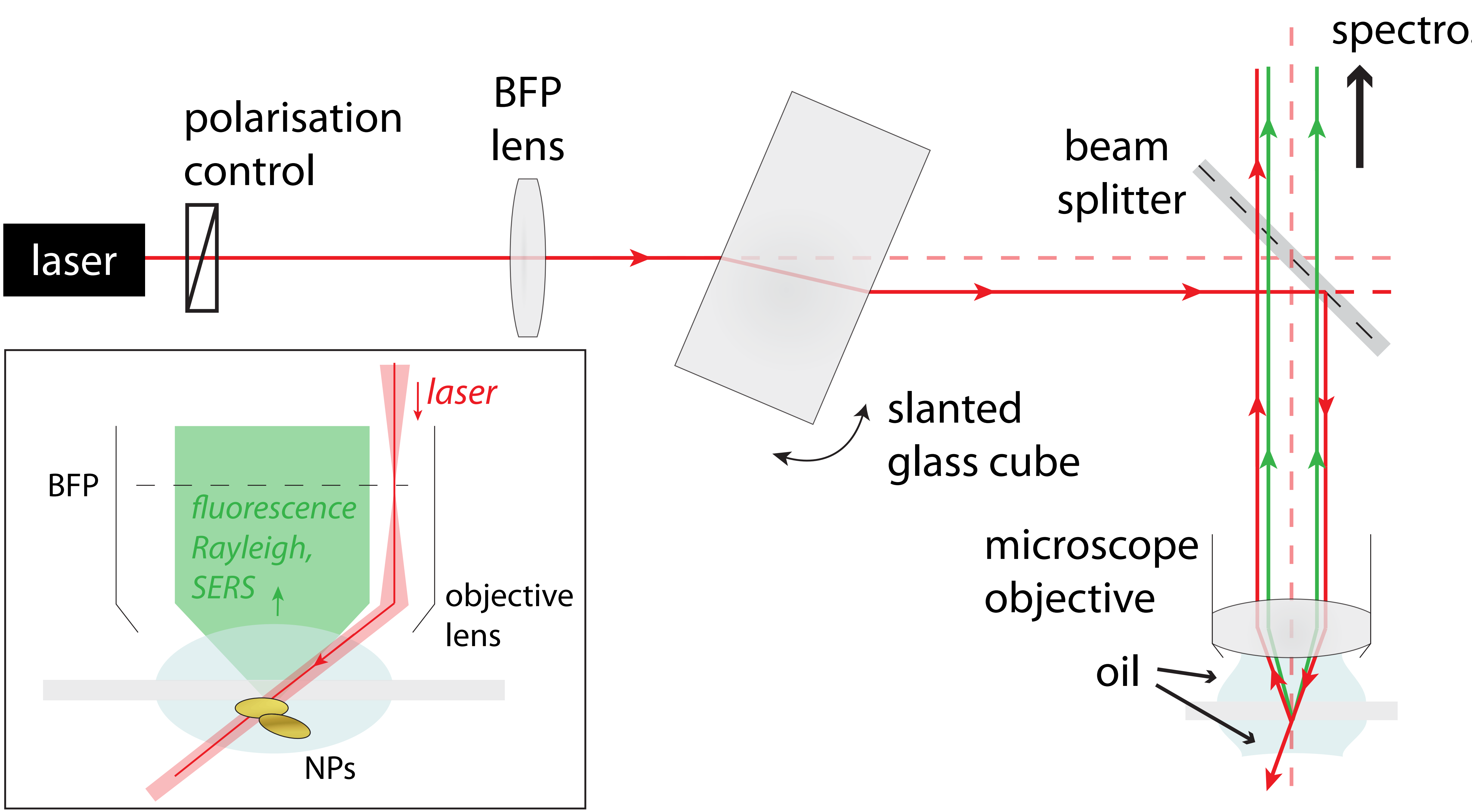


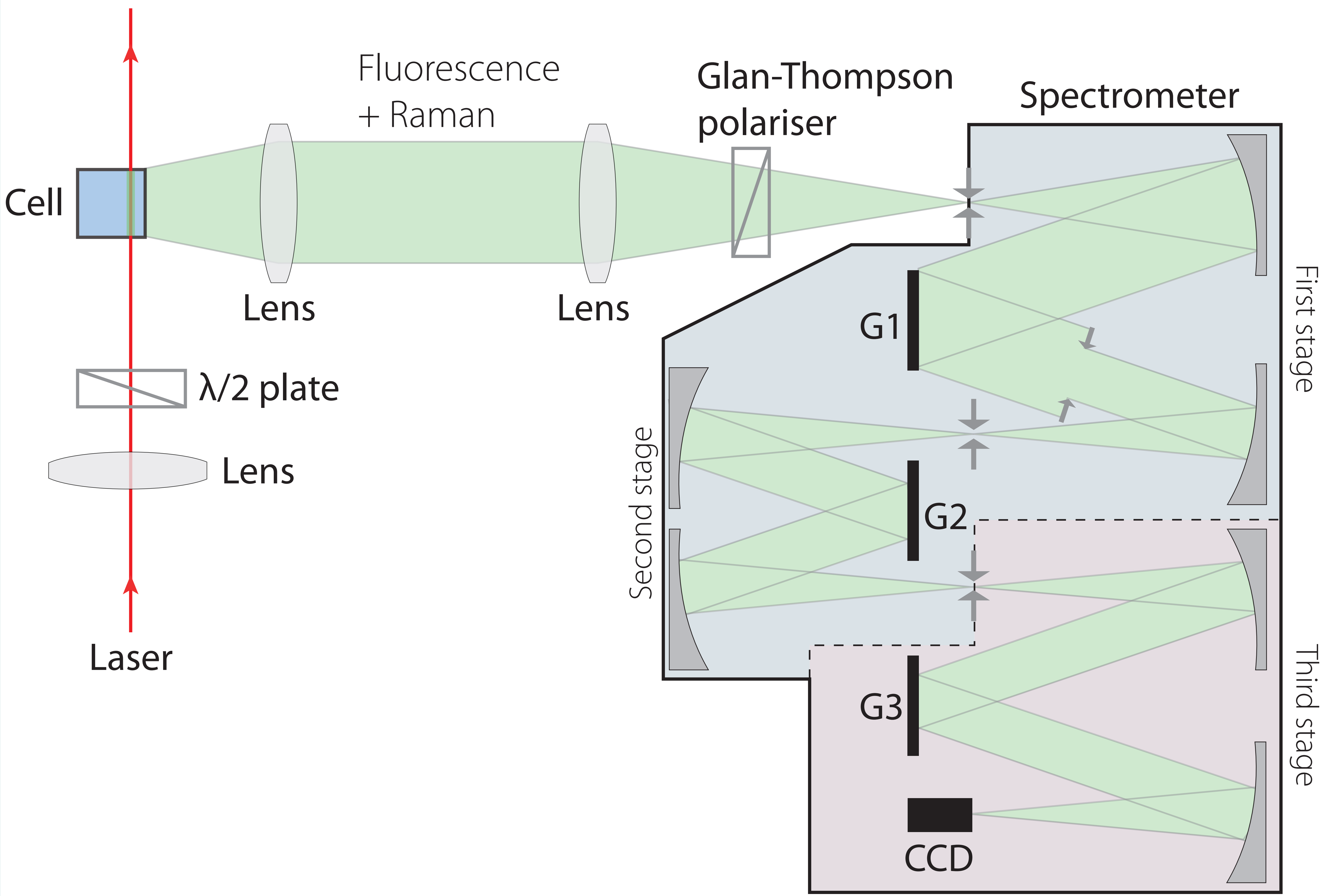


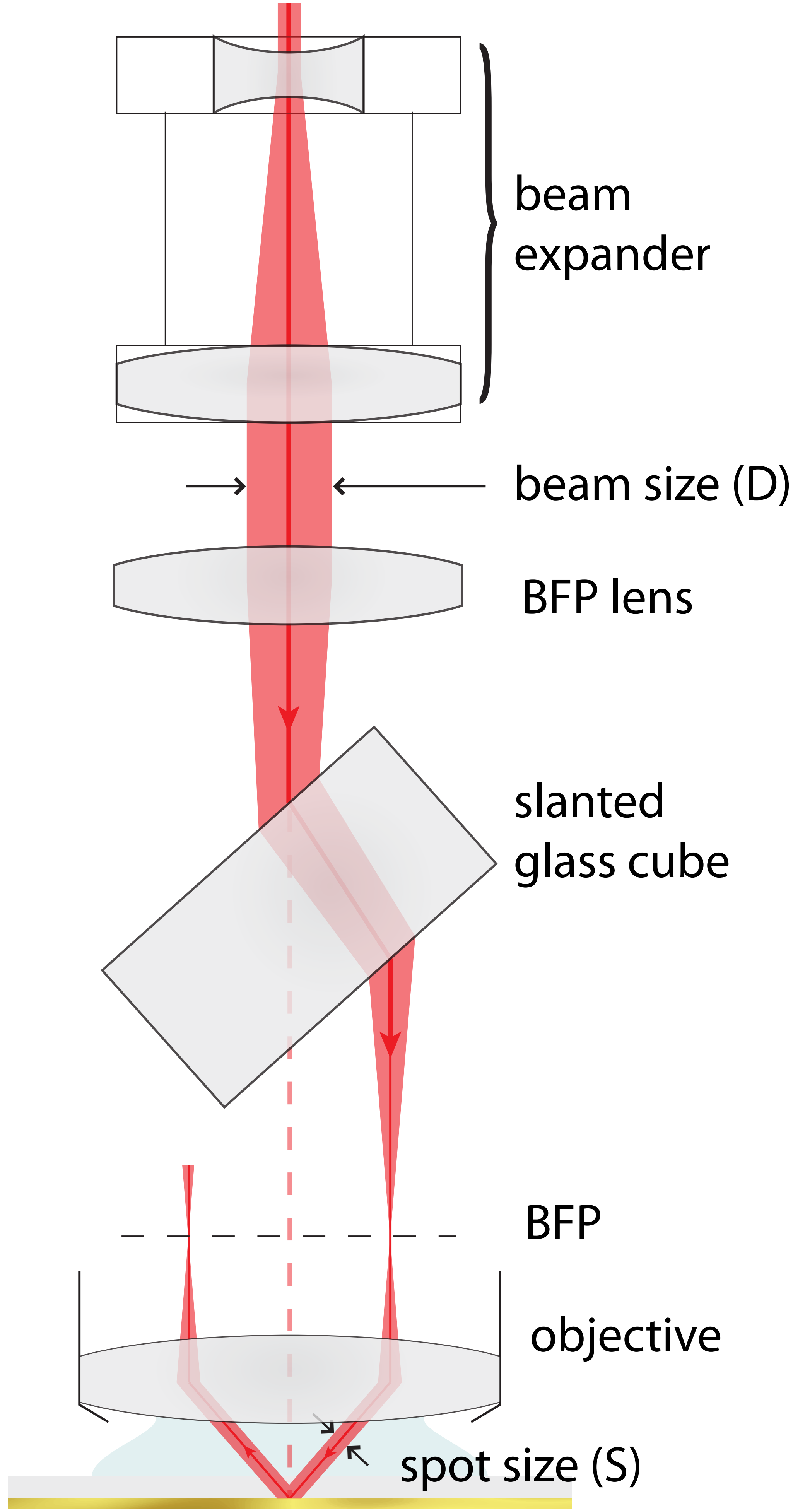


Nile Blue in water
Raman cross-section /10⁻²⁶ cm² sr⁻¹
200
100
0
500
550
600
650
700
Wavelength /nm
595 cm⁻¹
1647 cm⁻¹

Schematics: minimal & annotated

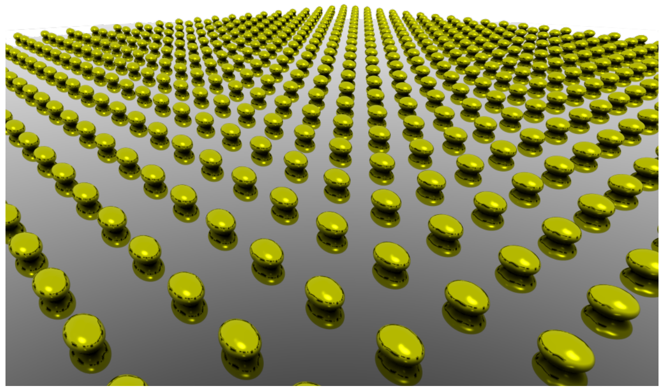



Fluorescence
+ Raman
Glan-Thompson
polariser
Spectrometer
Cell
Lens
Lens
G1
First stage
λ/2 plate
Lens
Second stage
G2
G3
Third stage
Laser
CCD


beam
expander
beam size (D)
BFP lens
slanted
glass cube
BFP
objective
spot size (S)

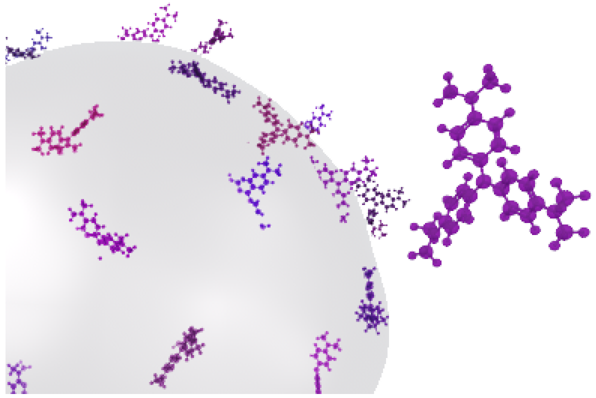
GRAPHICS FOR PRESENTATION SLIDES

PARTICLE ARRAYS

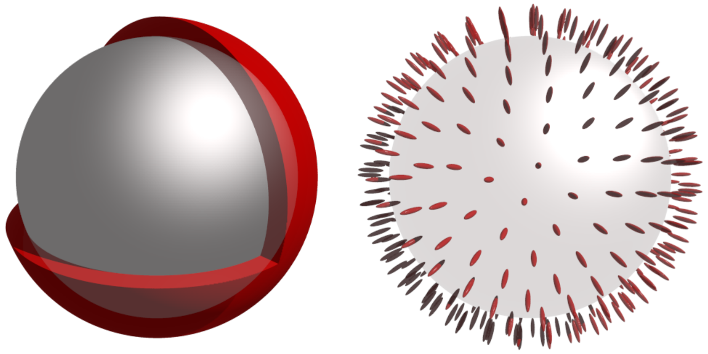


CHIRAL NANO-STRUCTURE

MOLECULES ON COLLOIDS

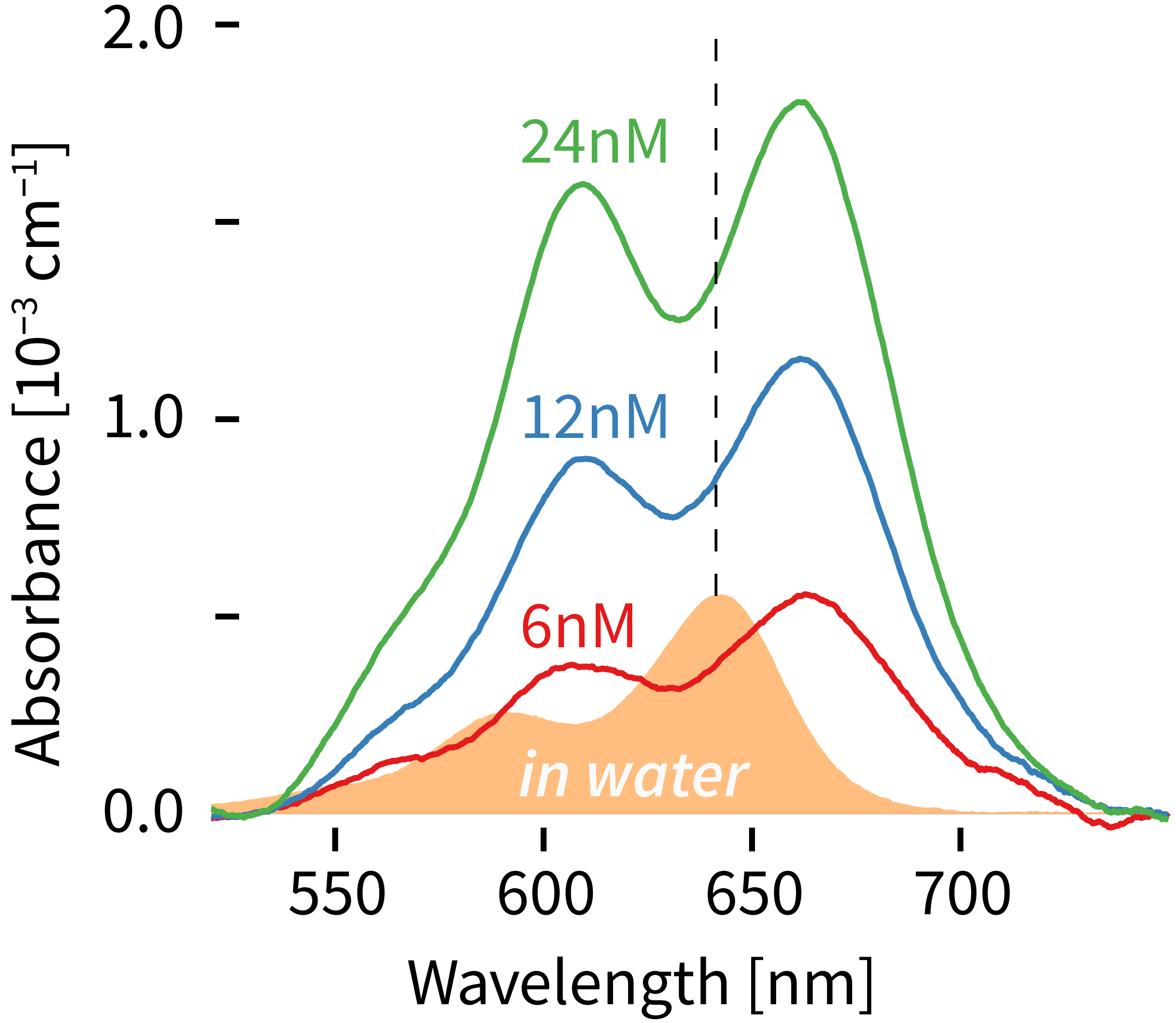


SHELLS OF INTERACTING DYES



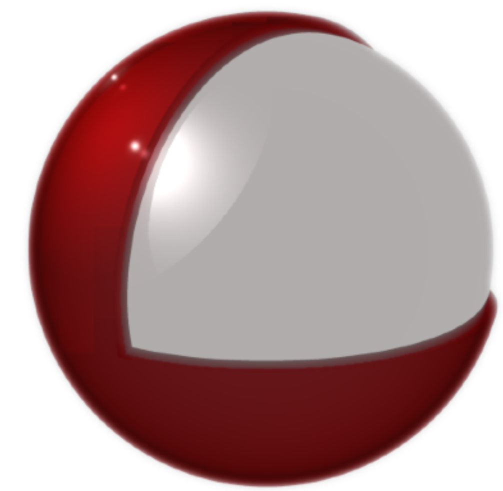
Graphics for slides – minimalist

Experiments

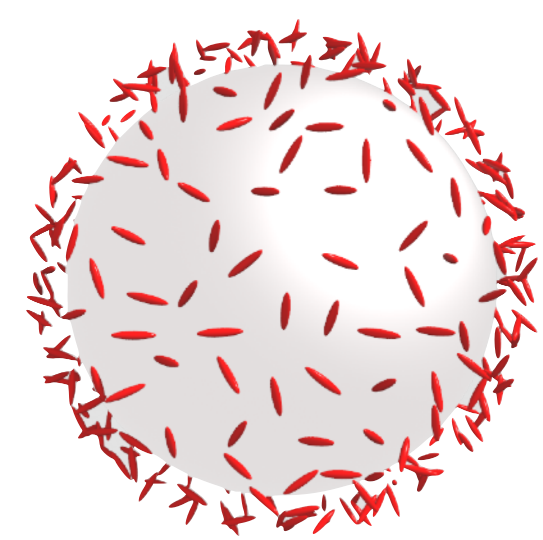


Theory

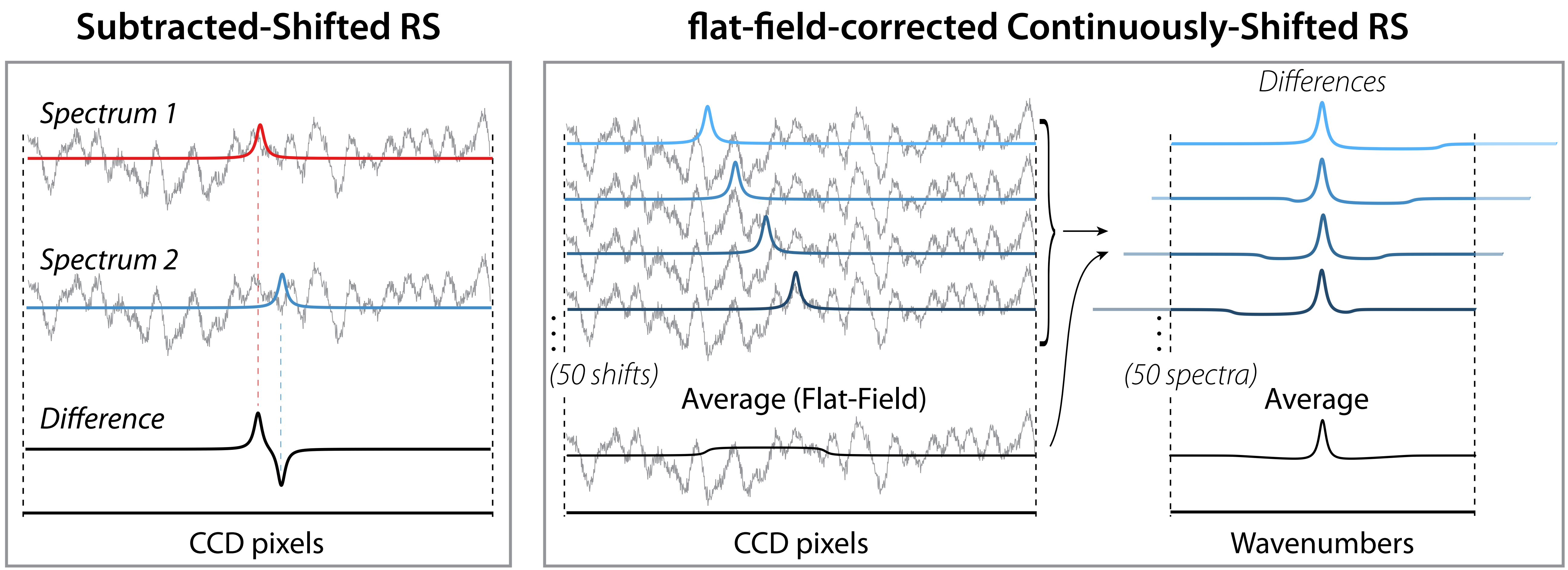
continous shell
(Mie theory)



dipoles
&
Mie theory



SLIDES – MINIMALIST



Transition Matrix

$$\mathbf{E}_{\mathrm{inc}} = E_0 \sum_{n,m} a_{nm}\mathbf{M}^{(1)}_{nm}(k_1\mathbf{r}) + b_{nm}\mathbf{N}^{(1)}_{nm}(k_1\mathbf{r})$$

$$\mathbf{E}_{\mathrm{sca}} = E_0 \sum_{n,m} p_{nm}\mathbf{M}^{(3)}_{nm}(k_1\mathbf{r}) + q_{nm}\mathbf{N}^{(3)}_{nm}(k_1\mathbf{r})$$

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

$$\mathbf{T} = \begin{pmatrix}\mathbf{T}^{11} & \mathbf{T}^{12}\\ \mathbf{T}^{21} & \mathbf{T}^{22}\end{pmatrix}$$

electric–electric
magnetic–electric
electric–magnetic
magnetic–magnetic

POSTERS

Tell them to work on a better abstract next time

JH

What are posters for?

DEVIL'S ADVOCATE

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

- **A SPECTRUM OF USES**
  - Interactive discussion vs individual viewing
  - Serious vs introductory – consider your audience
  - ¿A lesser oral presentation?


FRANCIS FORD COPPOLA
PRESENTS
Apocalypse Now
MARLON BRANDO ROBERT DUVALL MARTIN SHEEN in APOCALYPSE NOW
FREDERIC FORREST ALBERT HALL SAM BOTTOMS LARRY FISHBURNE and DENNIS HOPPER
Produced and Directed by FRANCIS COPPOLA
Written by JOHN MILIUS and FRANCIS COPPOLA Narration by MICHAEL HERR
Co-Produced by FRED ROOS, GRAY FREDERICKSON and TOM STERNBERG
Director of Photography VITTORIO STORARO Production Designer DEAN TAVOULARIS Editor RICHARD MARKS
Sound Design by WALTER MURCH Music by CARMINE COPPOLA and FRANCIS COPPOLA
R TECHNICOLOR® DOLBY STEREO United Artists AN OMNI ZOETROPE PRODUCTION


The world
will never be the same
once you've
seen it through the eyes of
Forrest Gump.
Tom
Hanks is
Forrest
Gump
July 6

Guidelines for posters

- **Tell a compelling story**
  - Focus on main points
  - Attract the viewer's attention
  - Use few words, lists
- **Test for effectiveness**
- **Posters are a hybrid medium**
  - Complement with discussion (prepare it)
  - Consider other supports (tablet, 3D model, …)
  - Be original, but not distracting (message first)

POSTER TIPS

- **BE MINIMALIST**
  - 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, think of negative space
  - Be ready to present

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

Designing nanoparticles for sensing

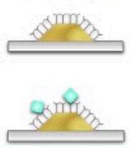
Baptiste Auguié (†)
Andy Murray
Bill Barnes

†: ba208@ex.ac.uk
University of Exeter
Stocker Road,
Exeter, Devon, EX4 4QL, UK

Goal:

to optimize the optical detection of biomolecules using metallic nanoparticles

- *defining sensitivity: how small an amount of material can we detect above the noise level*
- *sensitivity depends on the setup: distinction between intrinsic sensitivity and technical limitations*



the gold particles are immobilized on a substrate,

When the target molecules bind to the surface, the change in local refractive index is seen in the optical response (scattering, extinction).

Exploiting sub-wavelength localisation of optical fields

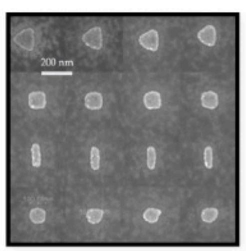
Optimizing the particle shape, size, and configuration,

- *evaluate the influence of each parameter on the sensitivity*
- *appreciate technical constraints (camera sensitivity, size, sources of noise, reproducibility)*

-> trade-off for real-life application

A variety of fabrication and characterisation techniques

e-beam lithography (EBL) scanning electron microscopy (SEM)



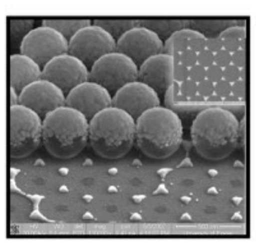
- *a 10 nm fabrication resolution is easily achieved using EBL*
- *by changing the particle shape and size, we tune the resonance to favorable spectral regions.*
- *polycrystalline nature is the main limitation, both in terms of reproducibility and material properties: surface roughness and grain boundaries broaden and flatten the resonance for high aspect ratio*

Producing large areas

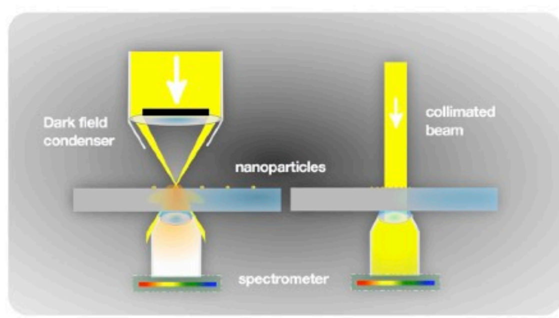
Three techniques allow us to fabricate over large areas,

- *nanosphere lithography*
- *thin film evaporation and annealing*
- *colloidal growth and drop-coating deposition*

Despite their relative ease of manufacture, variability in particle size and shapes lead to strong inhomogeneous broadening, and issues of reproducibility.



Spectroscopy



- single particle optical characterisation using dark field spectroscopy
- epi-illumination allows the use of a flow cell to detect changes in the spectral response in different biological environments
- extinction measurements at normal incidence

Single particle response

Aspect ratio and spectral position

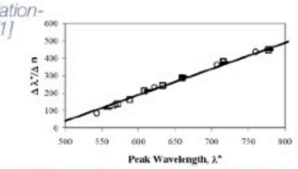
- *a gold sphere has a broad resonance (LSPR)*
- *changing the aspect ratio red-shifts the resonance, where gold behaves more like a Drude metal*
- *trade off between radiative damping and signal intensity*

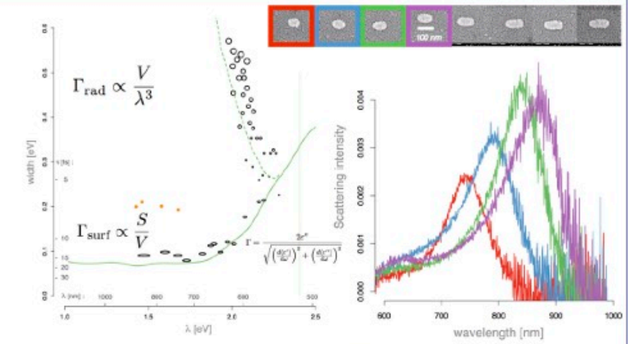
Sensitivity to refractive index

- *bulk index change: depends only on resonance position*
- *thin layer: influence of the near-field extent ("hot spots")*

bulk index sensitivity: linear relationship with resonance position. [1]

Data: *nanocylinders (circles), nanodisks (squares, hollow nanoshells (diamonds)*

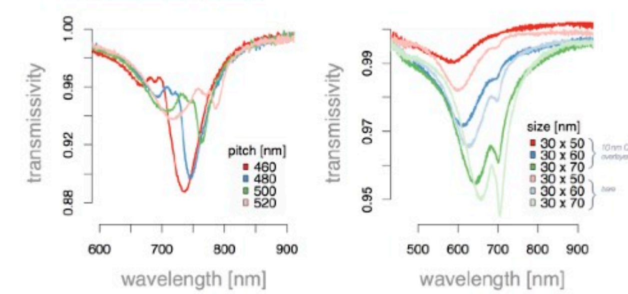




Left: *the width of dipolar resonances. The green curve is the theoretical limit accounting for gold's material properties (Landau damping), while the dashed line is the result of Mie modelling for spheres of increasing diameter. Black points are taken from the literature [2], for gold spheres and nanorods (circles and ellipses resp.). Orange points are taken from our particles.*

Right: *gold nanorods SEMs and scattering spectra. The aspect ratio dictates the position of the LSP resonance.*

Particle arrays spectra



Left: *effect of varying the pitch on the transmission spectra. The particles are of constant size and shape. Surrounding medium is homogeneous, n=1.52.*

Right: *transmission spectra at normal incidence for three gold nanorod arrays (pitch 460 nm). Sizes range from 30 x 50 to 30 x 70 nm. A duplicate array shows a consistent change after deposition of a thin CaF_2 layer (15 nm, n=1.44).*

Many particles: collective response

Additional freedom in design

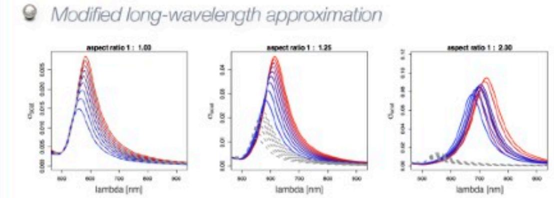
Building upon the knowledge of single particles response, new challenges and opportunities arise from the interaction of a collection of particles

- *dimers lead to a splitting of the dipolar mode*
- *short-range interactions can lead to high field enhancement*
- *ordered arrays can exhibit diffractive coupling [3]. We study the influence of particle shape, separation, and refractive index of the environment*

Modelling

Several numerical schemes have been used

- *Discrete Dipole Approximation, coupled dipole approximation*
- *T-matrix*
- *Mie theory*
- *Modified long-wavelength approximation*



T-matrix calculations of the scattering cross-section for gold ellipsoids coated by a thin layer (n=1.5) of increasing thickness (step 5nm), for three different aspect ratio. The surrounding medium is water. Grey curves are for incident polarisation along the short axis, colored curves are for the long axis.

Future directions

Investigate ordered and disordered arrays

- *adapt to the asymmetric environment (substrate/water)*
- *effect of particle variability*
- *study of polarisation conversion*

References

1. Plasmonic Nanoparticles: Factors Controlling Refractive Index Sensitivity. PhD thesis. M. Miller , 2007
2. Sonnishen et al. "Drastic Reduction of Plasmon Damping in Gold Nanorods". Phys. Rev. Lett., 88(7):077402, Jan 2002.
3. Hick et al. "Controlling plasmon line shapes through diffractive coupling in linear arrays of cylindrical nanoparticles fabricated by electron beam lithography". Nano Lett, 5(6):1065–70, Jun 2005.

Attogram

2D Attogram Surface Plasmon Resonance Imaging

University of Exeter

The University of Nottingham

Plasmonic Optical Activity

Baptiste Auguié

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Co-workers:
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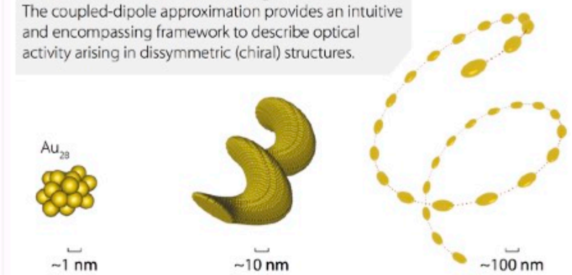
Luis M. Liz-Marzán
Química Orgánica
José Lorenzo Alonso-Gómez
M. Magdalena Cid

Motivation

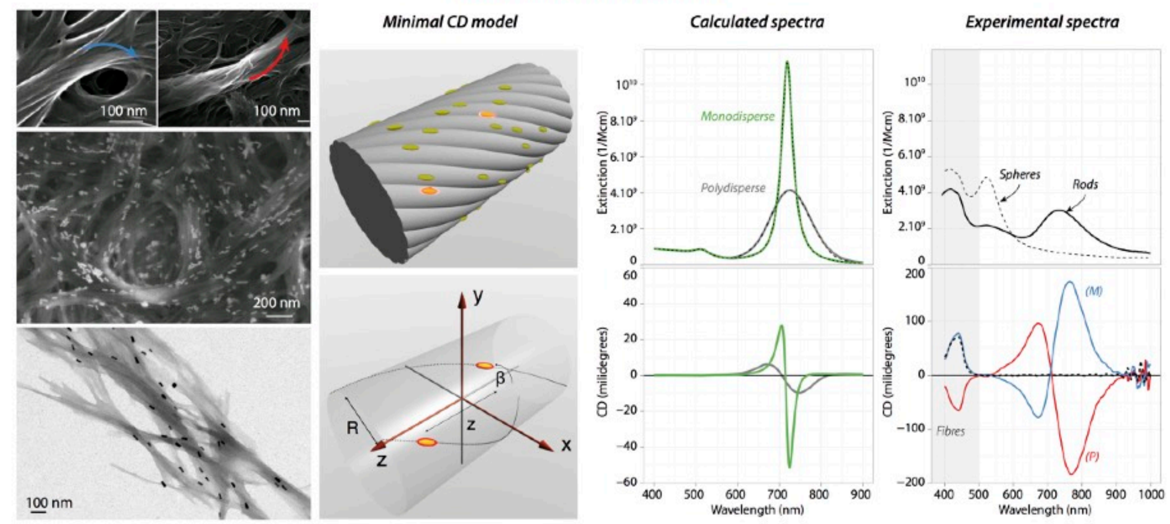
A natural pairing with stereochemistry and biological applications, conjointly with the pursuit of negative refraction, have triggered an intense activity in the design of chiral metamaterials, from microwave frequencies to the visible. In the vast array of proposed designs, the focus has been largely on periodic, often 2D structures. In contrast, colloidal synthesis offers the perspective of producing truly 3D chiral and isotropic structures *en masse*, with a versatile and complementary manufacturing process.

Different scales of metallic building blocks
The coupled-dipole approximation provides an intuitive and encompassing framework to describe optical activity arising in dissymmetric (chiral) structures.



Plasmonic nanostructures from colloidal chemistry can enrich the emerging field of metamaterials and widen its spread of applications with hybrid designs.

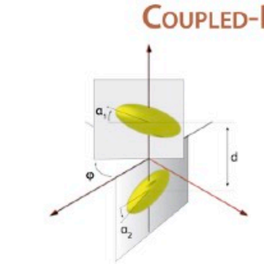
Experimental Results

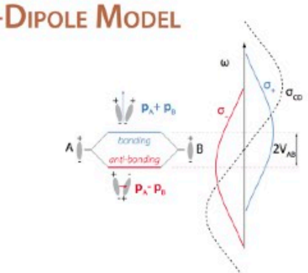


Highly-symmetric shapes such as nanorods do not generally produce optical activity, and an average ensemble of such particles freely moving in solution is intrinsically achiral. A rapidly expanding number of studies [1–3] (and refs. therein) have put forward the development of strong optical activity via a chiral conformation of aggregates ordered onto a suitable template.

The data reported above were obtained from assemblies of gold nanorods onto helical fibres [1]. The difference in extinction for left-handed and right-handed circularly polarised light, defined as circular dichroism (CD), presents a mirror-image spectrum for the two fibre enantiomorphs. Modelling suggests such optical activity results from electromagnetic interaction between nanorods.

Coupled-Dipole Model





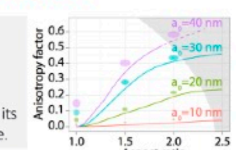
Chiral dimer of nanorods
Minimal model of plasmonic optical activity [2–4]. Coupling between the plasmon modes + chirality.

Exciton-coupling
Original theory of coupled-dipoles, recently revisited in the context of plasmon hybridisation.

The intense CD signals coincide with the excitation of localised plasmon resonances, and offer a promising avenue of research at the interface between nano-optics, plasmonics, and stereochemistry. The characteristic bisignated lineshape of the CD spectra is reminiscent of a parent mechanism known as exciton-coupling in organic chemistry.

Outlook

Beyond what we know –
Building on these rich analogies, assemblies of plasmonic particles provide new perspectives into the mechanisms of optical activity and its relation to chirality at the nanoscale.



g-factor
Increase or CDA break-down?

With regards to nano-optics and plasmonics, we propose:

- *T-matrix modelling, beyond the coupled-dipole approximation (CDA)*
- *Contribution of higher-order modes; influence of scattering/absorption ratio*
- *EE(G|L)S / Cathodoluminescence mapping of a single chiral cluster*
- *CD spectroscopy as a tool to investigate the symmetry of plasmonic assemblies*
- *Large-scale numerical optimisation of optical activity in nanoparticle clusters*

References

[1] A. Guerrero-Martinez *et al.* Angew. Chem. **50** (2011)
[2] B. Auguié *et al.* J. Phys. Chem. Lett. **2** (2011)
[3] A. Guerrero-Martinez *et al.* Nano Today **6** (*Review*, 2011)
[4] http://cran.r-project.org/web/packages/cda (*open-source*)

Thanks: Javier García de Abajo (CSIC, Madrid)

Radiative Correction for Electromagnetic Scattering

Eric Le Ru, Walter Somerville, Baptiste Auguié

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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 $P_{\text{ext}} = ½\omega\text{Im}(\alpha_0)|E_{\text{inc}}|^2$
- Also the power absorbed, P_{abs}, in the electrostatics approximation
- Energy conservation $P_{\text{ext}} = P_{\text{abs}} + P_{\text{sca}}$ is violated for optical properties

Self-field corrected polarizability

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

- Enforces energy conservation, but G is infinite…
- Common prescription: use the finite, imaginary part

$$\alpha = \frac{\alpha_0}{1 - i\frac{k_1^3}{6\pi\epsilon_0\epsilon_1}\alpha_0}$$

— 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

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

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

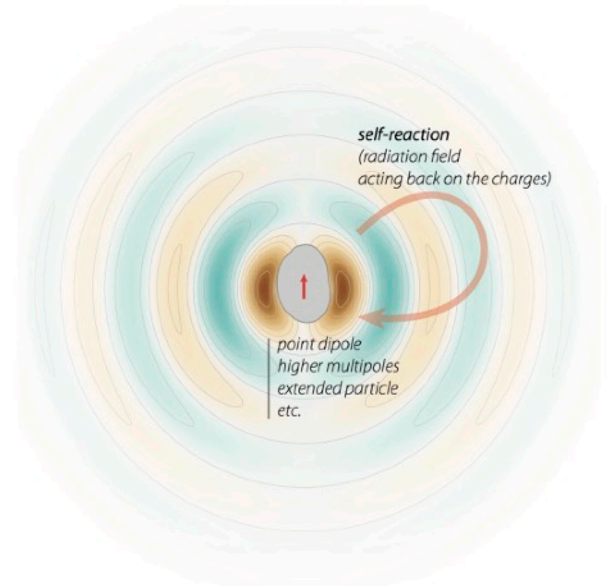
Cayleigh transform

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 impression of self-reaction

— Rigorous RC in the T-matrix Framework —

- Energy conservation is expressed as $\mathbf{K}=\mathbf{K}^\dagger$ (non-absorbing)
- Absorbing particles: $i\mathbf{K}-i\mathbf{K}^\dagger$ is Hermitian positive semi-definite (**K** is *dissipative*) (generalizes $\text{Im}(K) \geq 0$ 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, $K_d^{(0)} = -iT_d^{(0)} = \frac{k_1^3\alpha_0}{6\pi\epsilon_0\epsilon_1}$

We justify

$$\alpha = \frac{\alpha_0}{1 - i\frac{k_1^3}{6\pi\epsilon_0\epsilon_1}\alpha_0}$$

Recent examples scattered in the literature

General multipole correction from Mie theory [5]

$$\alpha_n = \left[1 - \frac{i(n+1)k^{2n+1}}{n(2n-1)!!(2n+1)!!}\alpha_n\right]^{-1}\alpha_n$$

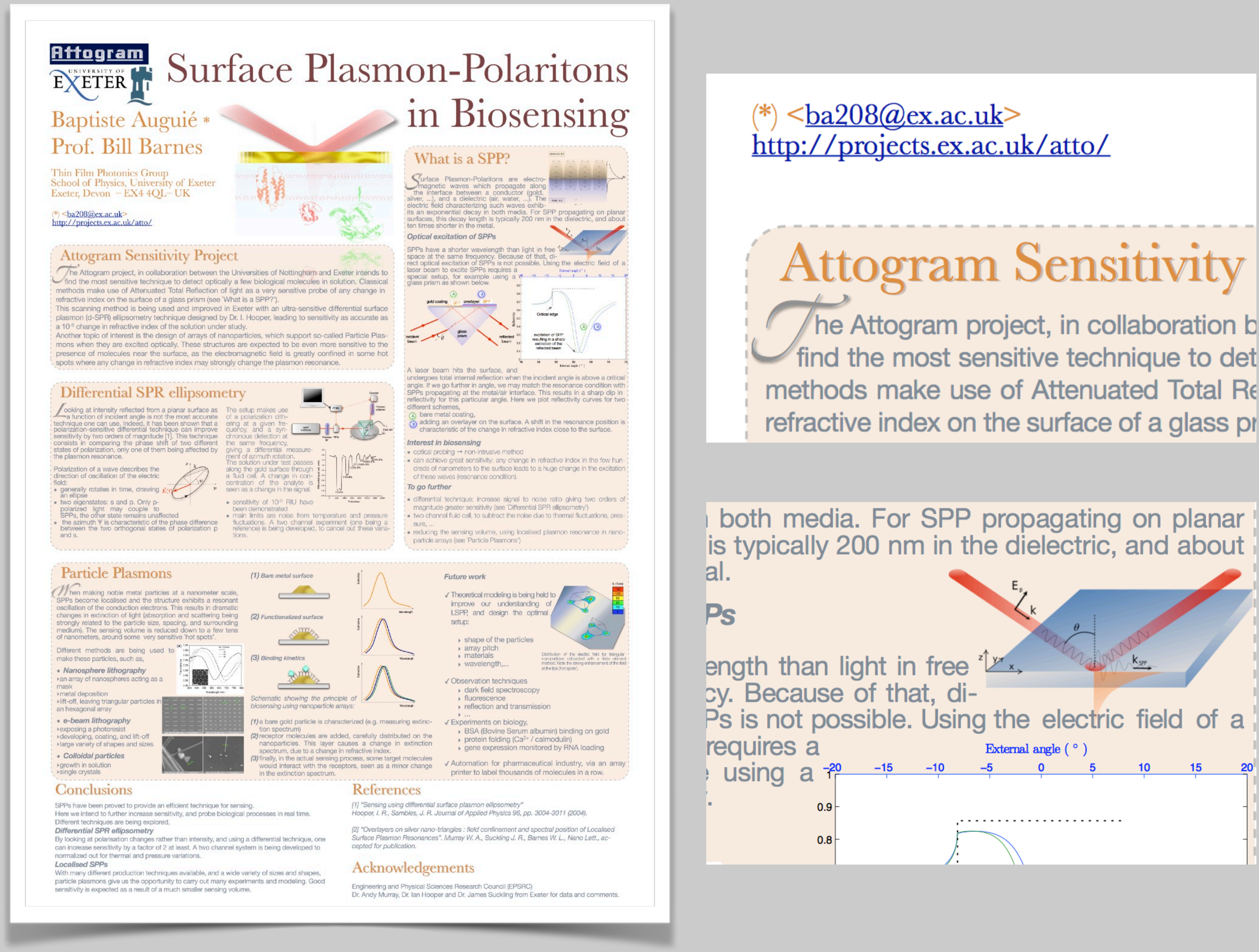
Bianisotropic lossless scatterers [6] also [7] with magnetoelectric coupling

$$\alpha^{-1} - (\alpha^{-1})^\dagger = -\frac{ik^3}{3\pi}\begin{pmatrix}\mathbf{I}/\epsilon_0 & 0\\ 0 & \mathbf{I}/\mu_0\end{pmatrix}$$

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 (1982)
[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**, 3931 (2009)
[6] P. A. Belov *et al*, Tech. Phys. Lett. **29**, 718 (2003)
[7] I. Sersic *et al*, Phys. Rev. B **83**, 245102 (2011)


Attogram
UNIVERSITY OF EXETER
Surface Plasmon-Polaritons in Biosensing
Baptiste Auguié *
Prof. Bill Barnes
Thin Film Photonics Group
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(*) <ba208@ex.ac.uk>
http://projects.ex.ac.uk/atto/
Attogram Sensitivity Project
The Attogram project, in collaboration between the Universities of Nottingham and Exeter intends to find the most sensitive technique to detect optically a few biological molecules in solution. Classical methods make use of Attenuated Total Reflection of light as a very sensitive probe of any change in refractive index on the surface of a glass prism (see 'What is a SPP?').
This scanning method is being used and improved in Exeter with an ultra-sensitive differential surface plasmon (d-SPR) ellipsometry technique designed by Dr. I. Hooper, leading to sensitivity as accurate as a 10⁻⁶ change in refractive index of the solution under study.
Another topic of interest is the design of arrays of nanoparticles, which support so-called Particle Plasmons when they are excited optically. These structures are expected to be even more sensitive to the presence of molecules near the surface, as the electromagnetic field is greatly confined in some hot spots where any change in refractive index may strongly change the plasmon resonance.
Differential SPR ellipsometry
What is a SPP?
Surface Plasmon-Polaritons are electromagnetic waves which propagate along the interface between a conductor (gold, silver, ...), and a dielectric (air, water, ...). The electric field characterizing such waves exhibits an exponential decay in both media. For SPP propagating on planar surfaces, this decay length is typically 200 nm in the dielectric, and about ten times shorter in the metal.
Optical excitation of SPPs
Interest in biosensing
To go further
Particle Plasmons
Future work
Conclusions
References
Acknowledgements
Engineering and Physical Sciences Research Council (EPSRC)
Dr. Andy Murray, Dr. Ian Hooper and Dr. James Suckling from Exeter for data and comments.
(*) <ba208@ex.ac.uk>
http://projects.ex.ac.uk/atto/
Attogram Sensitivity
The Attogram project, in collaboration b
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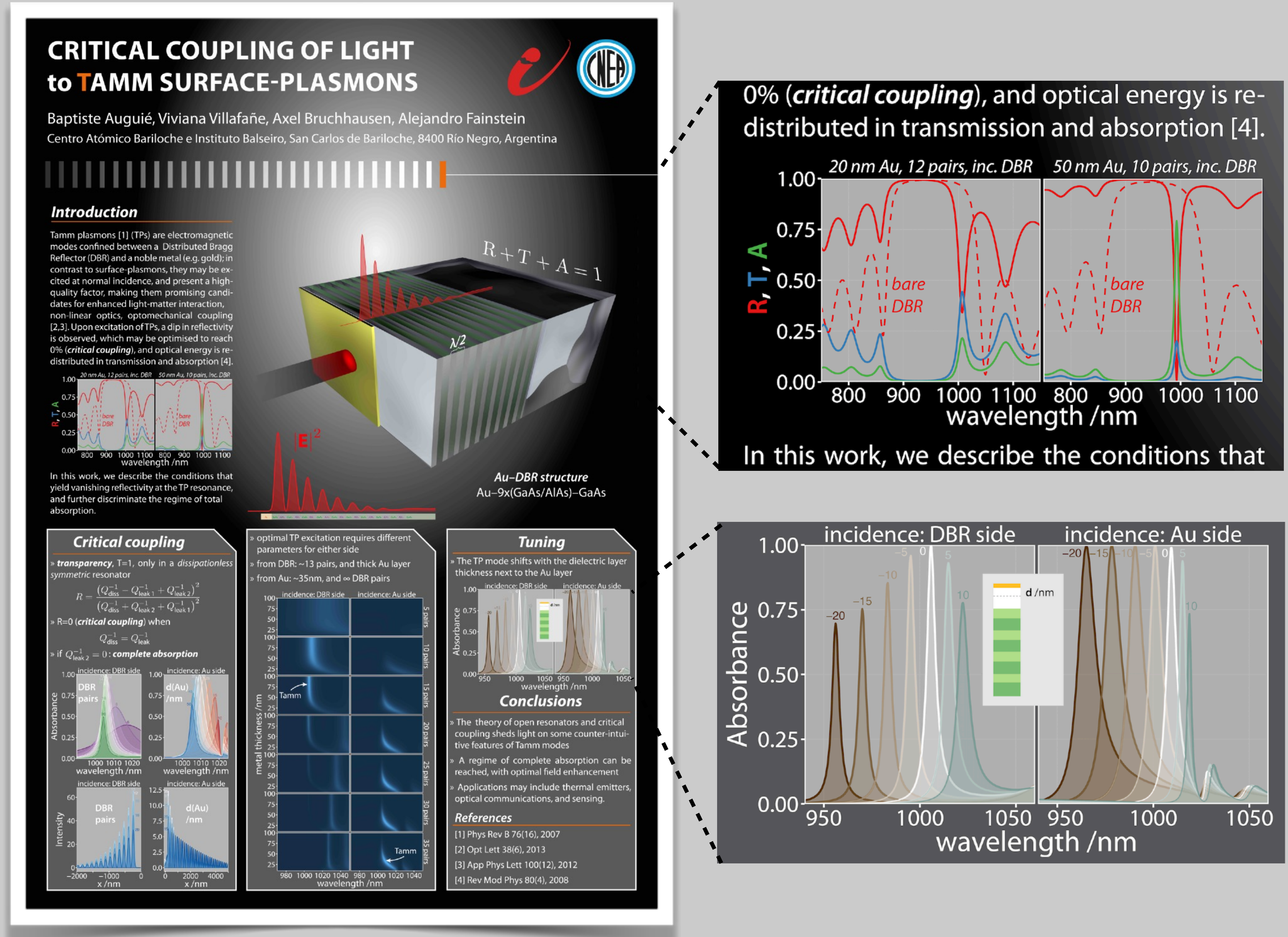
CRITICAL COUPLING OF LIGHT
to TAMM SURFACE-PLASMONS
Baptiste Auguié, Viviana Villafañe, Axel Bruchhausen, Alejandro Fainstein
Centro Atómico Bariloche e Instituto Balseiro, San Carlos de Bariloche, 8400 Río Negro, Argentina
Introduction
Tamm plasmons [1] (TPs) are electromagnetic modes confined between 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, non-linear optics, optomechanical coupling [2,3]. Upon excitation of TPs, a dip in reflectivity is observed, which may be optimised to reach 0% (critical coupling), and optical energy is re-distributed in transmission and absorption [4].
20 nm Au, 12 pairs, inc. DBR
50 nm Au, 10 pairs, inc. DBR
R, T, A
bare DBR
wavelength /nm
In this work, we describe the conditions that yield vanishing reflectivity at the TP resonance, and further discriminate the regime of total absorption.
R + T + A = 1
λ/2
$|E|^2$
Au–DBR structure
Au–9x(GaAs/AlAs)–GaAs
Critical coupling
» transparency, T=1, only in a dissipationless symmetric resonator
$R=\frac{(Q_{diss}^{-1}-Q_{leak\,1}^{-1}+Q_{leak\,2}^{-1})^2}{(Q_{diss}^{-1}+Q_{leak\,2}^{-1}+Q_{leak\,1}^{-1})^2}$
» R=0 (critical coupling) when
$Q_{diss}^{-1}=Q_{leak}^{-1}$
» if $Q_{leak\,2}^{-1}=0$: complete absorption
incidence: DBR side
incidence: Au side
DBR pairs
d(Au) /nm
Absorbance
Intensity
x /nm
» optimal TP excitation requires different parameters for either side
» from DBR: ~13 pairs, and thick Au layer
» from Au: ~35nm, and ∞ DBR pairs
metal thickness /nm
Tamm
5 pairs
10 pairs
15 pairs
20 pairs
25 pairs
30 pairs
35 pairs
Tuning
» The TP mode shifts with the dielectric layer thickness next to the Au layer
d /nm
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 76(16), 2007
[2] Opt Lett 38(6), 2013
[3] App Phys Lett 100(12), 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
incidence: DBR side
incidence: Au side
Absorbance
wavelength /nm

CSRS — Continuously-Shifted Raman Spectroscopy

Needles in a haystack: recovering tiny signals in bright-lit CCD detectors

Baptiste Auguié, Antoine Reigue, Eric Le Ru, Pablo Etchegoin

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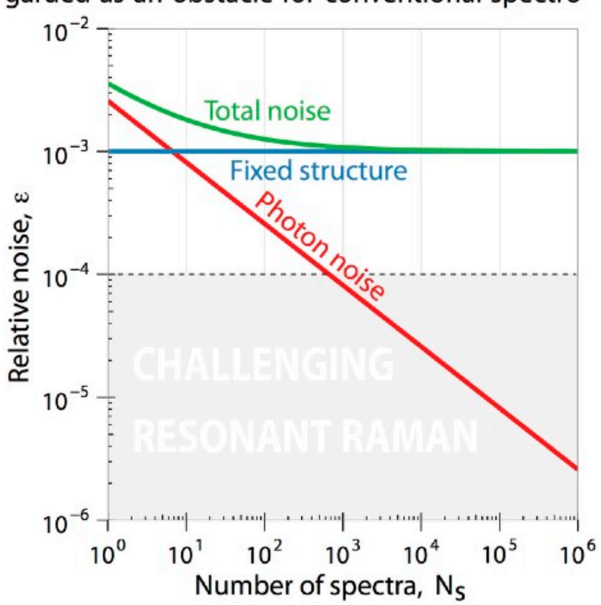
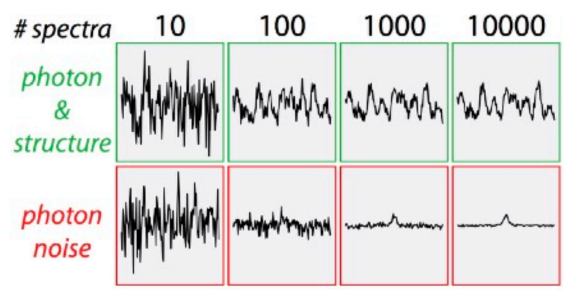
School of Chemical and Physical Sciences
Victoria University, Wellington, New Zealand

— Motivation —

In many important applications, excitation of a dye near an absorption line conjointly produces intense fluorescence that overwhelms the Raman peaks [1]. This practical difficulty is commonly regarded as an obstacle for conventional spectroscopic tools. The general issue we seek to address is how to retrieve comparatively small features in a large background using a standard spectrometer equipped with a CCD detector.





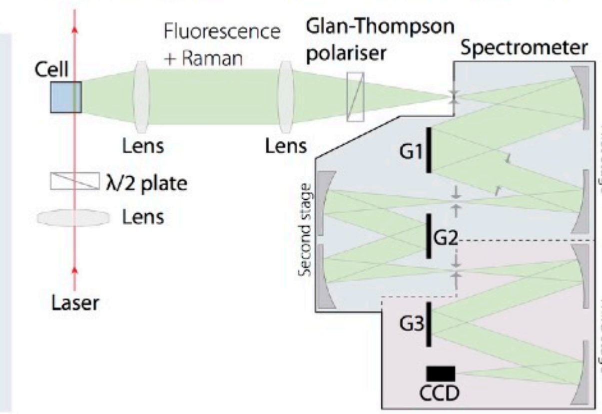
Beating the average — *The signal-to-noise ratio that limits the detection level of Raman peaks in the fluorescence background can be improved by averaging many spectra. However, this procedure rapidly meets a major obstacle [1,2], a fixed-structure noise that is insensitive to the photon counts, limiting detectable Raman signals to Raman-to-fluorescence ratios below 10^{-3}.*

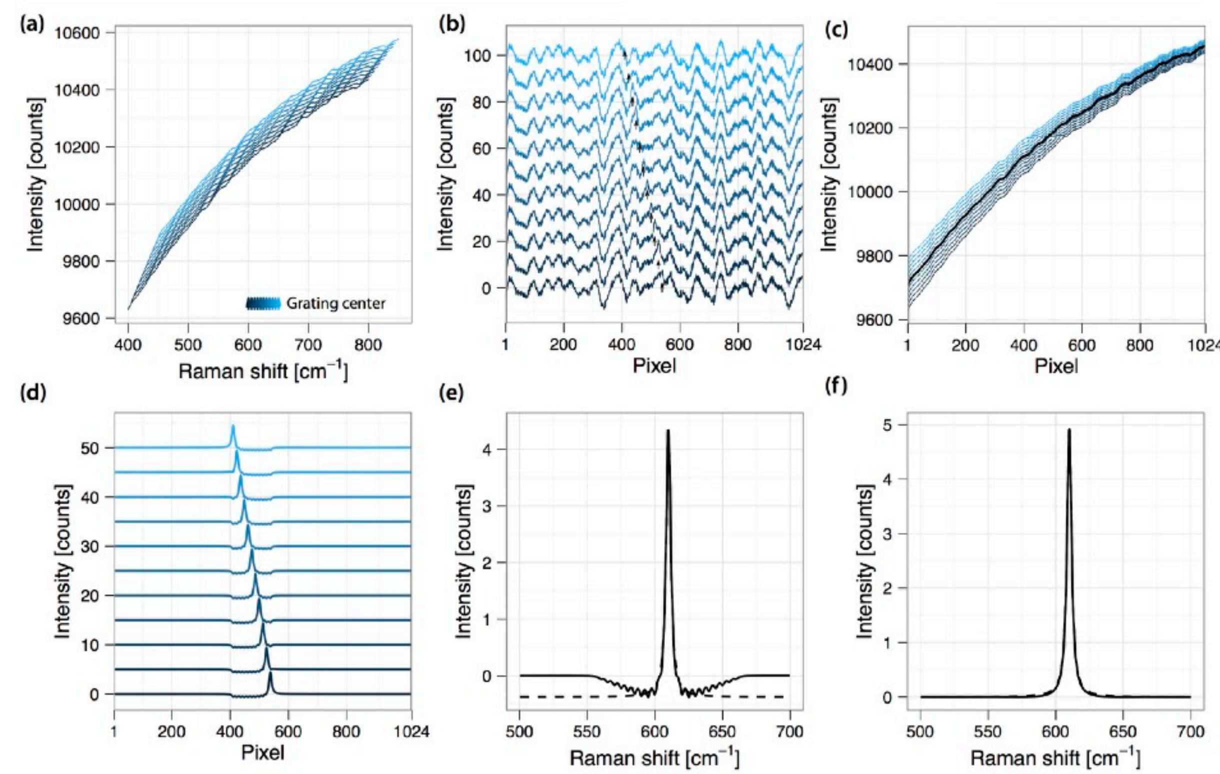
If a flat-field correction scheme can be devised to eliminate the fixed-structure contribution from the CCD counts [1,2], the acquisition of multiple spectra will regain photon-limited statistics, whereby the relative rms noise, and therefore the detectable Raman- to-fluorescence ratio, can reach $\varepsilon \sim 10^{-5}$.

— Methodology —

Using a standard CCD-based spectrometer, we present a practical method that enables *routine resonant Raman measurements* of dyes with high quantum yield. With multiple shifts of the diffraction gratings the pixel-dependent noise structure is captured and used as a flat-field correction.

Experimental setup — *Schematic representation of the triple-subtractive spectrometer (T64000, Horiba Jobin-Yvon), and the 90º scattering configuration used in our experiments. A Glan-Thompson polariser is used at the entrance of the spectrometer, the incident linear polarisation is selected by a λ/2-waveplate.*
In a typical experiment, multiple spectra are acquired for ~50 positions of the gratings, each totalling ~10^4 counts at the central wavelength.





CSRS flat-field correction — *Peak-retrieval methodology on simulated data.* ***(a)*** *11 shifts of 5 cm^{-1} each.* ***(b)*** *Fixed-structure noise after removal of a 4th-order polynomial. A black arrow indicates the position of the Raman peak.* ***(c)*** *Same as in* ***(a)****, plotted against CCD pixels. The black curve is the average of all spectra (**flat-field**).* ***(d)*** *Recovered spectra after flat-field correction.* ***(e)*** *Average spectrum from* ***(d)****, plotted against wavenumbers.* ***(f)*** *Second background subtraction and original Lorentzian .*

CONCLUSIONS

References & further reading

- William Cleveland • *The Elements of Graphing Data*
- Edward Tufte • *The visual display of quantitative information*
- Jan White • *Graphic design for the electronic age*
- H. Wainer • *How to Display Data Badly*

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/

Suggested software

- **Plots**
  - Python, R (static)
  - D3, plot.ly (interactive)
  - Tableau (expensive)
- **Schematics & layout**
  - Inkscape (open-source)
  - Adobe Illustrator, Indesign (expensive)