

Baptiste Auguie

~ 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



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*

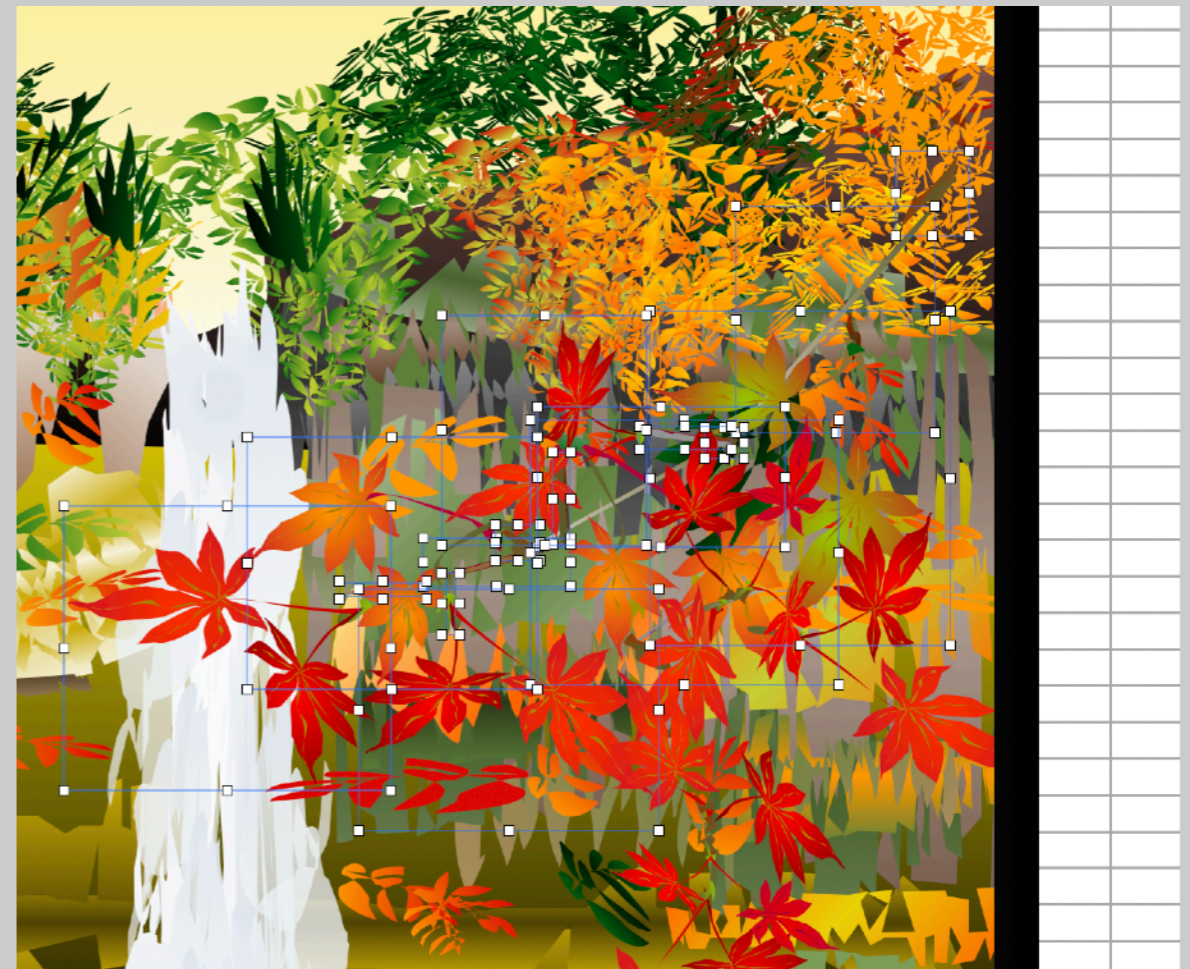
▶ **A VISION FOR GRAPHICS**

- *Aesthetics and impact*
- *TOC figures, slides, posters*

Tools don't matter
(but they do)

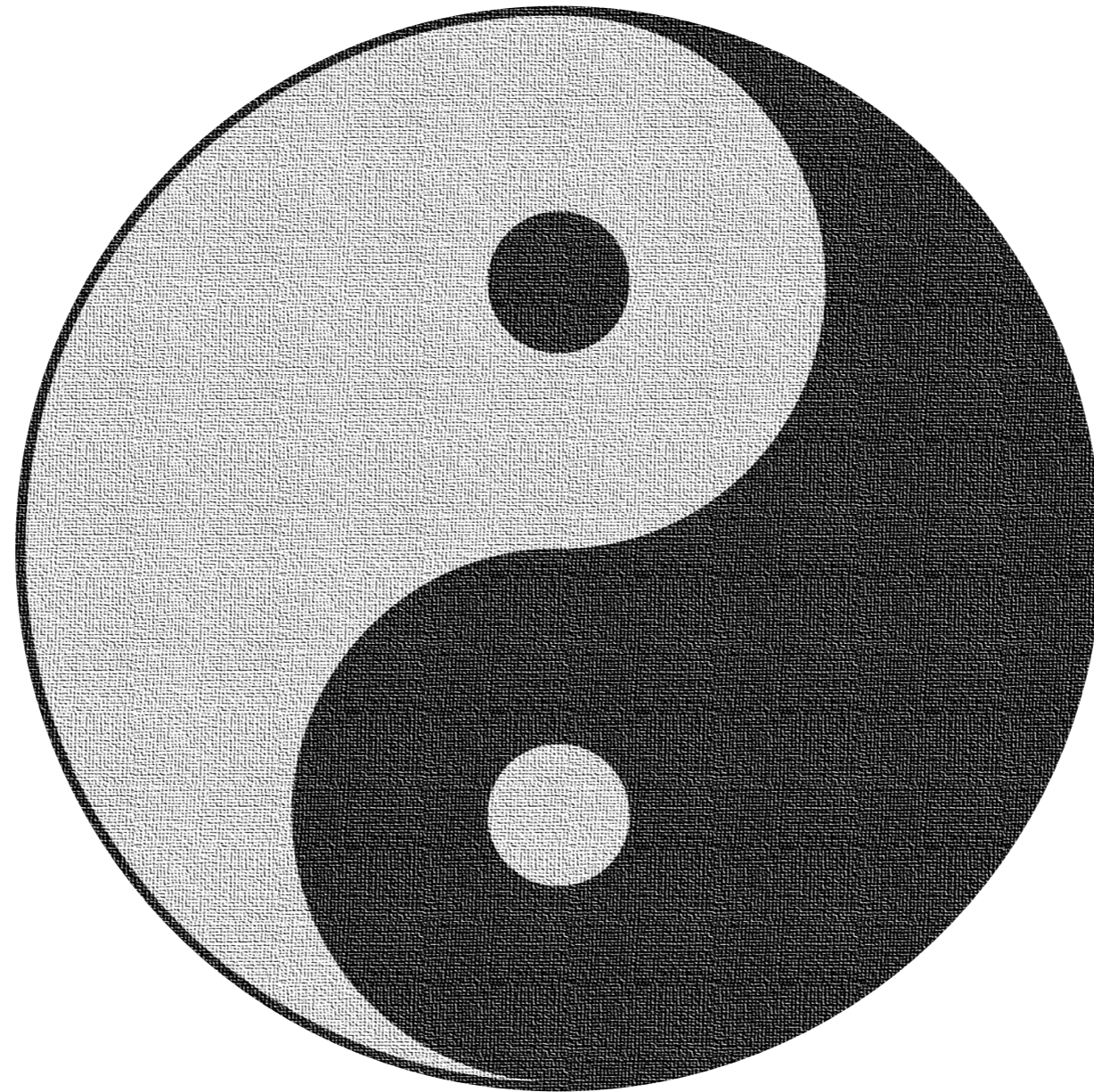


Tatsuo Horiuchi
Excel artist



PART I • A PHILOSOPHY OF GRAPHICS

ANALYTIC

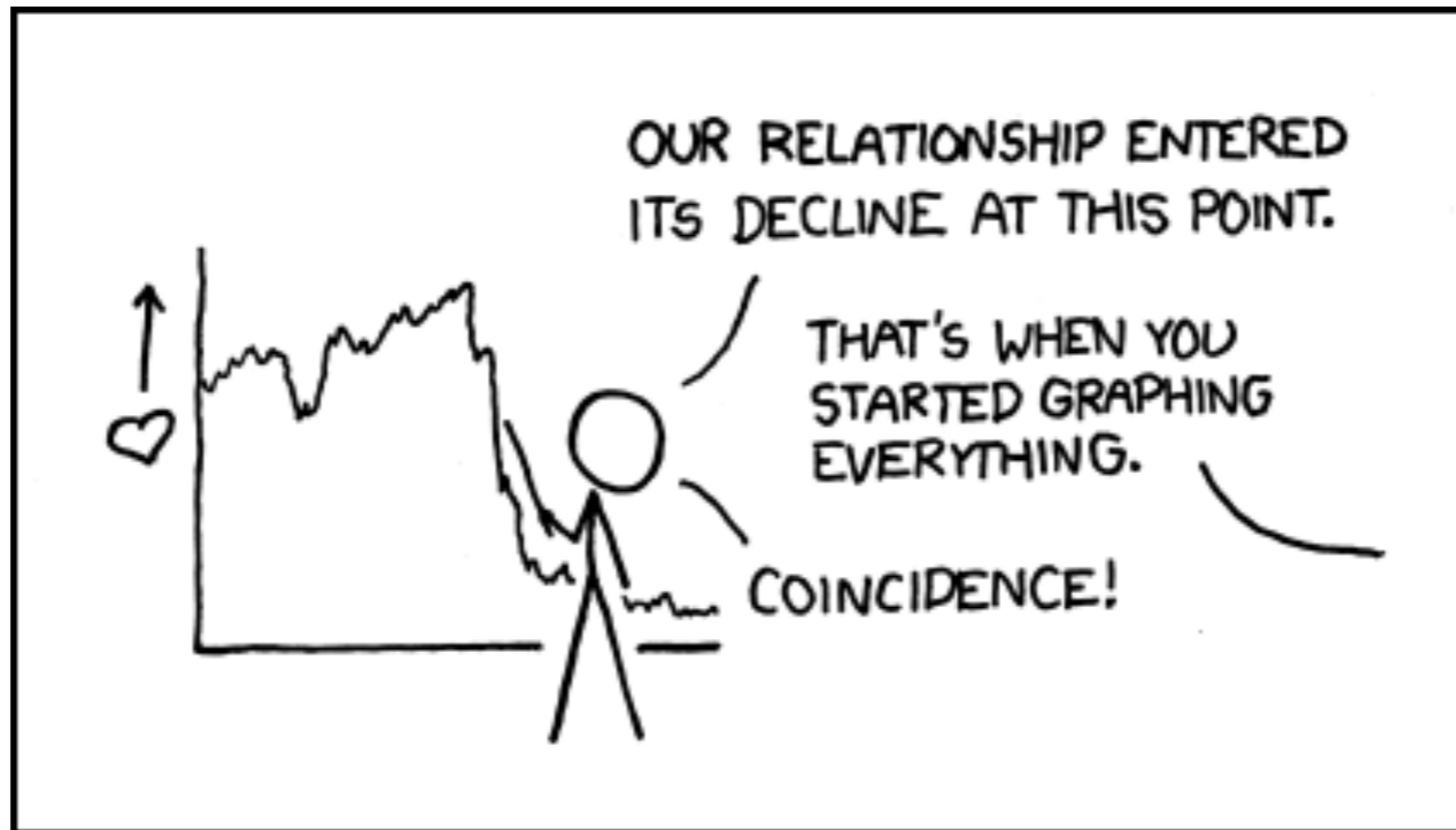


VISUAL

Clarity:

data-to-ink ratio

GRAPH ALL THE THINGS?



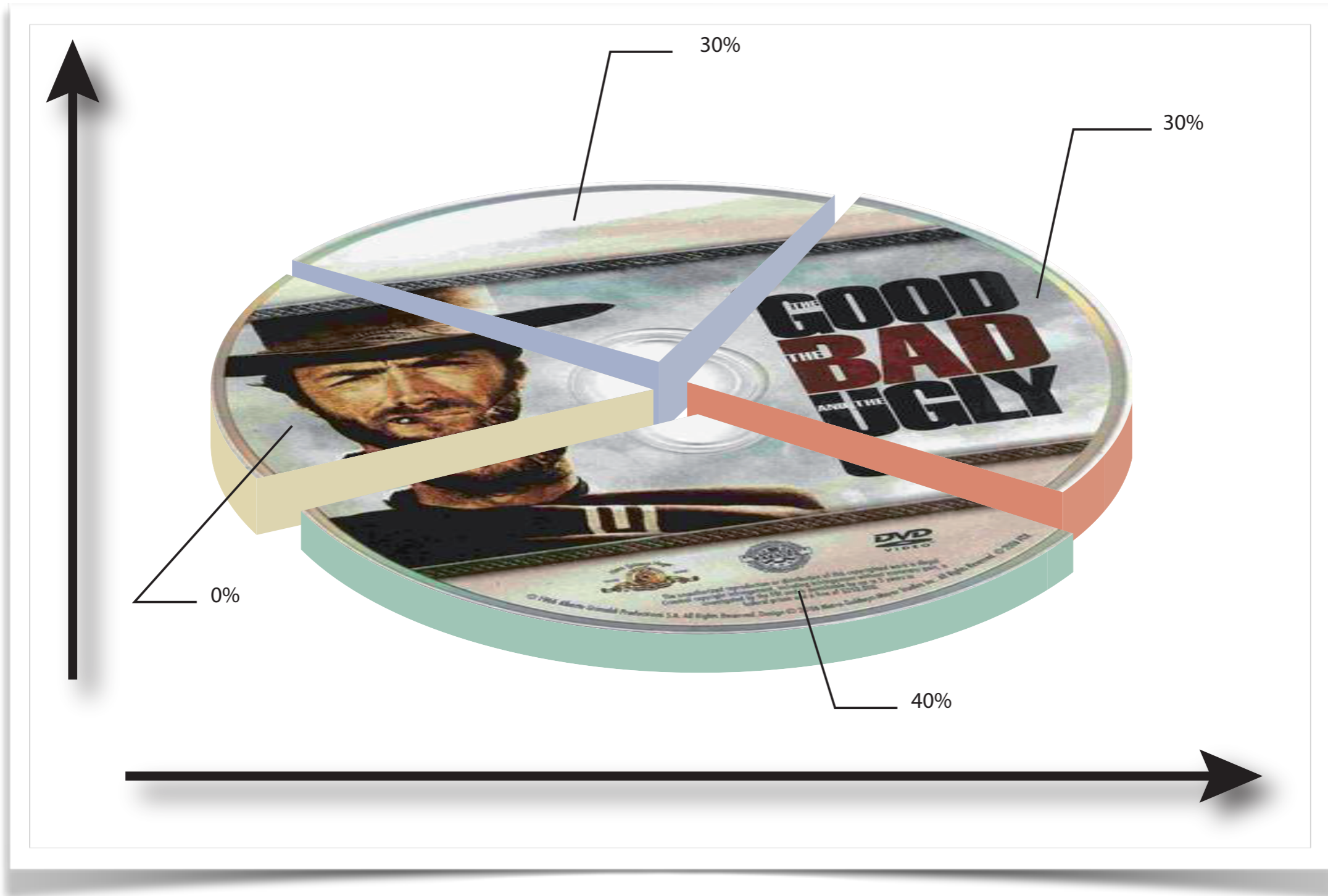
xkcd.com

CONSIDER A TABLE

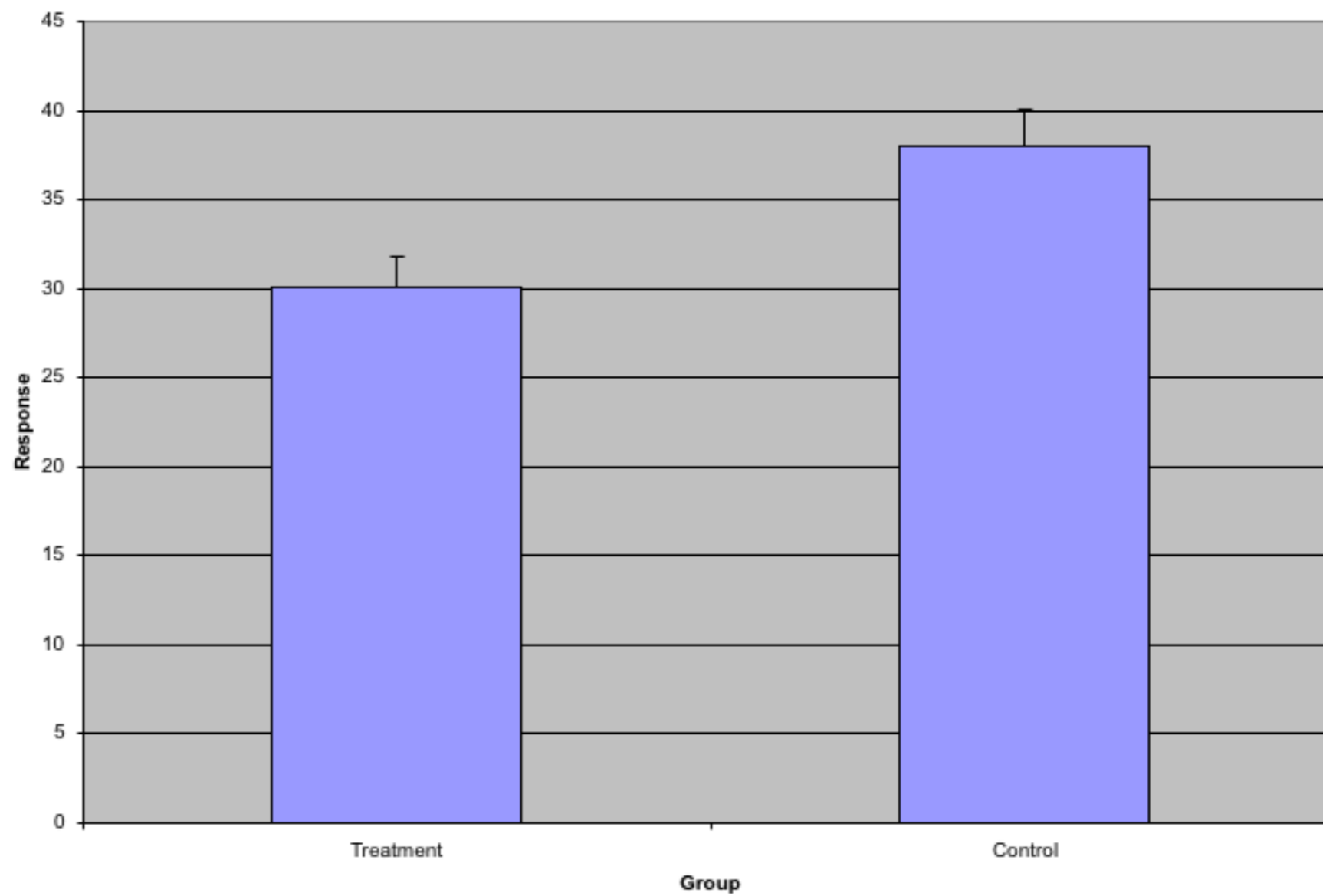
n	Arbitrary precision	Double precision
1	(1.351522998772148 +0.002682327826796 <i>i</i>)	(1.351522998772154 +0.002682327826791 <i>i</i>)
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3	(3.267511781081814 +0.354044762711458 <i>i</i>) $\times 10^{-3}$	(3.267511780908656 +0.354044762723604 <i>i</i>) $\times 10^{-3}$
4	(8.234338861126748 +1.361708455386841 <i>i</i>) $\times 10^{-5}$	(8.234338230741085 +1.361708446137377 <i>i</i>) $\times 10^{-5}$
5	(15.30077682100172 +3.20759658015824 <i>i</i>) $\times 10^{-7}$	(15.30004712362165 +3.2074636639992 <i>i</i>) $\times 10^{-7}$
6	(23.34600724021963 +6.186419274080092 <i>i</i>) $\times 10^{-9}$	(25.42872582340277 +5.90596678628629 <i>i</i>) $\times 10^{-9}$
7	(29.40892160067281 +9.22544630049269 <i>i</i>) $\times 10^{-11}$	(24.3107199444863 -1.13271331394081 <i>i</i>) $\times 10^{-8}$
8	(3.204531139340317 +1.186184482330857 <i>i</i>) $\times 10^{-12}$	(177.439991438448 -2.0214735003898 <i>i</i>) $\times 10^{-7}$
9	(3.038290261597983 +1.287101819776947 <i>i</i>) $\times 10^{-14}$	(67.0727643316326 +1.57033685336724 <i>i</i>) $\times 10^{-5}$
10	(2.5674093425467 +1.240871523988642 <i>i</i>) $\times 10^{-16}$	-0.03959069252015016 +0.00071876916602068 <i>i</i>
11	(1.94474203713492 +1.055179886196251 <i>i</i>) $\times 10^{-18}$	-10.11371972337842 -0.13925596567256 <i>i</i>
12	(13.38699265450917 +8.13464528498008 <i>i</i>) $\times 10^{-21}$	-1132.655389072814 +0.299642890755 <i>i</i>
13	(8.417729528036757 +5.677389217679542 <i>i</i>) $\times 10^{-23}$	(-86.48807724977711 +1.50271433683522 <i>i</i>) $\times 10^3$
14	(4.876046808254036 +3.644961564953527 <i>i</i>) $\times 10^{-25}$	(-29.88742021522111 +6.65835422187729 <i>i</i>) $\times 10^5$
15	(2.613375843631903 +2.154801883308382 <i>i</i>) $\times 10^{-27}$	(34.54711402938201 +8.19472138834448 <i>i</i>) $\times 10^7$
16	(1.303141351977849 +1.184738044986223 <i>i</i>) $\times 10^{-29}$	(45.78317881557951 +9.731545021815603 <i>i</i>) $\times 10^9$
17	(6.067251546625191 +6.069699524562945 <i>i</i>) $\times 10^{-32}$	(-3.816711620949946 +1.082670199384622 <i>i</i>) $\times 10^{12}$
18	(2.647391356803932 +2.916878553003213 <i>i</i>) $\times 10^{-34}$	(-154.3422495126499 +7.8521375375244 <i>i</i>) $\times 10^{13}$
19	(1.085651390657799 +1.317672507647534 <i>i</i>) $\times 10^{-36}$	(-166.490936601337536 -1.779710476225576 <i>i</i>) $\times 10^{15}$
20	(4.194570626830792 +5.621507702515121 <i>i</i>) $\times 10^{-39}$	(21.346348083272847360-1.199678065337379840 <i>i</i>) $\times 10^{18}$
21	(1.530005420781641 +2.269669591435182 <i>i</i>) $\times 10^{-41}$	(100.285925474474 -3.244785438691 <i>i</i>) $\times 10^{20}$

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
1.1	N	5	5	7	9	11	11	13	15	17	17	21	23	27	35	41	47	63	77	95	127	111
	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}
1.3	N	5	5	9	11	11	13	15	15	19	19	23	27	31	37	45	53	69	93	115		
	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}		
2	N	5	7	11	13	15	15	19	19	21	23	25	27	33	41	49	61	75	103			
	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}			
4	N	5	7	11	15	17	19	21	23	23	25	29	31	35	45	51	57	59				
	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}				
7	N	5	7	11	15	19	19	19	23	25	27	31	35	37	41	47	47					
	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}					
10	N	5	7	13	15	19	19	21	25	27	27	31	33	41	45	43	47					
	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}					
20	N	5	7	13	15	19	21	23	23	27	29	33	37	43	43	49	41					
	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}					
50	N	5	7	13	17	19	21	23	25	27	29	33	35	39	45	47	45					
	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}					
100	N	5	7	13	17	19	21	23	25	27	27	33	35	47	53	47						
	N_θ	1000	1100	1000	1100	1000	1100	1100	1100	1100	1100	1100	1100	1300	1500	1400	1600	2000				
	error	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	10^{-9}					

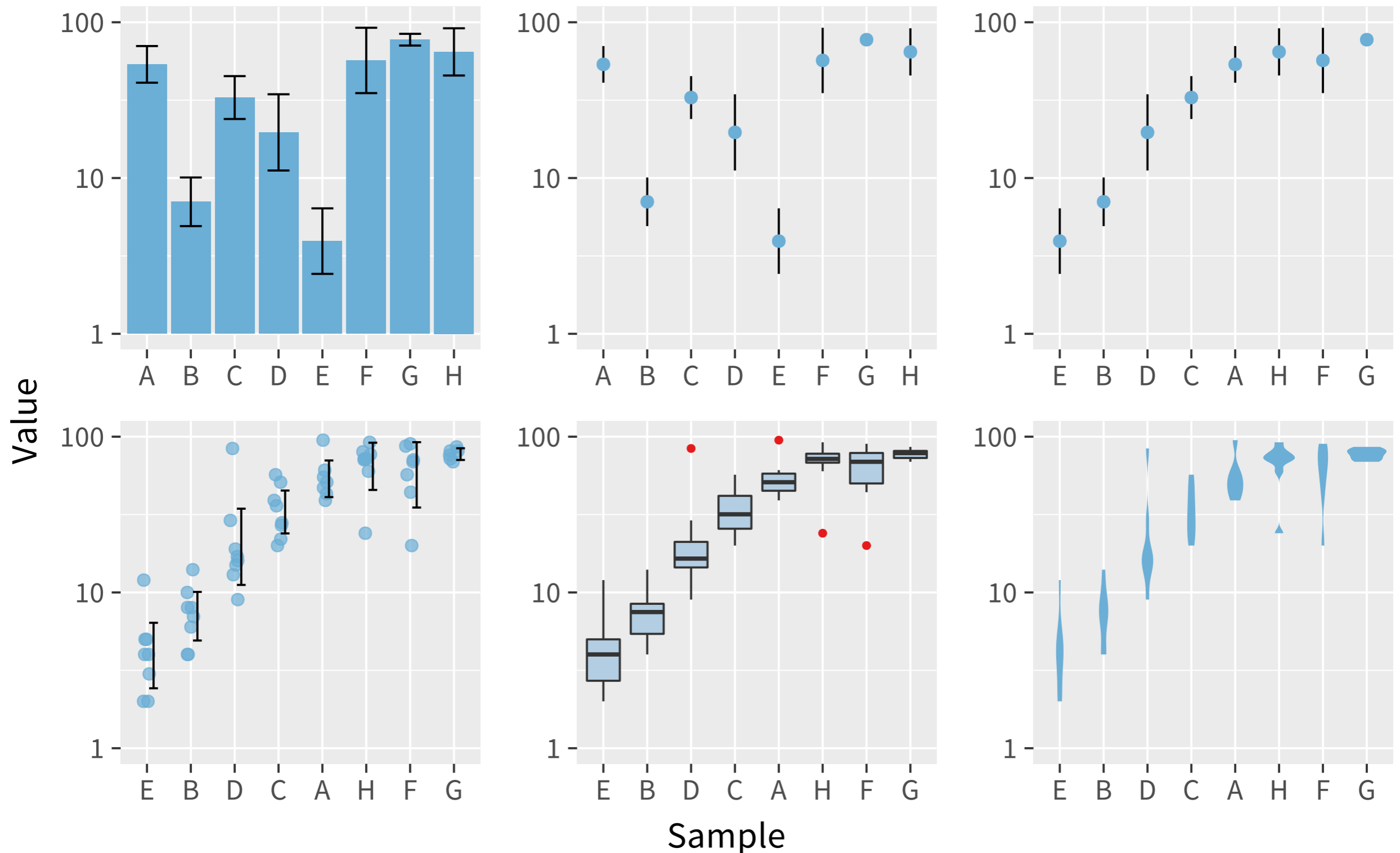
THE GOOD, THE BAD, AND THE UGLY



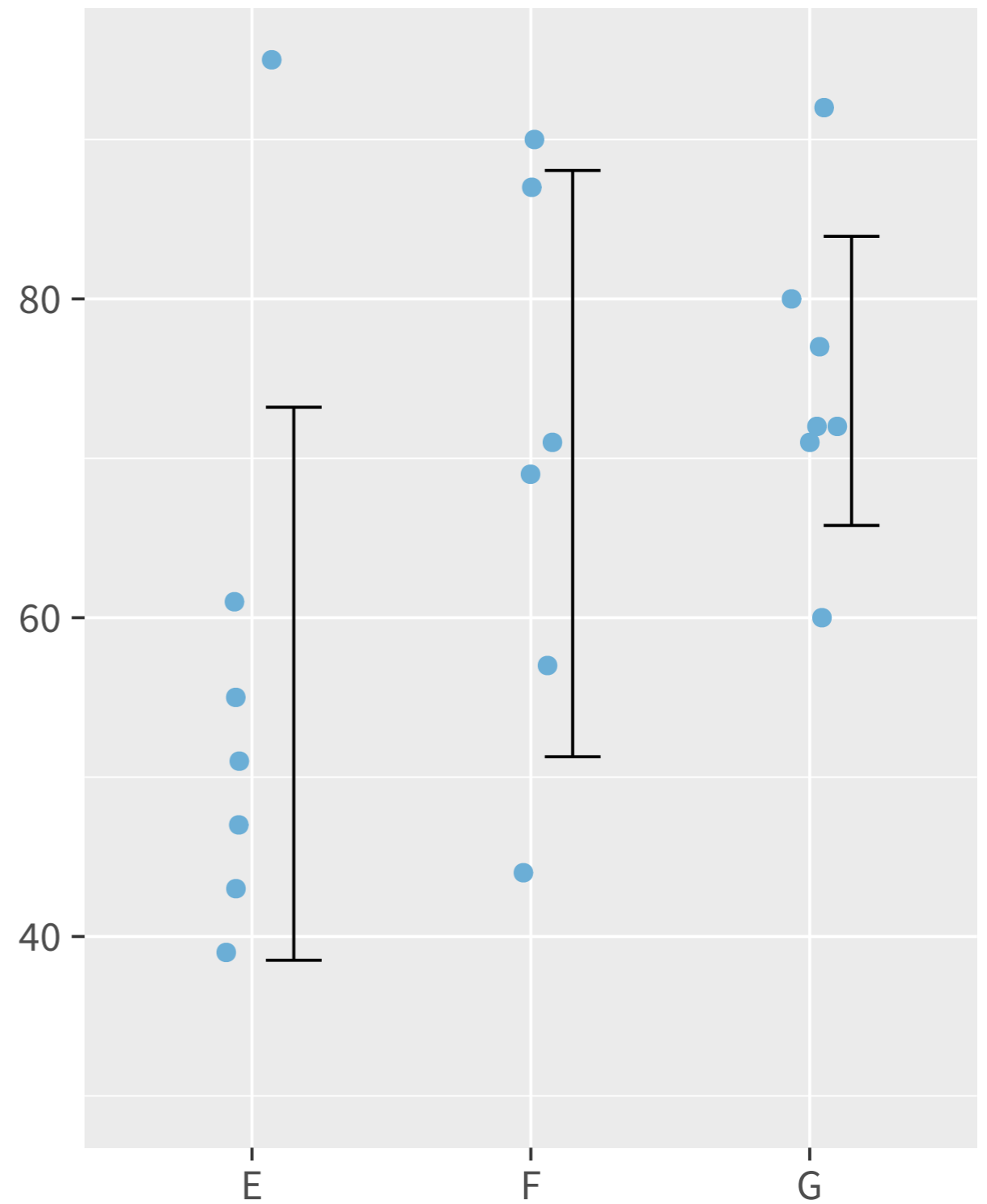
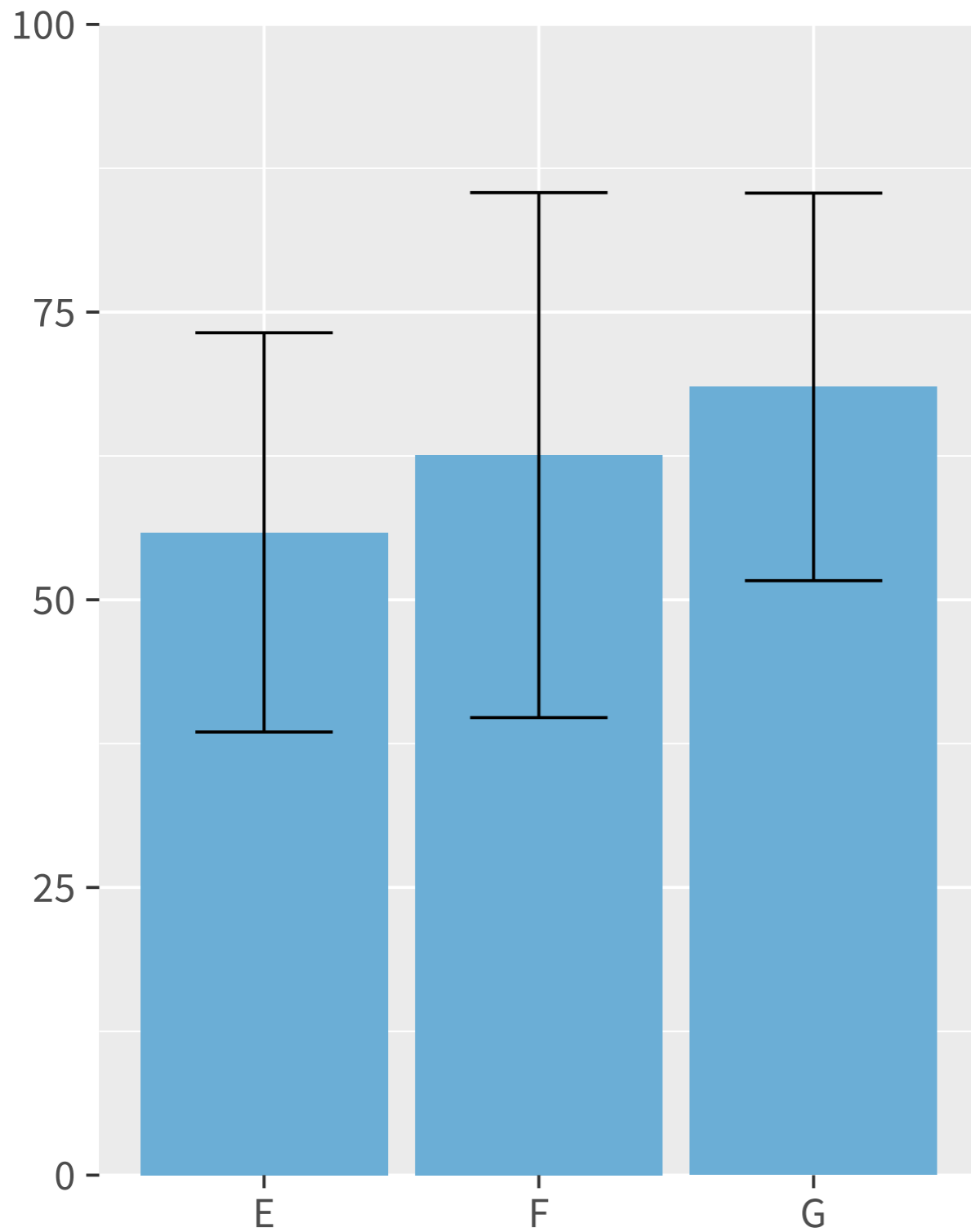
DYNAMITE PLOT

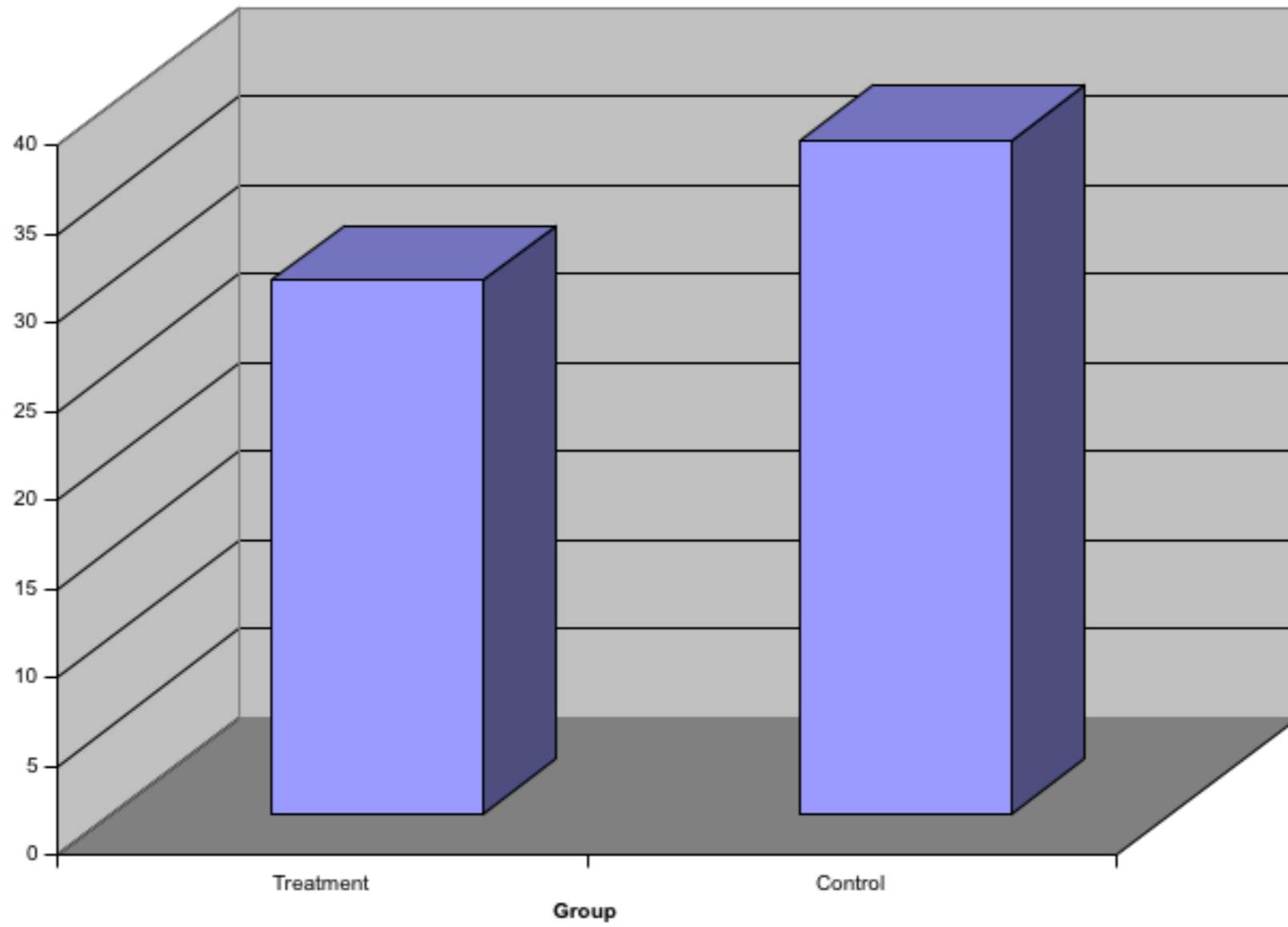


BARPLOT ALTERNATIVES: DOT PLOT, BOXPLOT



ALWAYS INCLUDE 0?





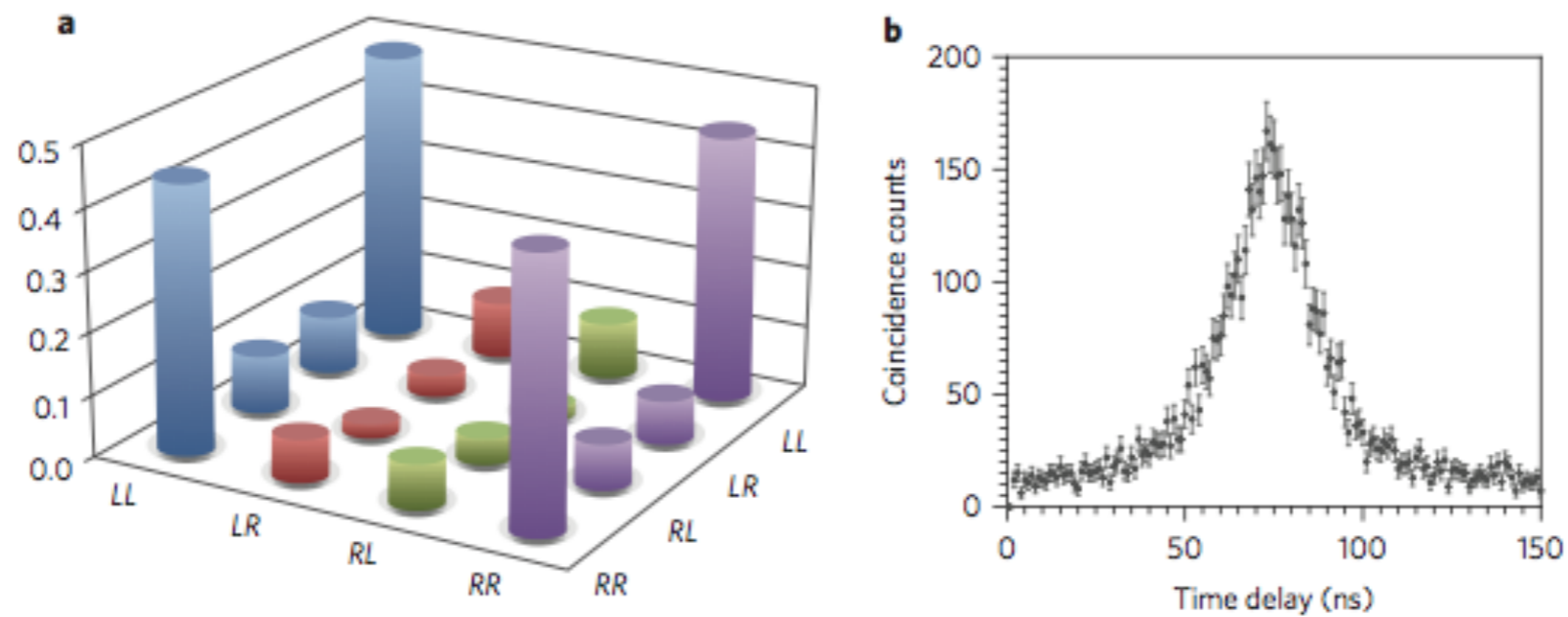
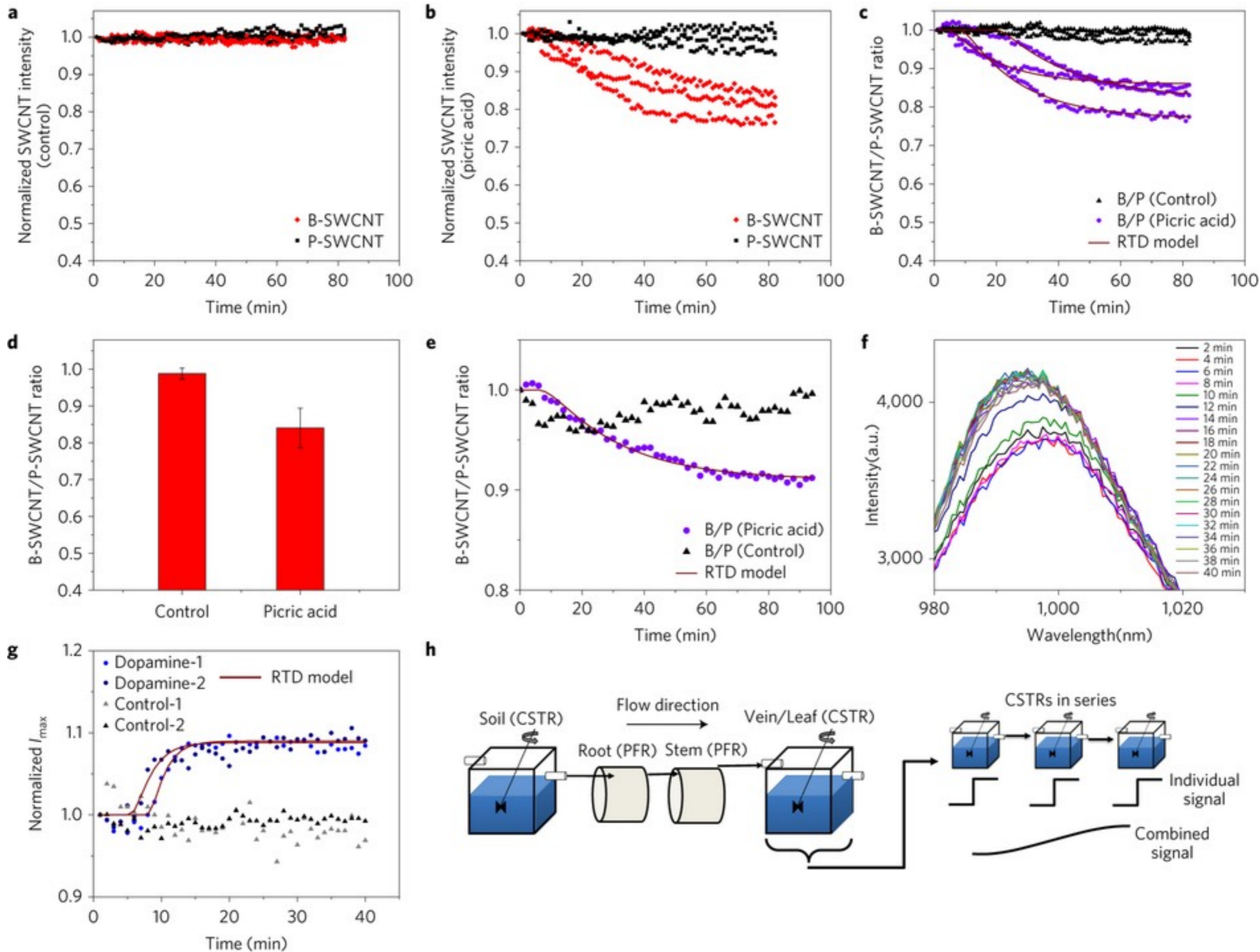
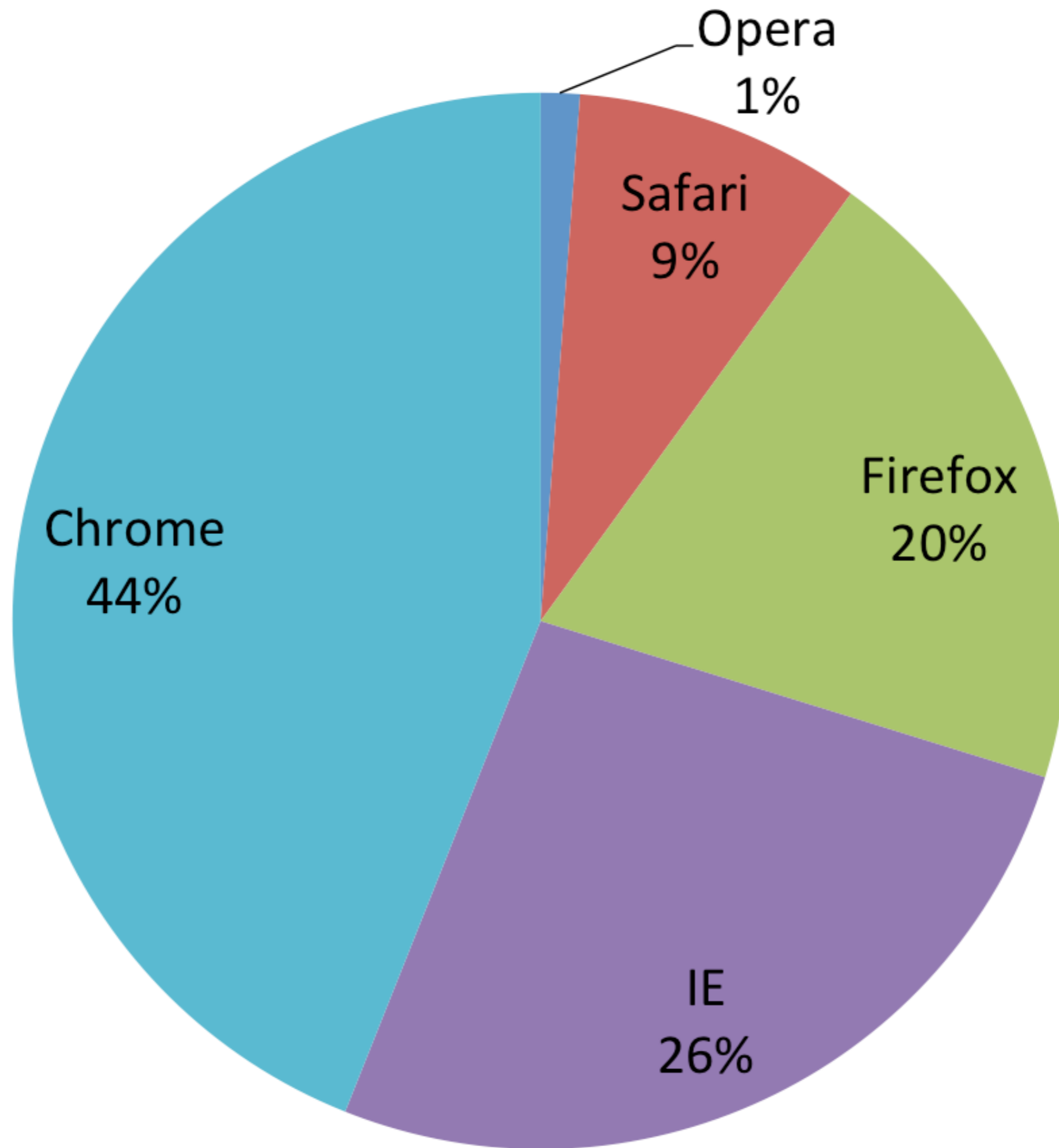





Figure 3 | NOON state characterization. **a**, Density matrix ρ (magnitudes only) from quantum state tomography, showing large coherence between $|LL\rangle$ and $|RR\rangle$ components. **b**, Measured correlation of the filtered CESPDC pairs (no background subtracted). The absence of modulation at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

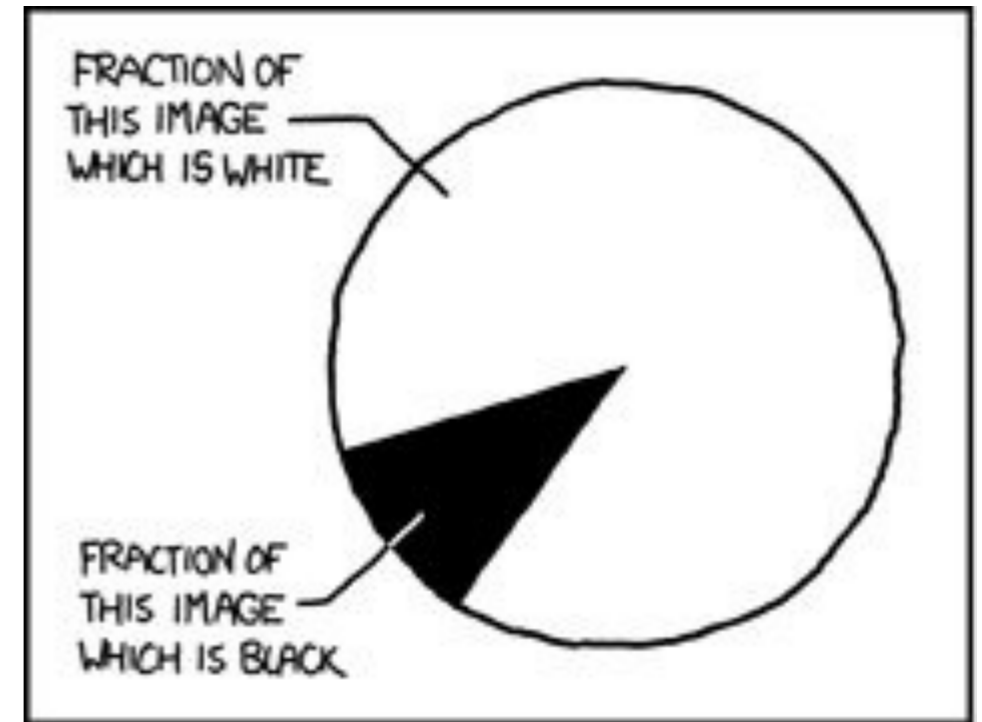






PIE CHARTS – LIMITED USE

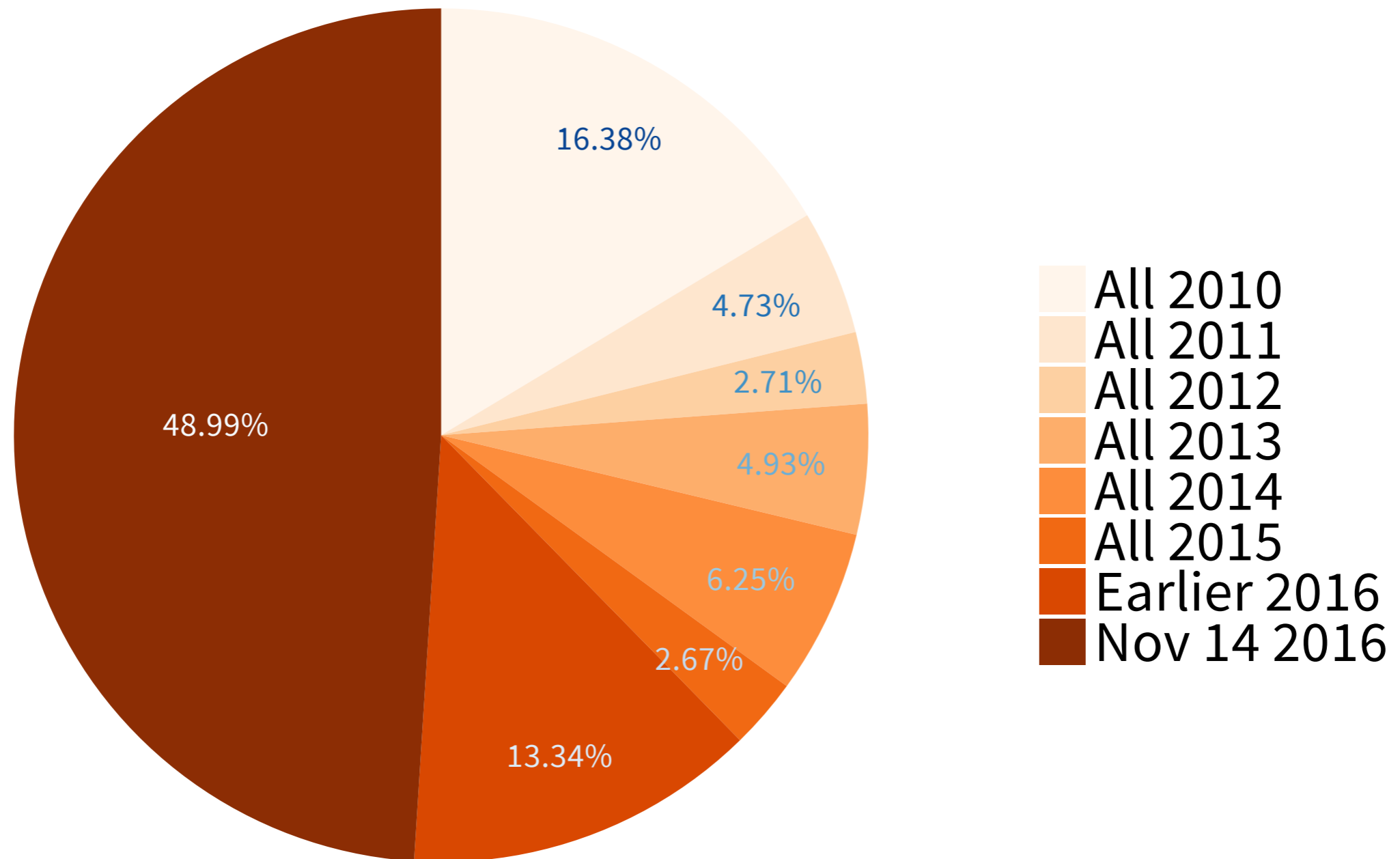


-  Sky
-  Sunny side of pyramid
-  Shady side of pyramid

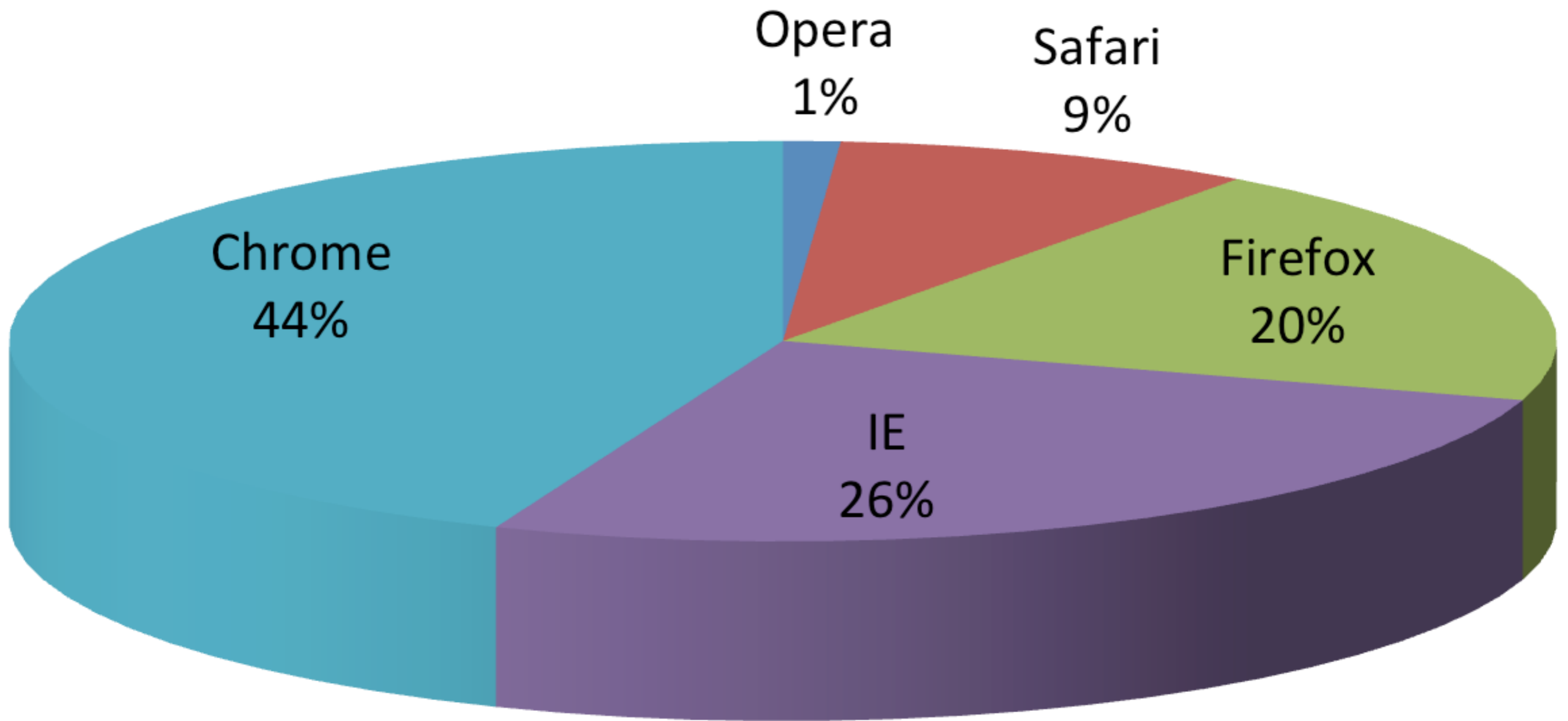


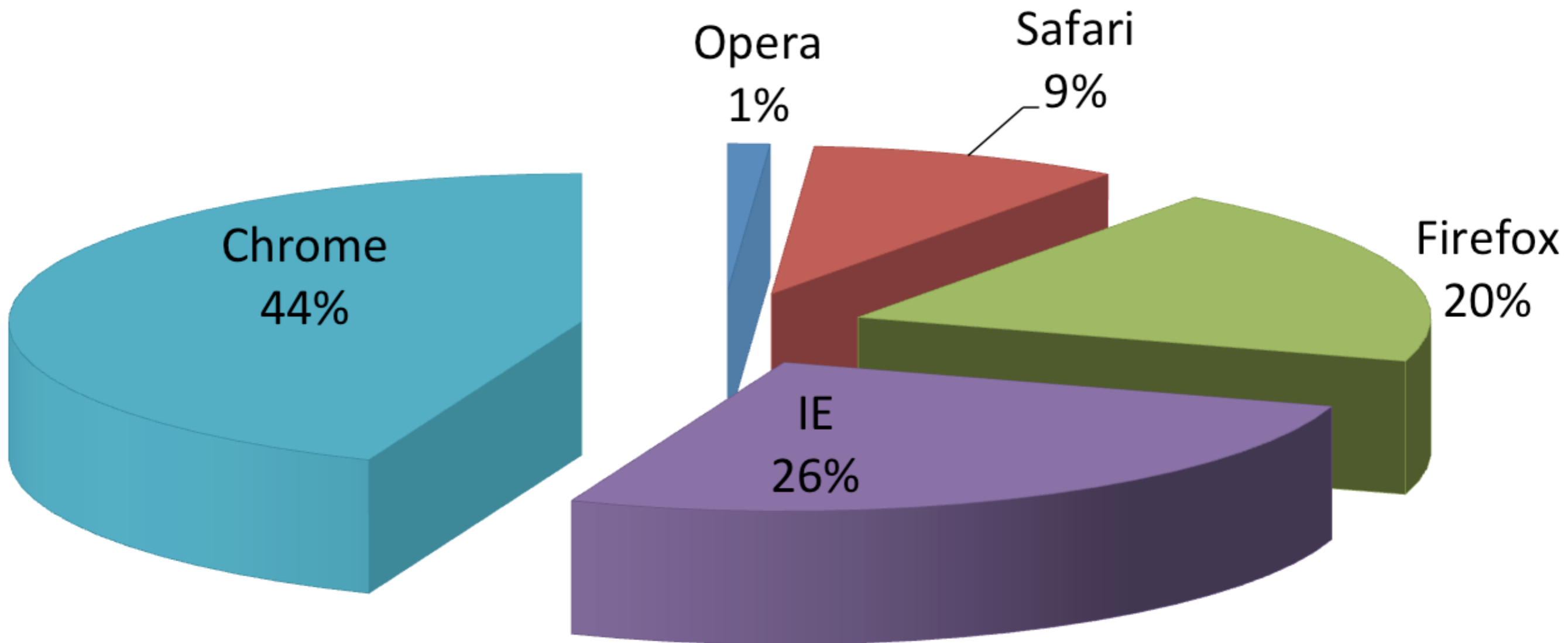
-  Pacman
-  Not Pacman

ENERGY RELEASED IN EARTHQUAKES SINCE 2010

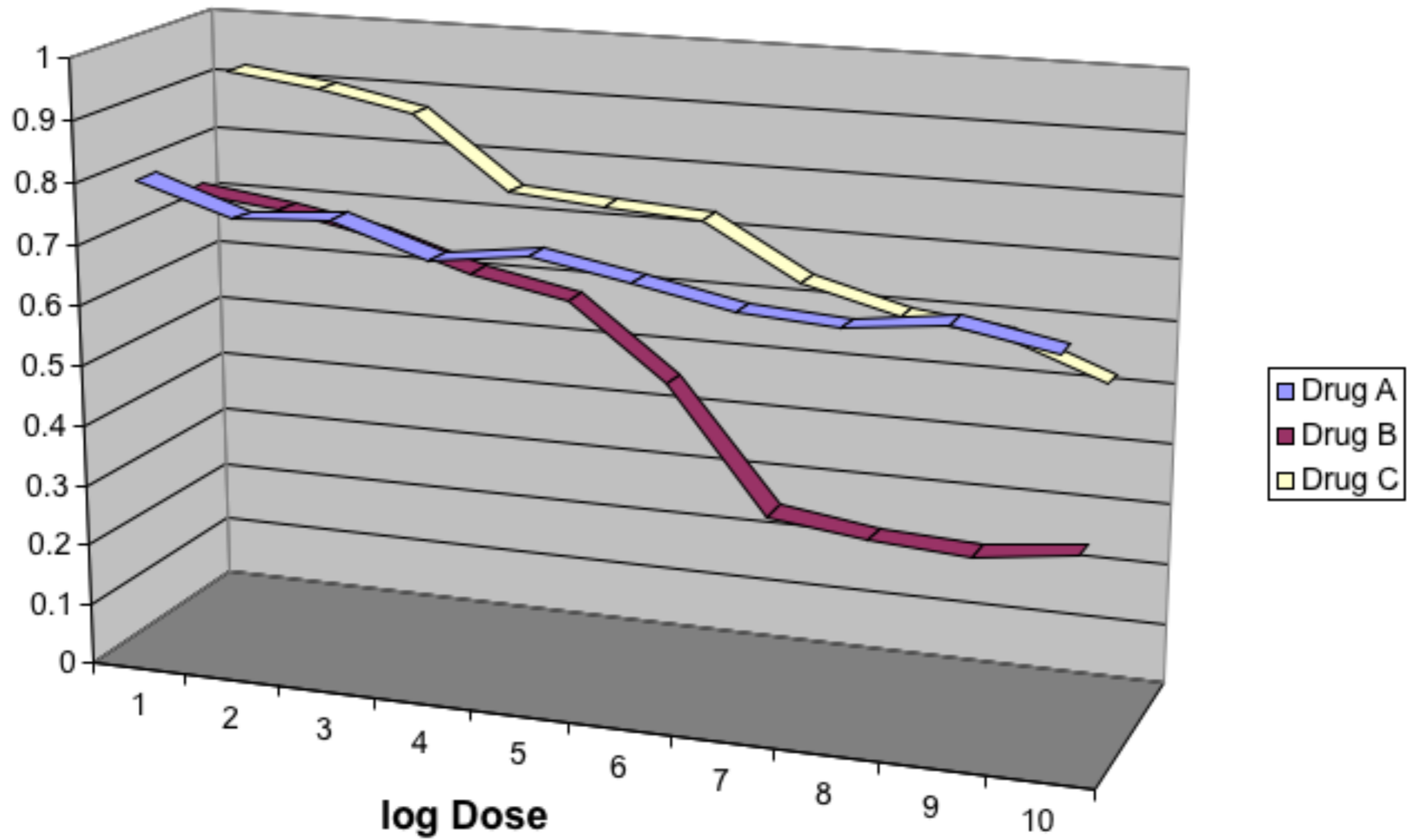


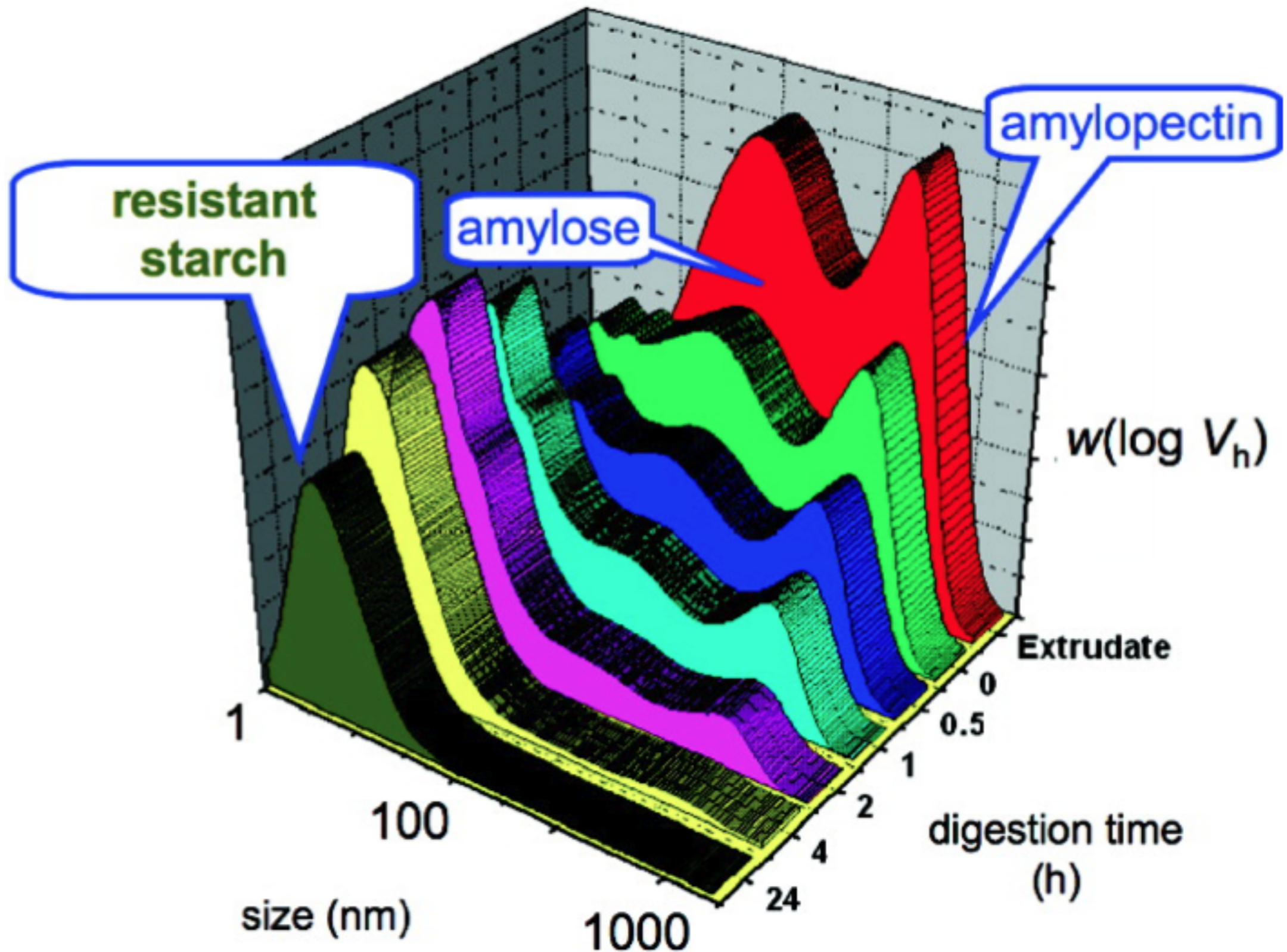
ellisp.github.io





Proportion survived





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*

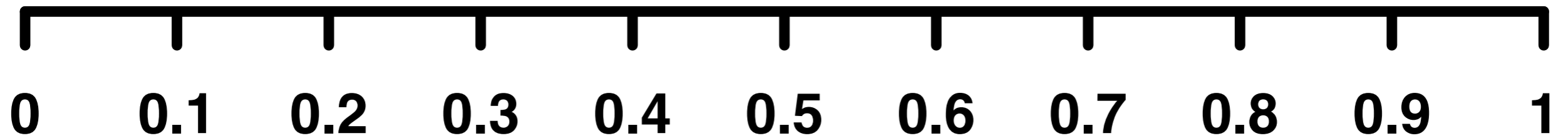
▶ **A VISION FOR GRAPHICS**

- *Aesthetics and impact*
- *TOC figures, slides, posters*

TIP #1 • GRAPHIC FORMATS

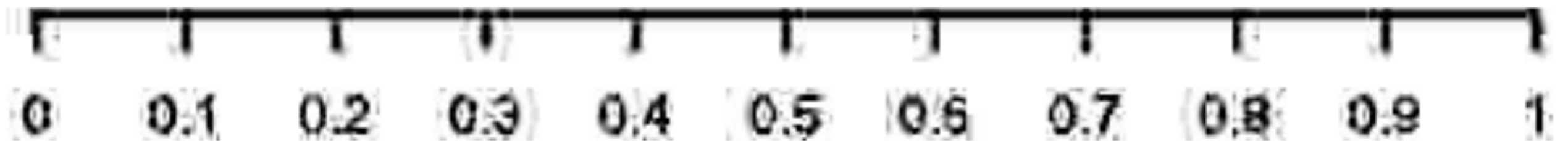
- ▶ **VECTOR FORMAT**
.eps, .svg, .pdf

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,

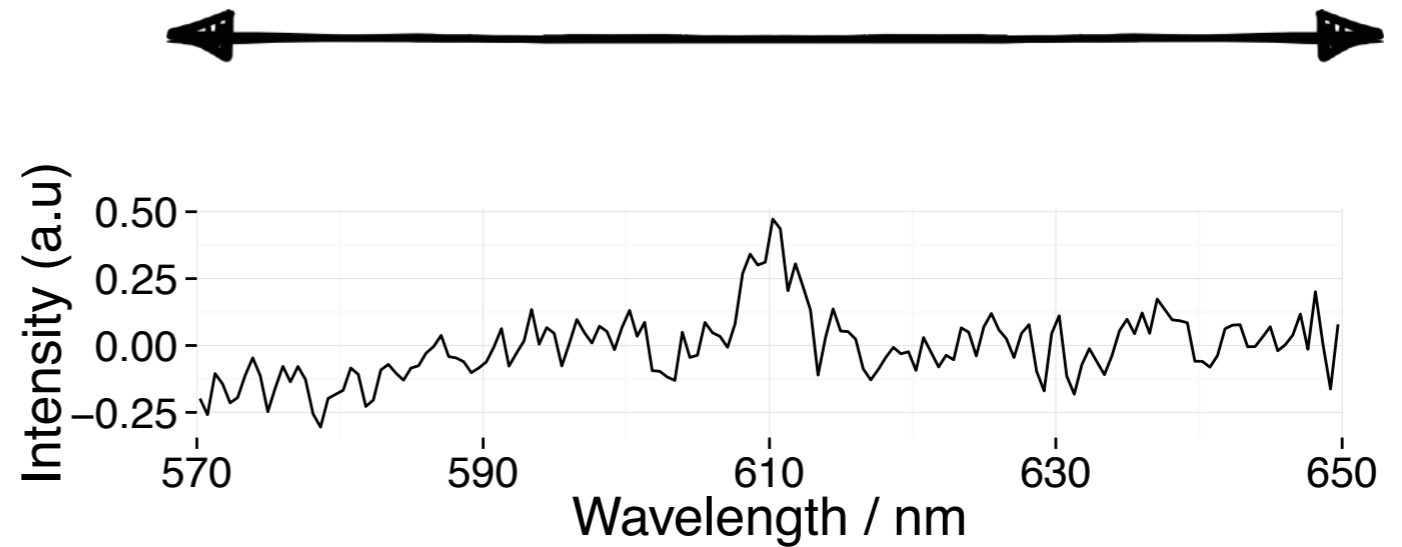
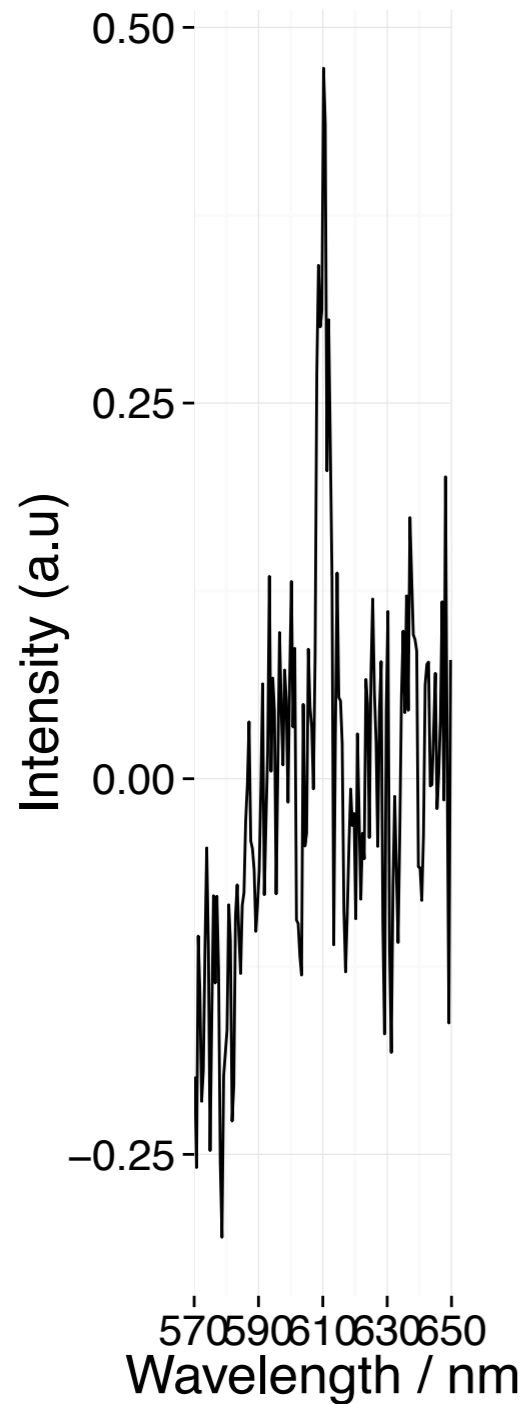
Figure 1: Nunc sed pede. Praesent vitae lectus. Praesent neque justo, vehicula eget, interdum id, facilisis et, nibh. Phasellus at purus et libero lacinia dictum. Fusce aliquet. Nulla eu ante placerat leo semper dictum. Mauris metus. Curabitur lobortis. Curabitur sollicitudin hendrerit nunc.

tus placerat pede. vivamus nunc nunc, molestie ut, ultricies vel, semper in, velit. Ut porttitor. Praesent in sapien. Lorem ipsum dolor sit amet, consectetur 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, consectetur 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, consectetur 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

L^AT_EX tip

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

TIP #3 • ASPECT RATIO



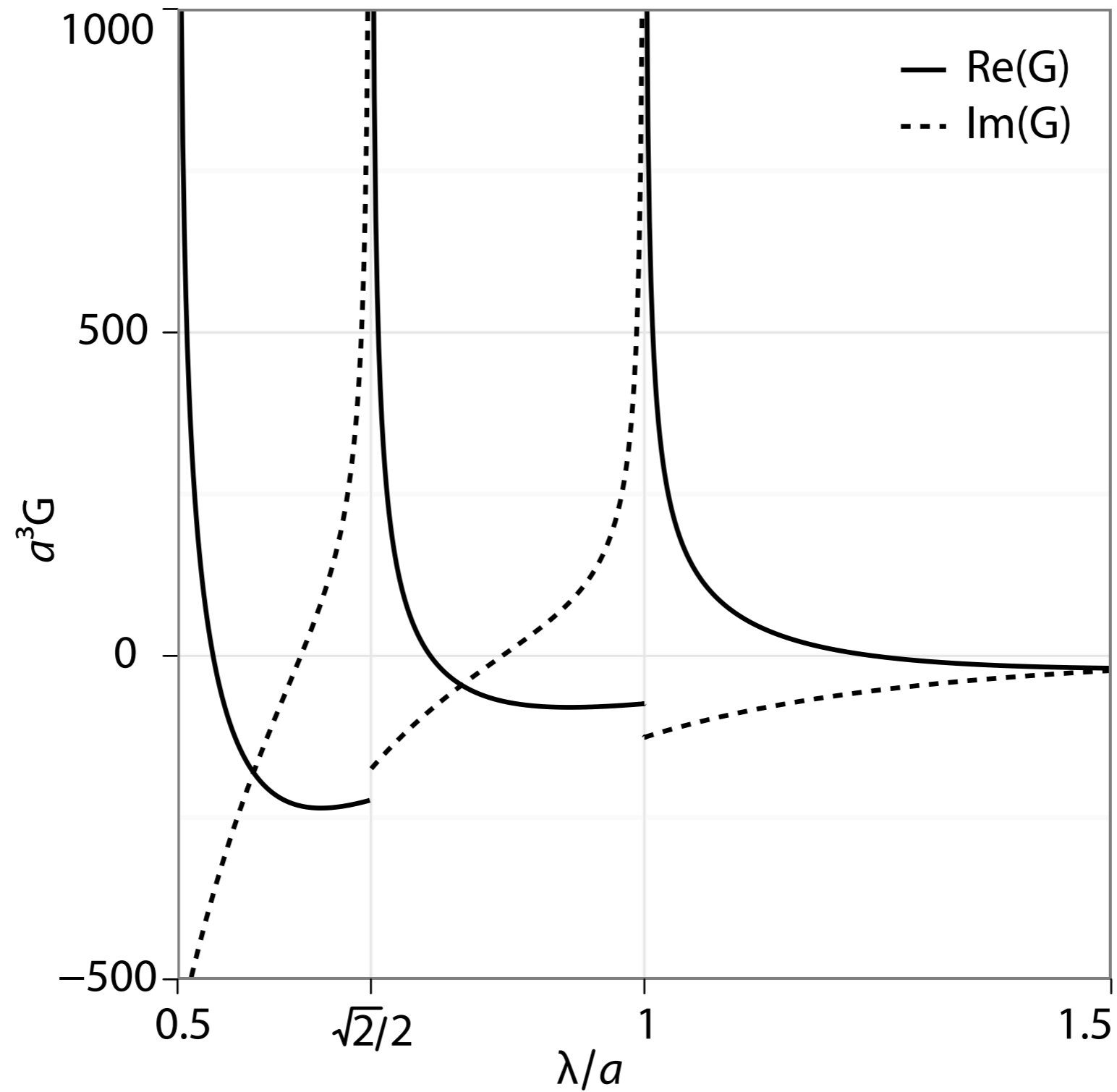
Try

- "banking" at 45°
- standard ratios

TIP #3 • ASPECT RATIO

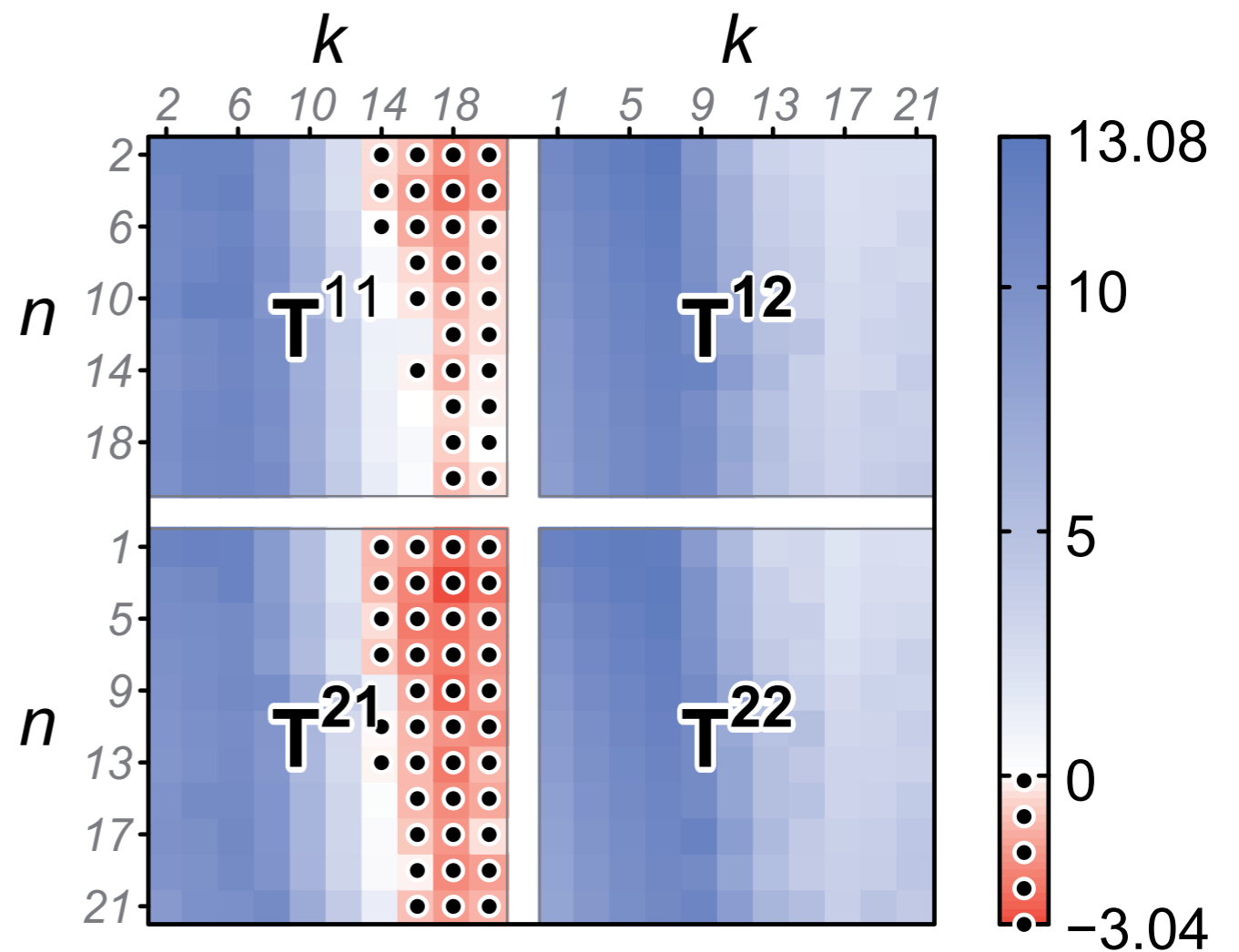
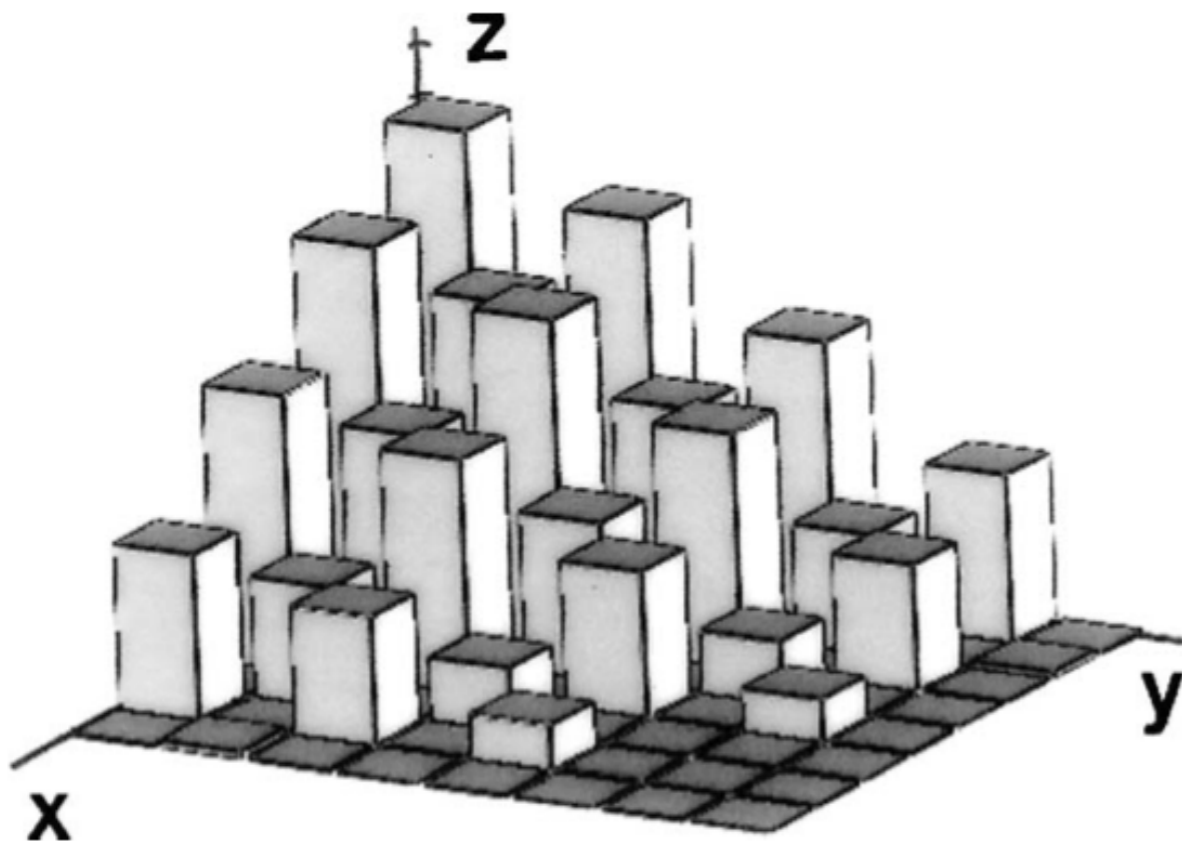
<https://xkcd.com/1732/>

TIP #4 • LESS IS MORE

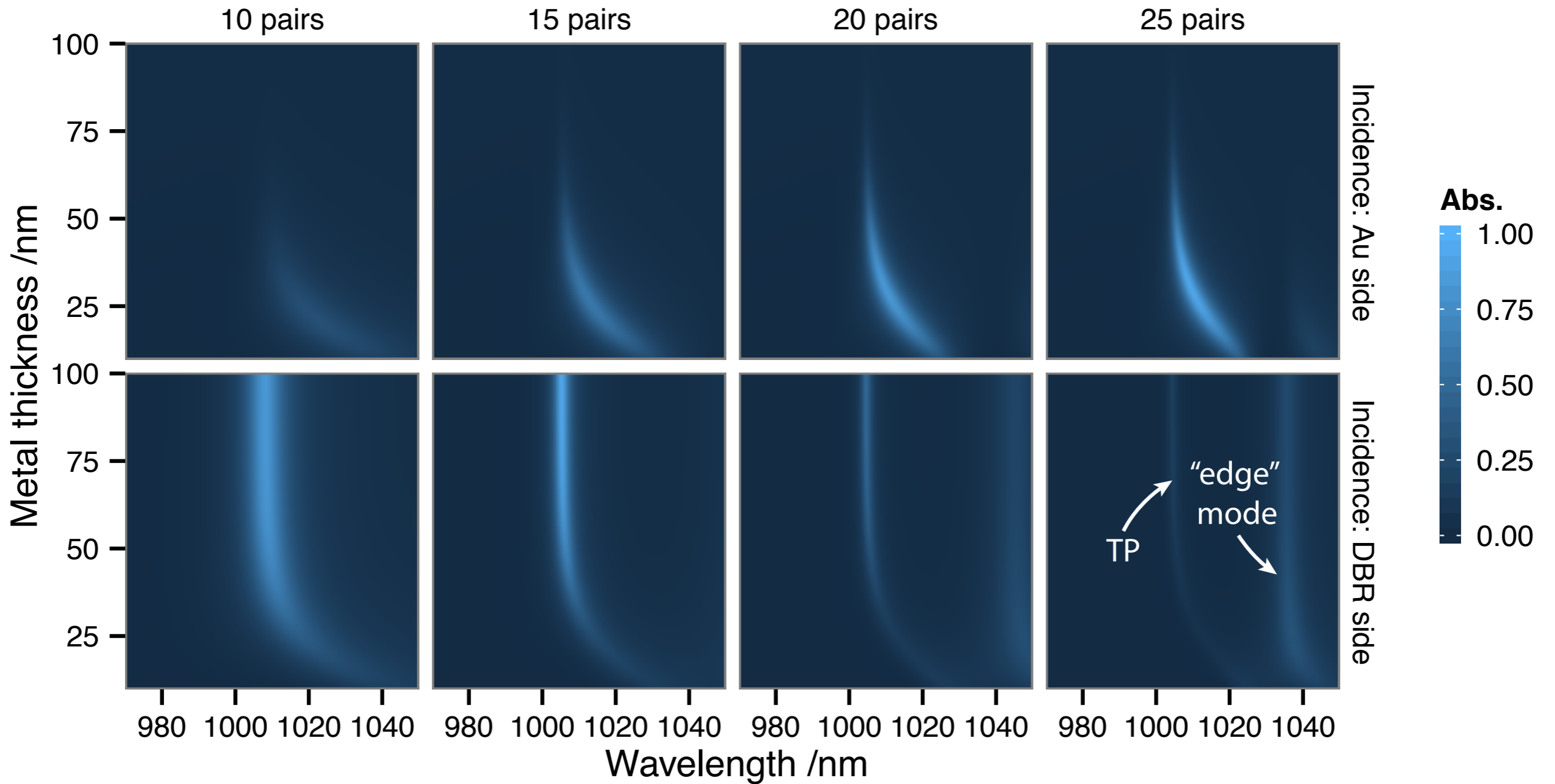


TIP #4 • LESS IS MORE

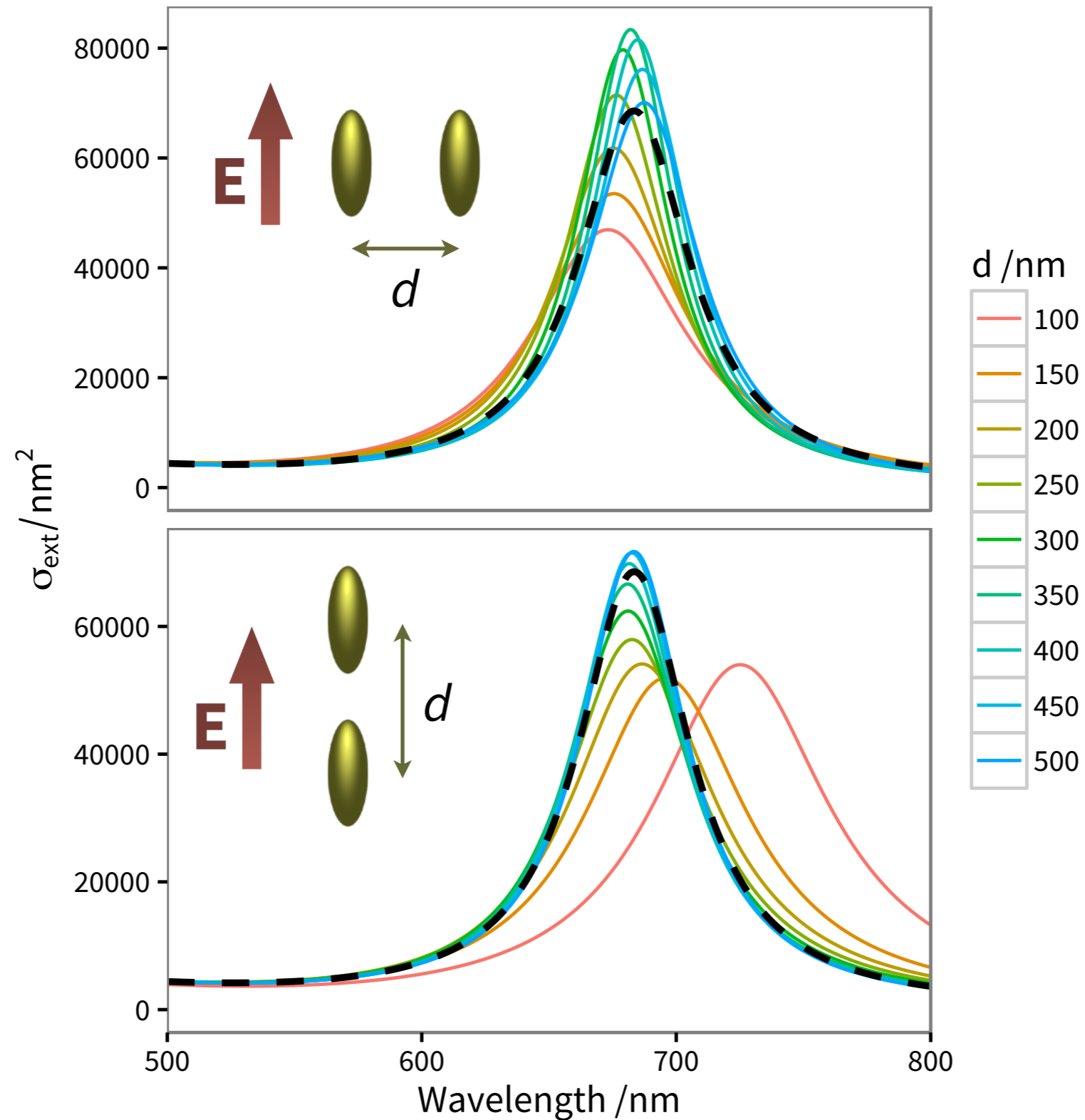
*Fake 3D is often
counterproductive*

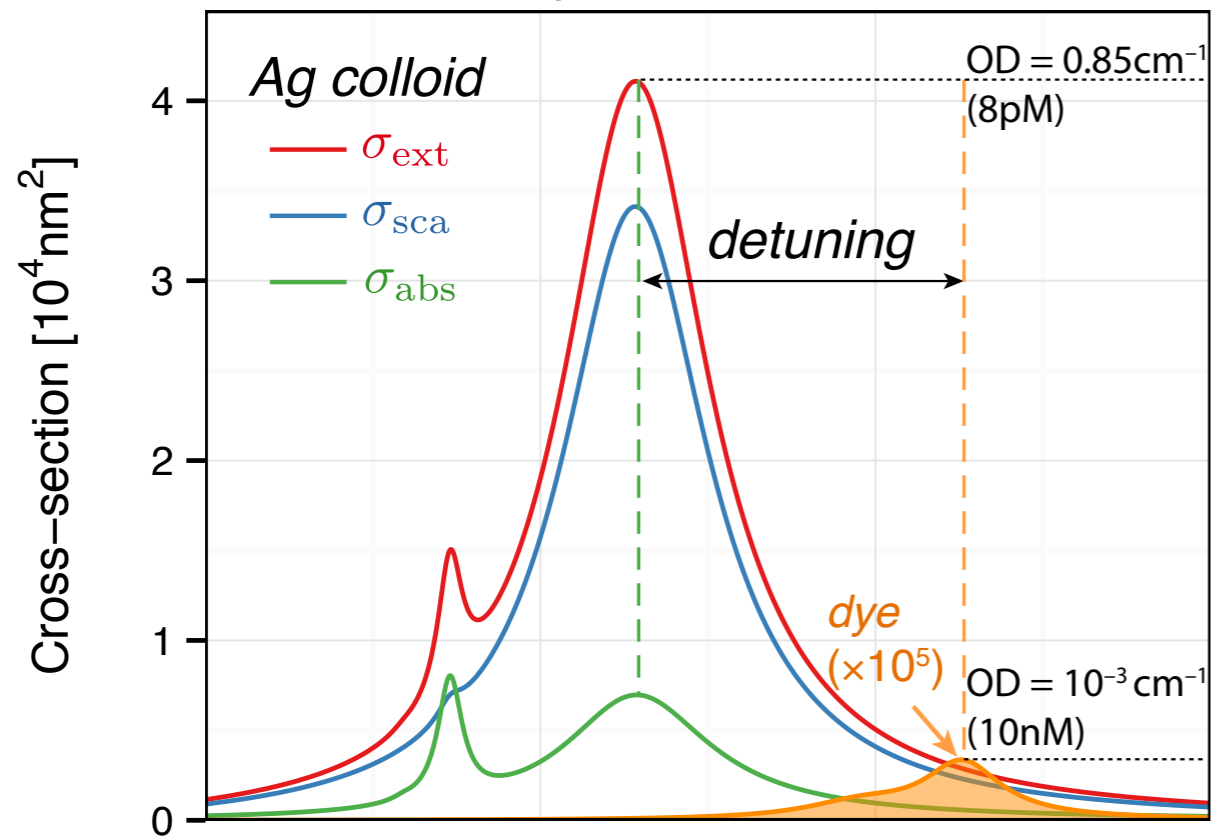
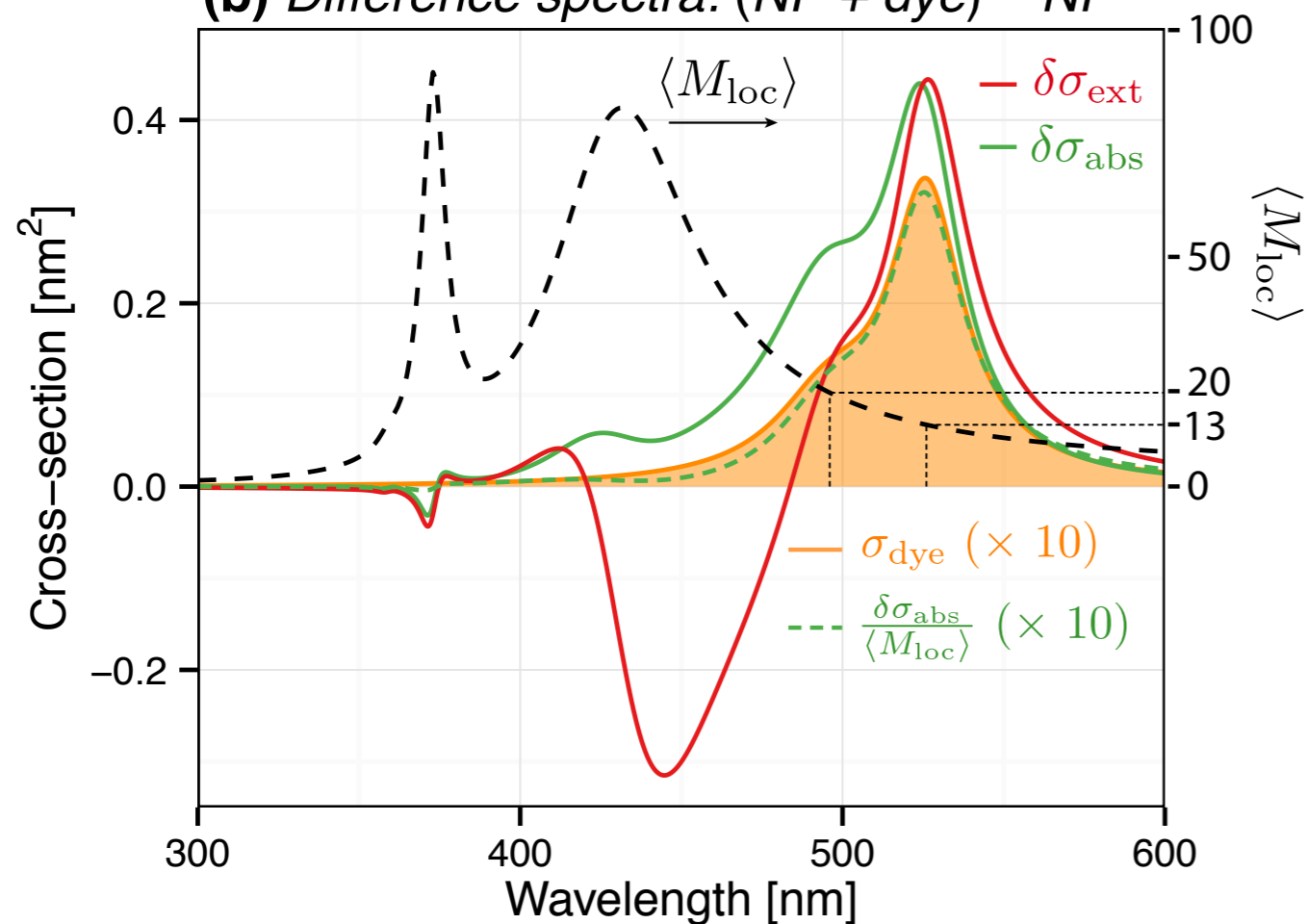
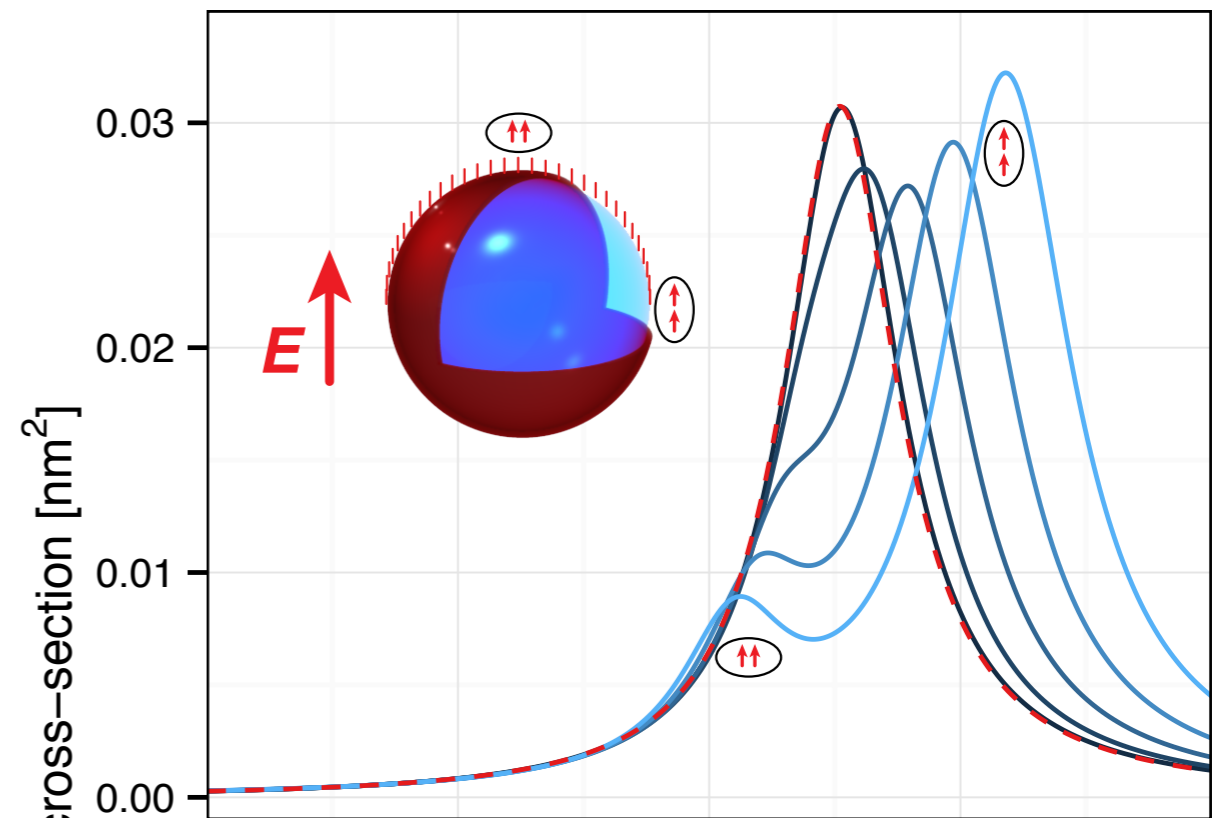
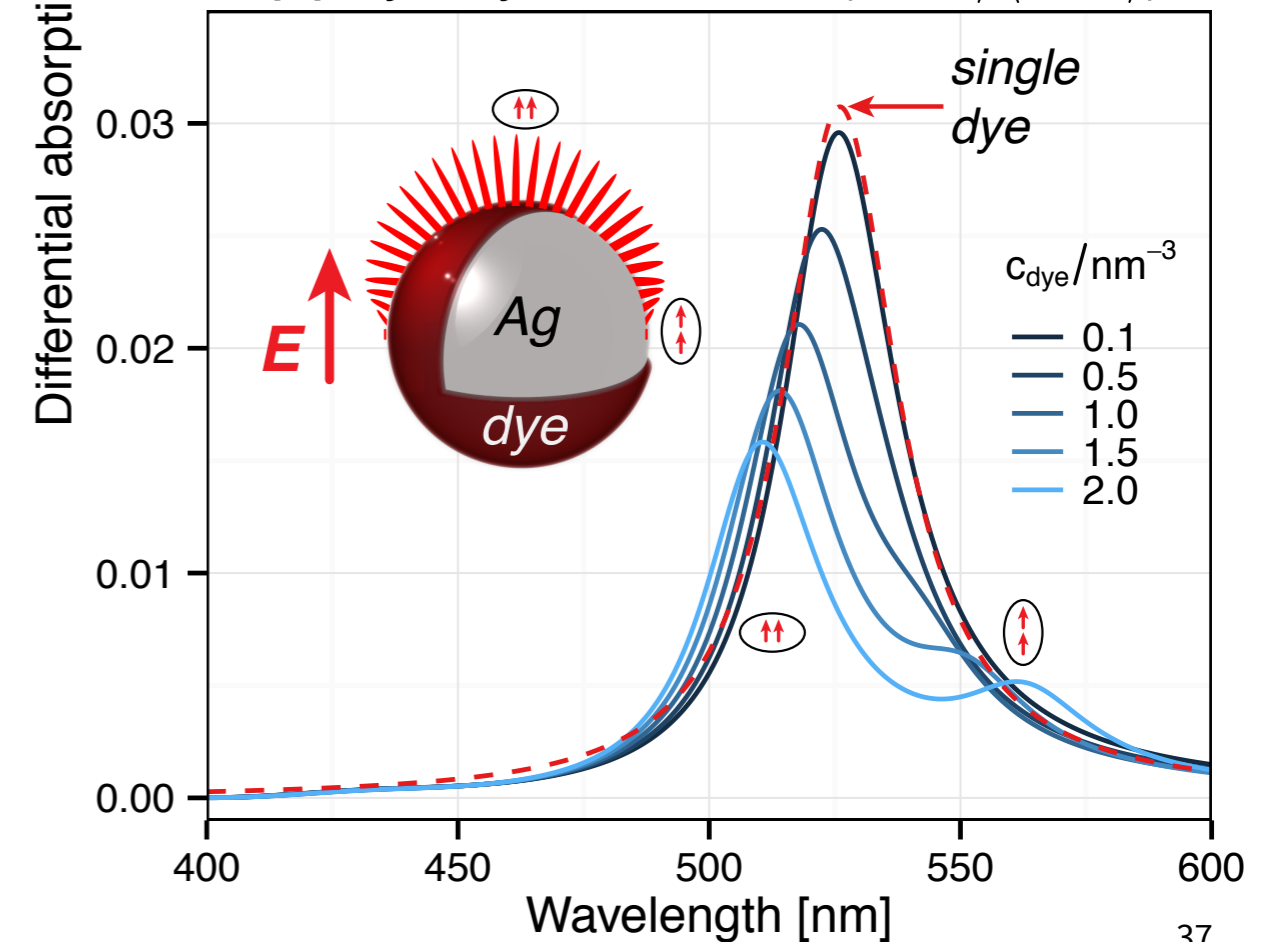


TIP #5 • SMALL MULTIPLES



TIP #6 • CONTEXTUAL ANNOTATIONS



(a) Bare components**(b) Difference spectra: (NP + dye) - NP****(c) Hollow dye shell ($\delta \sigma_{\text{abs}}$)****(d) Dye layer on colloid ($\delta \sigma_{\text{abs}} / \langle M_{\text{loc}} \rangle$)**

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

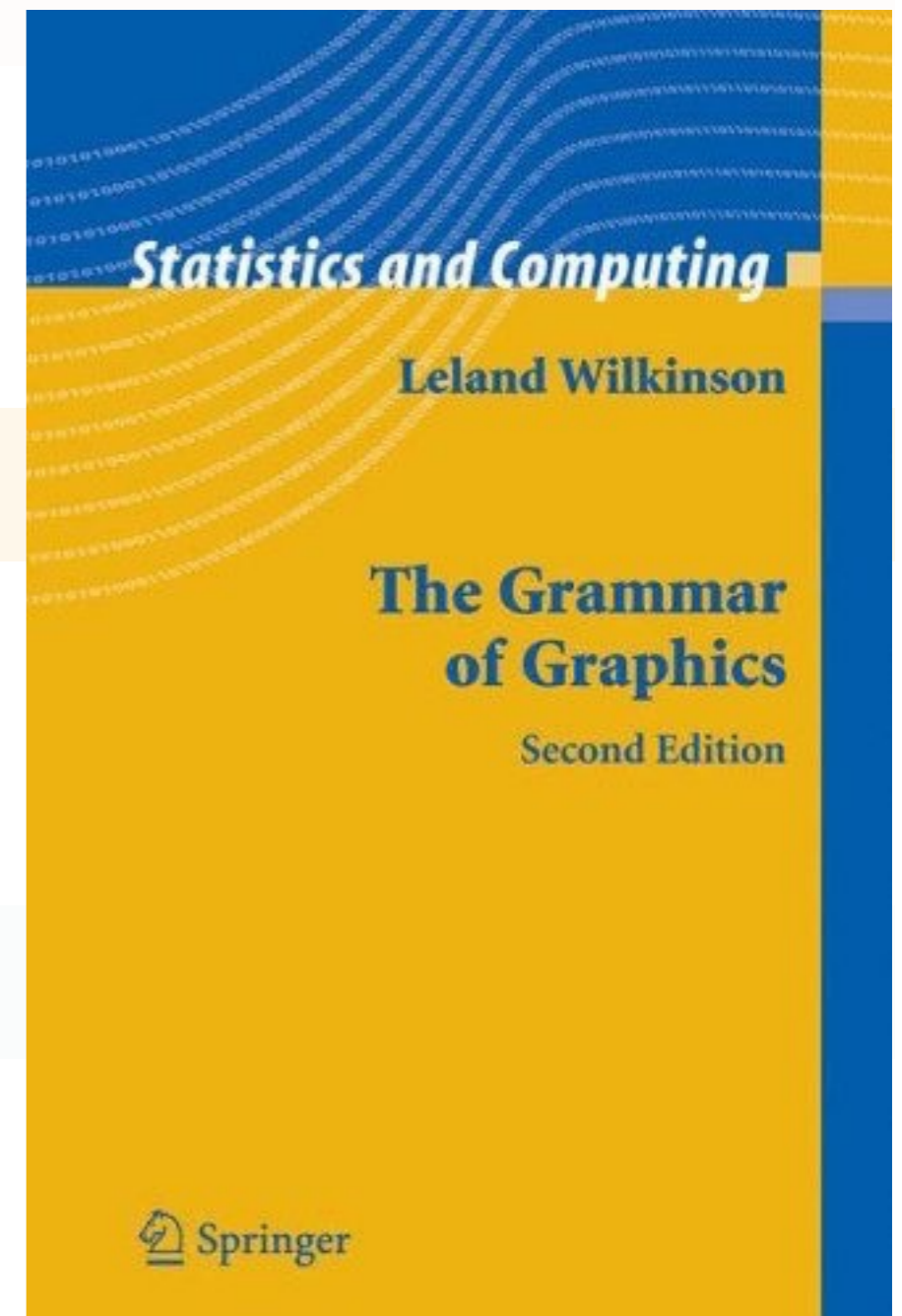
- *The good, the bad, and the ugly*
- *Tips and guidelines*

▶ 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.

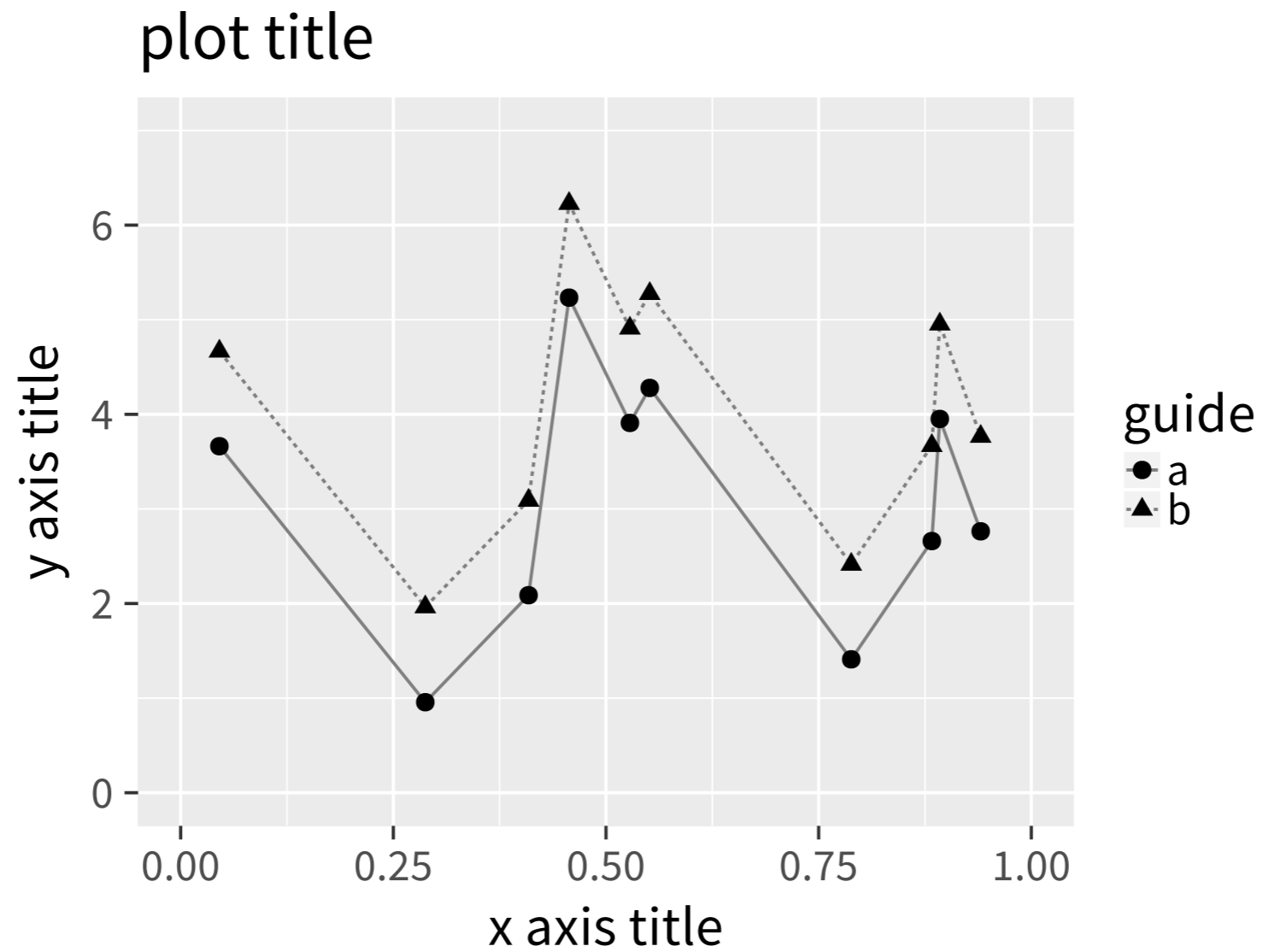
L. Wilkinson

TAXONOMY OF GRAPHICS

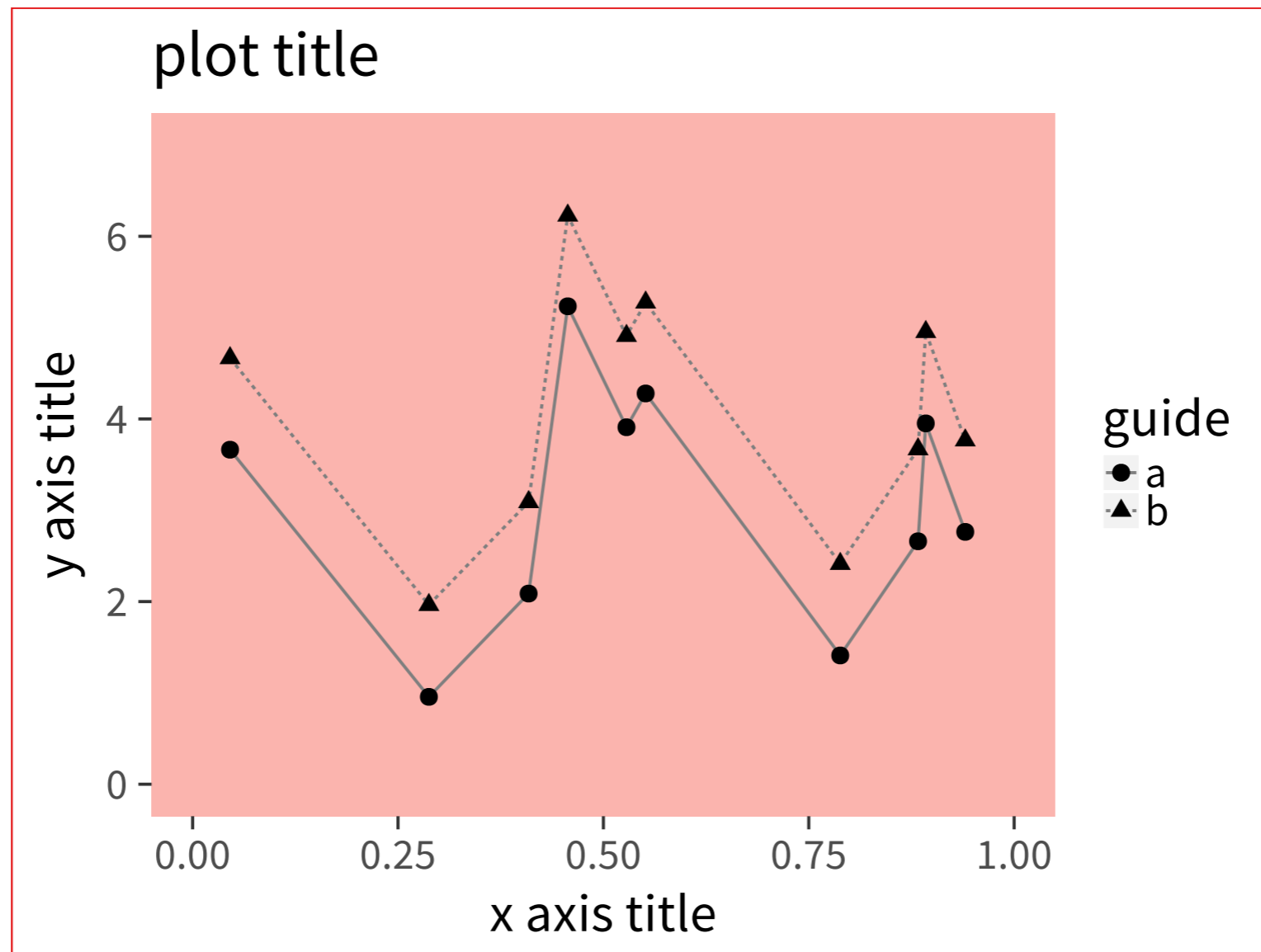
Deviation	Correlation	Ranking	Distribution	Change over Time	Part-to-whole	Magnitude	Spatial	Flow
<p>Emphasise variations (+/-) from a fixed reference point. Typically the reference point is zero but it can also be a target or a long-term average. Can also be used to show sentiment (positive/neutral/negative).</p> <p>Example FT uses Trade surplus/deficit, climate change</p>	<p>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).</p> <p>Example FT uses Inflation & unemployment, income & life expectancy</p>	<p>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.</p> <p>Example FT uses Wealth, deprivation, league tables, constituency election results</p>	<p>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.</p> <p>Example FT uses Income distribution, population (age/sex) distribution</p>	<p>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.</p> <p>Example FT uses Share price movements, economic time series</p>	<p>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.</p> <p>Example FT uses Fiscal budgets, company structures, national election results</p>	<p>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.</p> <p>Example FT uses Commodity production, market capitalisation</p>	<p>Used only when precise locations or geographical patterns in data are more important to the reader than anything else.</p> <p>Example FT uses Locator maps, population density, natural resource locations, natural disaster risk/impact, catchment areas, variation in election results</p>	<p>Show the reader volumes or intensity of movement between two or more states or conditions. These might be logical sequences or geographical locations.</p> <p>Example FT uses Movement of funds, trade, migrants, lawsuits, information; relationship graphs.</p>
<p>Diverging bar A simple standard bar chart that can handle both negative and positive magnitude values.</p> <p>Diverging stacked bar Perfect for presenting survey results which involve sentiment (eg disagree/neutral/agree).</p> <p>Spine chart Splits a single value into 2 contrasting components (eg Male/Female).</p> <p>Surplus/deficit filled line The shaded area of these charts allows a balance to be shown - either against a baseline or between two series.</p>	<p>Scatterplot The standard way to show the relationship between two continuous variables, each of which has its own axis.</p> <p>Line + Column A good way of showing the relationship between an amount (columns) and a rate (line).</p> <p>Connected scatterplot Usually used to show how the relationship between 2 variables has changed over time.</p> <p>Bubble Like a scatterplot, but adds additional detail by sizing the circles according to a third variable.</p> <p>XY heatmap A good way of showing the patterns between 2 categories of data, less good at showing fine differences in amounts.</p>	<p>Ordered bar Standard bar charts display the ranks of values much more easily when sorted into order.</p> <p>Ordered column See above.</p> <p>Ordered proportional symbol Use when there are big variations between values and/or seeing fine differences between data is not so important.</p> <p>Dot strip plot Dots placed in order on a strip are a space-efficient method of laying out ranks across multiple categories.</p> <p>Slope Perfect for showing how ranks have changed over time or vary between categories.</p> <p>Lollipop chart Lollipops draw more attention to the data value than standard bar/column and can also show rank and value effectively.</p>	<p>Histogram The standard way to show a changing time series. If data are irregular, consider markers to represent data points.</p> <p>Boxplot Summarise multiple distributions by showing the median (centre) and range of the data</p> <p>Violin plot Similar to a box plot but more effective with complex distributions (data that cannot be summarised with simple average).</p> <p>Population pyramid A standard way for showing the age and sex breakdown of a population distribution; effectively, back to back histograms.</p> <p>Dot strip plot Good for showing individual values in a distribution, can be a problem when too many dots have the same value.</p> <p>Dot plot A simple way of showing the change or range (min/max) of data across multiple categories.</p> <p>Barcode plot Like dot strip plots, good for displaying all the data in a table; they work best when highlighting individual values.</p> <p>Cumulative curve A good way of showing how unequal a distribution is; y axis is always cumulative frequency, x axis is always a measure.</p>	<p>Line The standard way to show a changing time series. If data are irregular, consider markers to represent data points.</p> <p>Column Columns work well for showing change over time - but usually best with only one series of data at a time.</p> <p>Line + column A good way of showing the relationship over time between an amount (columns) and a rate (line).</p> <p>Stock price Usually focused on day-to-day activity, these charts show opening/closing and hi/low points of each day.</p> <p>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.</p> <p>Area chart Use with care - these are good at showing changes to total, but seeing change in components can be very difficult.</p> <p>Fan chart (projections) Use to show the uncertainty in future projections - usually this grows the further forward to projection.</p> <p>Connected scatterplot A good way of showing changing data for two variables - at a relatively clear pattern of progression.</p> <p>Calendar heatmap A great way of showing temporal patterns (daily, weekly, monthly) - at the expense of showing precision in quantity.</p> <p>Priestley timeline Great when date and duration are key elements of the story in the data.</p> <p>Circle timeline Good for showing discrete values of varying size across multiple categories (eg earthquakes by continent).</p> <p>Seismogram Another alternative to the circle timeline for showing series where there are big variations in the data.</p>	<p>Stacked column A simple way of showing part-to-whole relationships but can be difficult to read with more than a few components.</p> <p>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.</p> <p>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.</p> <p>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).</p> <p>Treemap Use for hierarchical part-to-whole relationships; can be difficult to read when there are many small segments.</p> <p>Voronoi A way of turning points into areas - any point within each area is closer to the central point than any other centroid.</p> <p>Sunburst Another way of visualising hierarchical part-to-whole relationships. Use sparingly (if at all) for obvious reasons.</p> <p>Arc A hemicycle, often used for visualising political results in parliaments.</p> <p>Gridplot Good for showing % information, they work best when used on whole numbers and work well in multiple layout form.</p> <p>Venn Generally only used for schematic representation.</p> <p>Waterfall Can be useful for showing part-to-whole relationships where some of the components are negative.</p>	<p>Column The standard way to compare the size of things. Must always start at 0 on the axis.</p> <p>Bar See above. Good when the data are not time series and labels have long category names.</p> <p>Paired column As per standard column but allows for multiple series. Can become tricky to read with more than 2 series.</p> <p>Paired bar See above.</p> <p>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.</p> <p>Proportional symbol Use when there are big variations between values and/or seeing fine differences between data is not so important.</p> <p>Isotype (pictogram) Excellent solution in some instances - use only with whole numbers (do not slice off an arm to represent a decimal).</p> <p>Lollipop chart Lollipop charts draw more attention to the data value than standard bar/column - does not HAVE to start at zero (but preferable).</p> <p>Radar chart A space-efficient way of showing value of multiple variables - but make sure they are organised in a way that makes sense to reader.</p> <p>Parallel coordinates An alternative to radar charts - again, the arrangement of the variables is important. Usually benefits from highlighting values.</p>	<p>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.</p> <p>Proportional symbol (count/magnitude) Use for totals rather than rates - be wary that small differences in data will be hard to see.</p> <p>Flow map For showing unambiguous movement across a map.</p> <p>Contour map For showing areas of equal value on a map. Can use deviation colour schemes for showing +/- values</p> <p>Equalised cartogram Converting each unit on a map to a regular and equally-sized shape - good for representing voting regions with equal value.</p> <p>Scaled cartogram (value) Stretching and shrinking a map so that each area is sized according to a particular value.</p> <p>Dot density Used to show the location of individual events/locations - make sure they are reader should see.</p> <p>Heat map Grid-based data values mapped with an intensity colour scale. As choropleth map - but not snapped to an admin/political unit.</p>	<p>Sankey Shows changes in flows from one condition to at least one other; good for tracing the eventual outcome of a complex process.</p> <p>Waterfall Designed to show the sequencing of data through a flow process, typically budgets. Can include +/- components.</p> <p>Chord A complex but powerful diagram which can illustrate 2-way flows (and net winner) in a matrix.</p> <p>Network Used for showing the strength and inter-connectiveness of relationships of varying types.</p>

Source:
ft.com/vocabulary

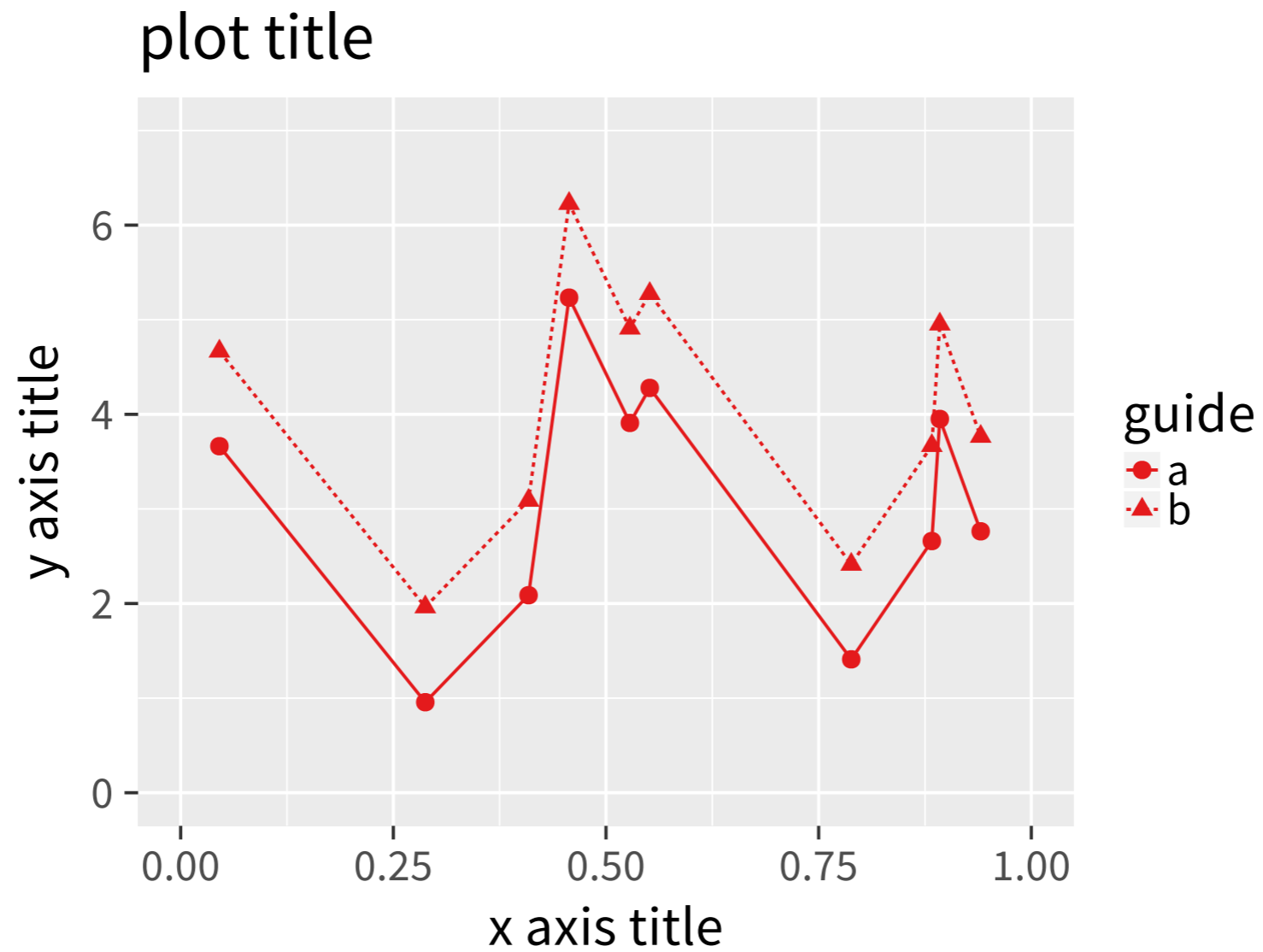
ANATOMY OF A PLOT



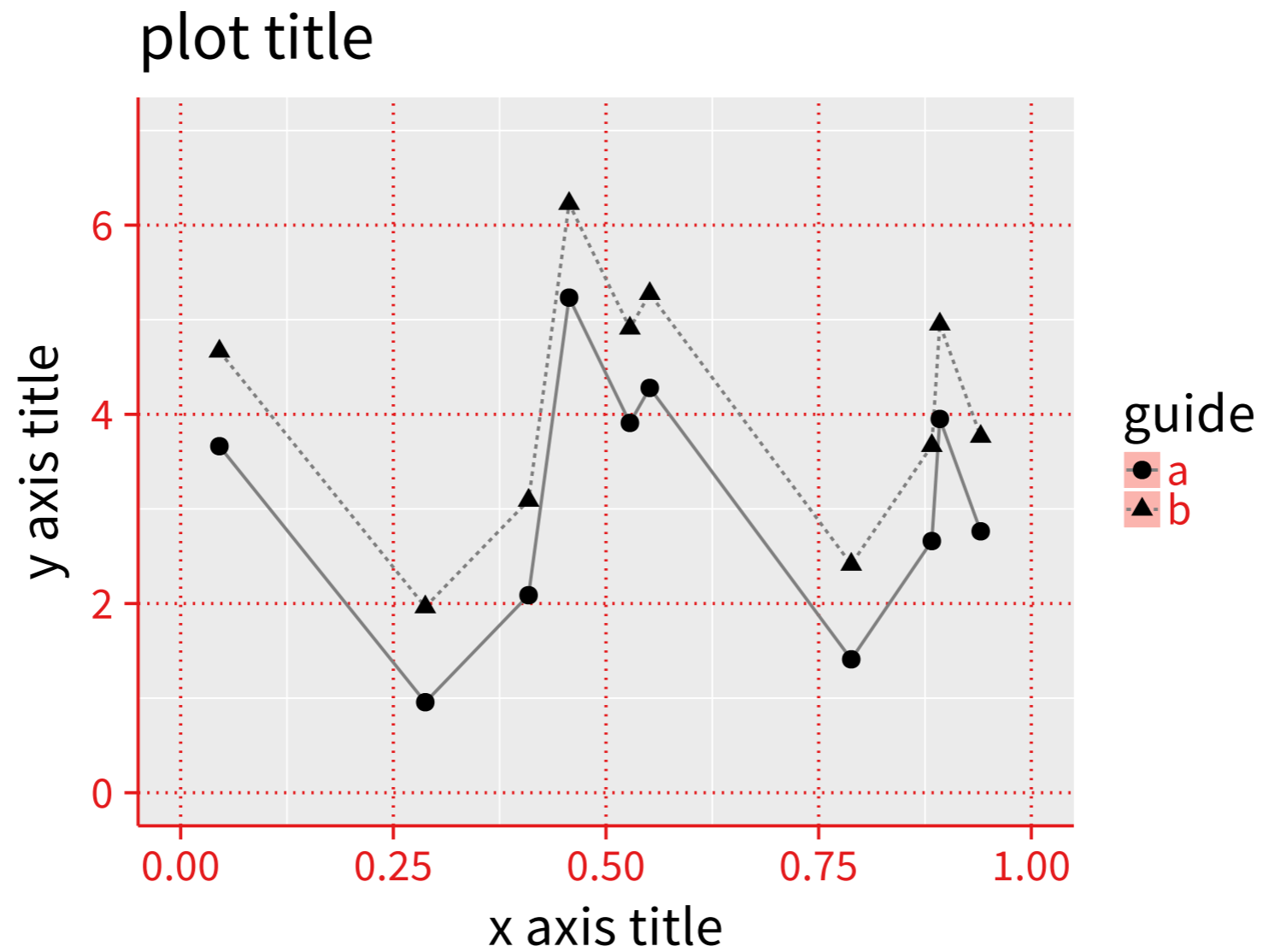
ANATOMY OF A PLOT • *PLOT PANEL*



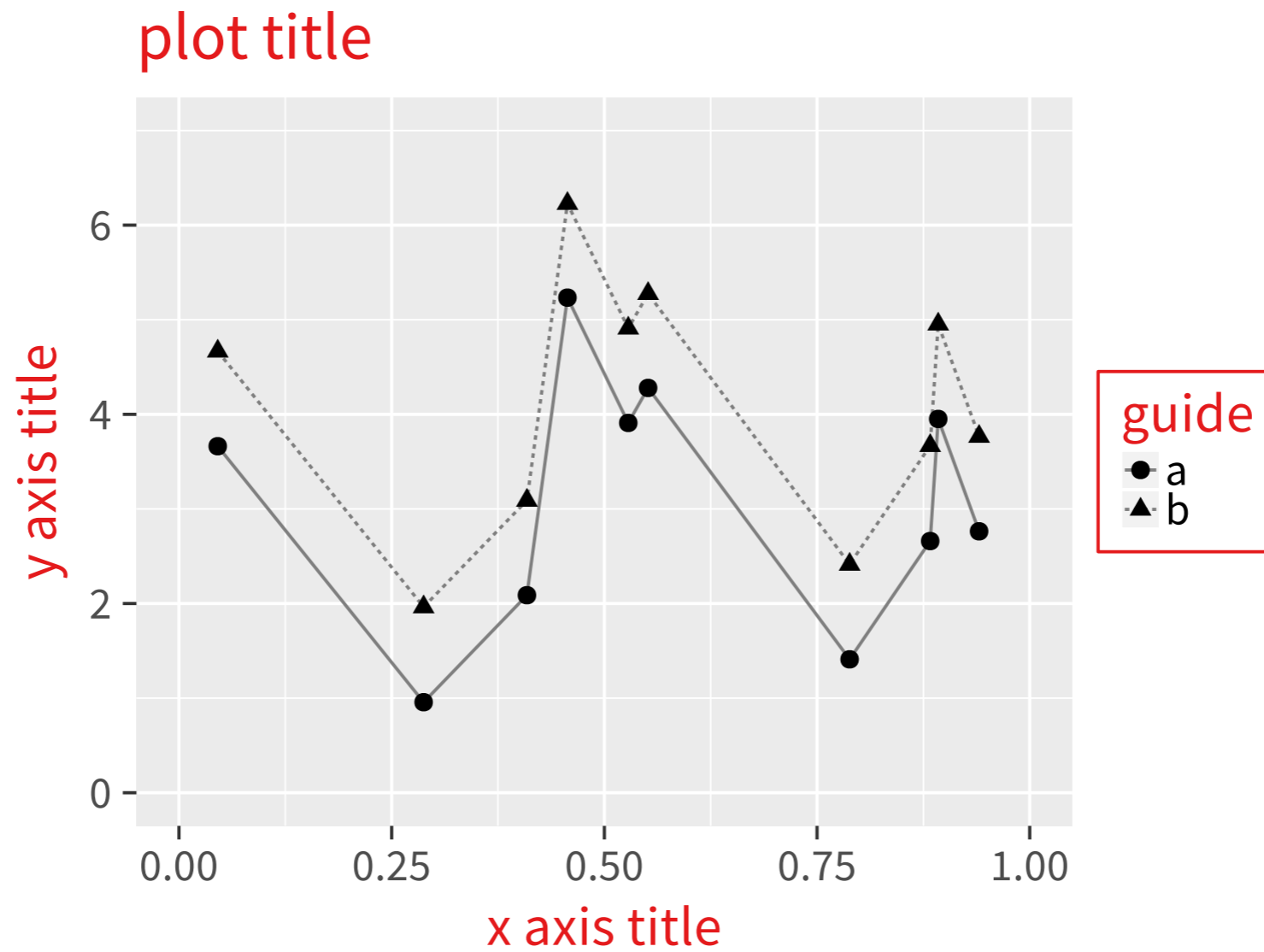
ANATOMY OF A PLOT • *THE DATA*



ANATOMY OF A PLOT • GUIDES

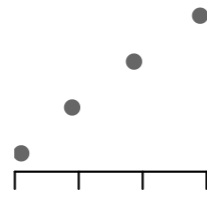


ANATOMY OF A PLOT • ANNOTATIONS

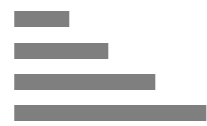


A GRAMMAR OF GRAPHICS – MAPPING DATA

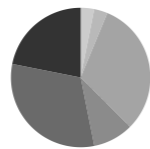
▶ **POSITION**



▶ **LENGTH**



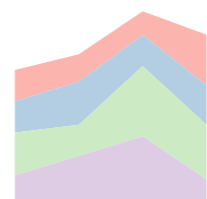
▶ **ANGLE**



▶ **AREA**



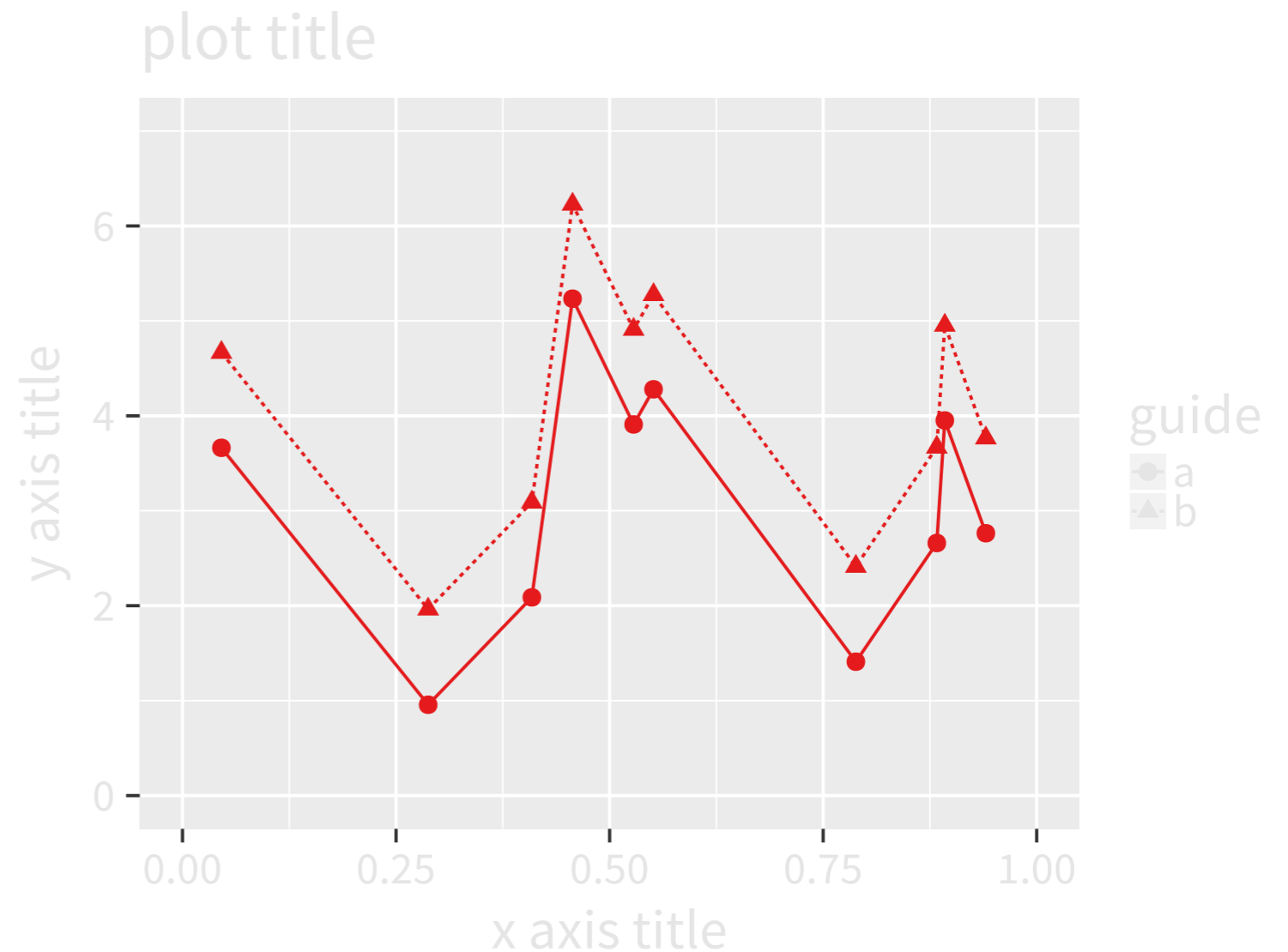
▶ **COLOUR**



▶ **SHAPE**



▶ **LINE TYPE, SIZE, TIME, ...**

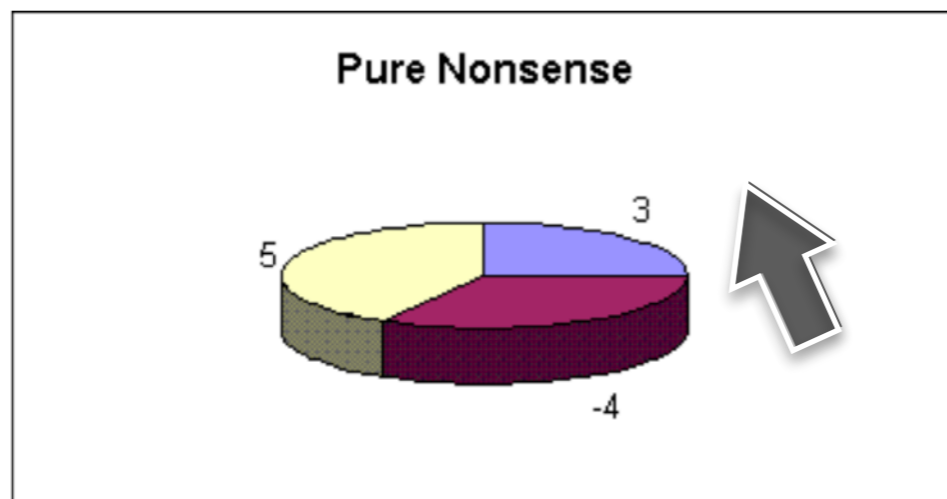


EXPRESSIVITY AND LEGIBILITY

▶ POINT N' CLICK

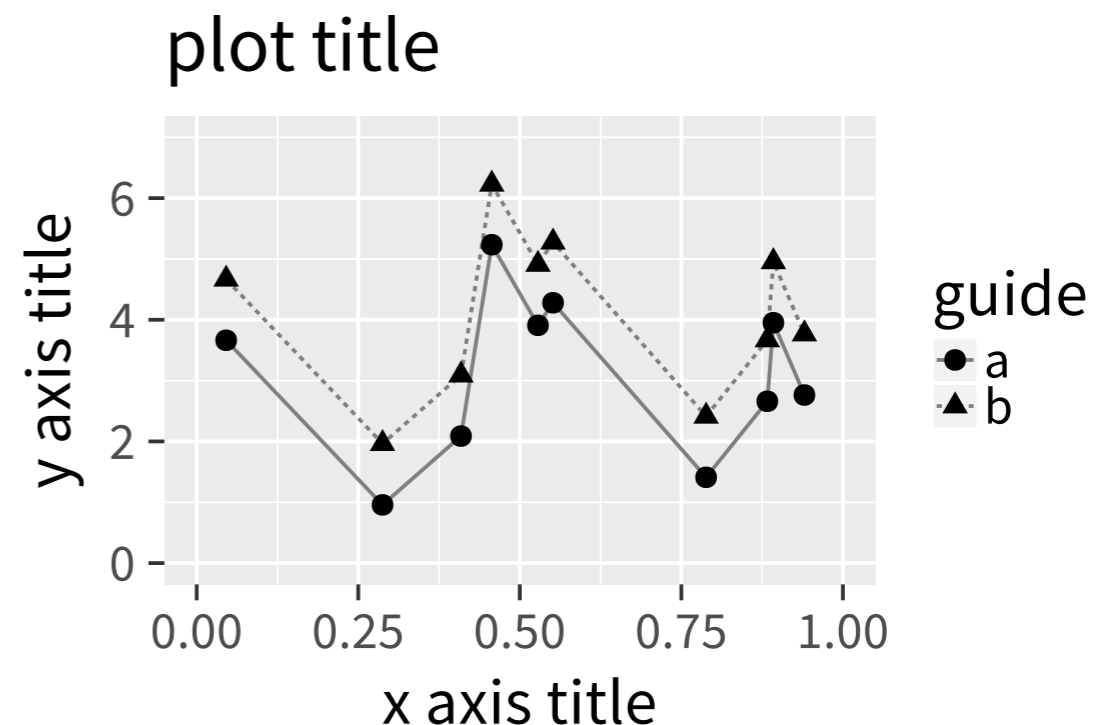
Yeah but, no but, yeah but, no but!!!
yeah but ... I swear * * * * *!!!!?!!!!
... but yeah _('ツ)_' / COMPUTER SAYS NO

Ctrl-Z



▶ GRAMMAR OF GRAPHICS

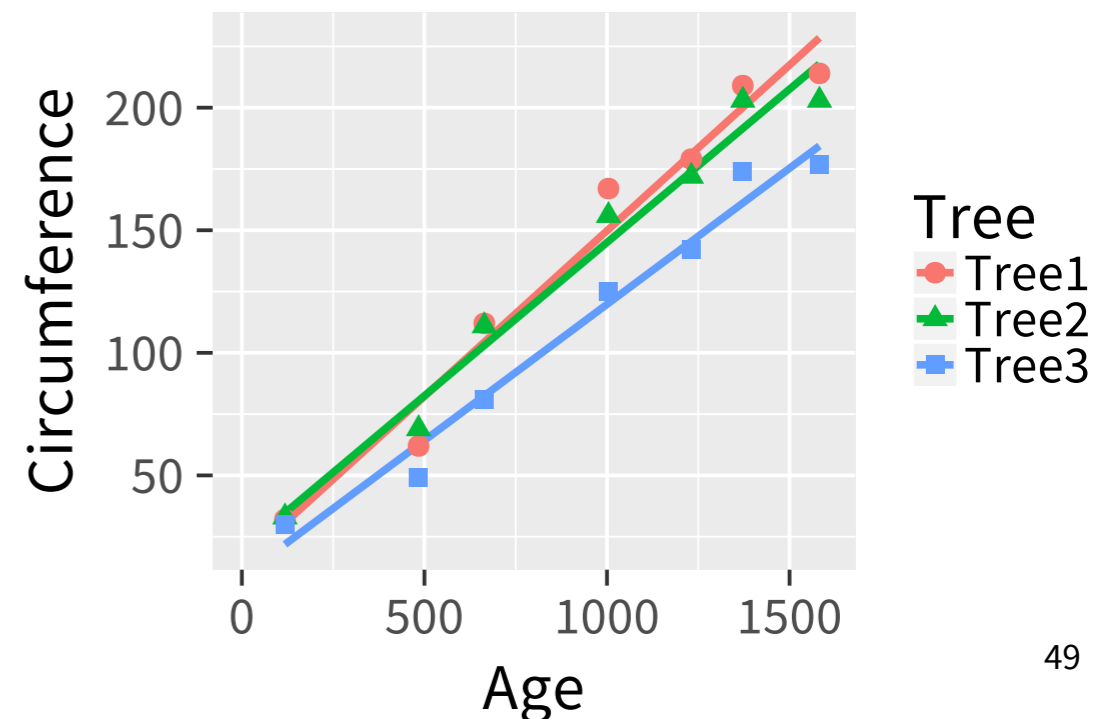
```
plot(data, map(x, y)) +  
  layer(point, map(colour = z)) +  
  layer(line, map(linetype = t)) +  
  theme(fontsize = 12)
```



MAPPING DATA TO GLYPHS

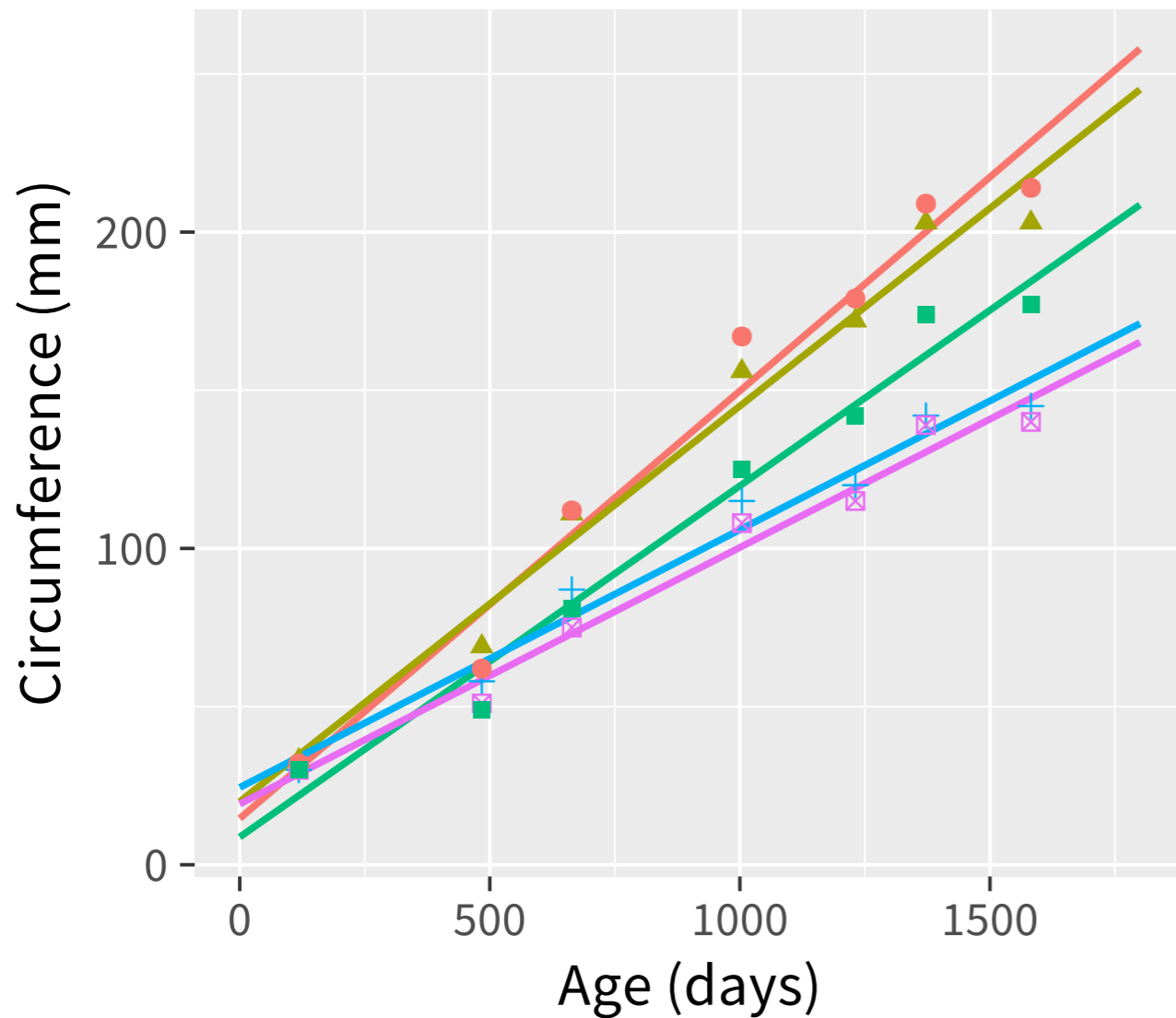
```
plot(data = d,  
      mapping = map(x = age,  
                    y = circumference)) +  
  layer(type = "point",  
        mapping = map(shape = Tree,  
                      colour = Tree)) +  
  layer(type = "line",  
        mapping = map(colour = Tree))
```

	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



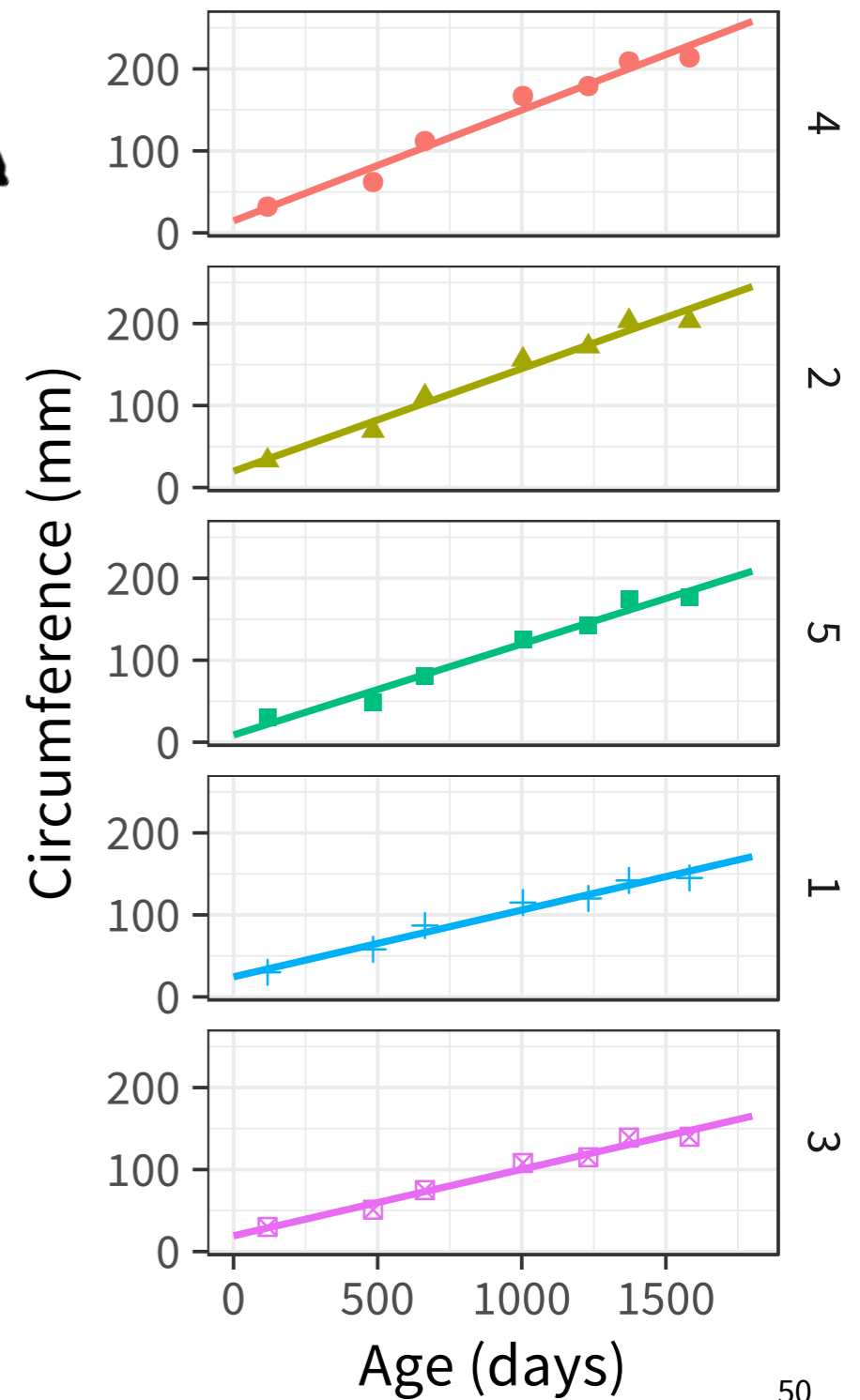
GRAPHICAL EXPLORATIONS

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

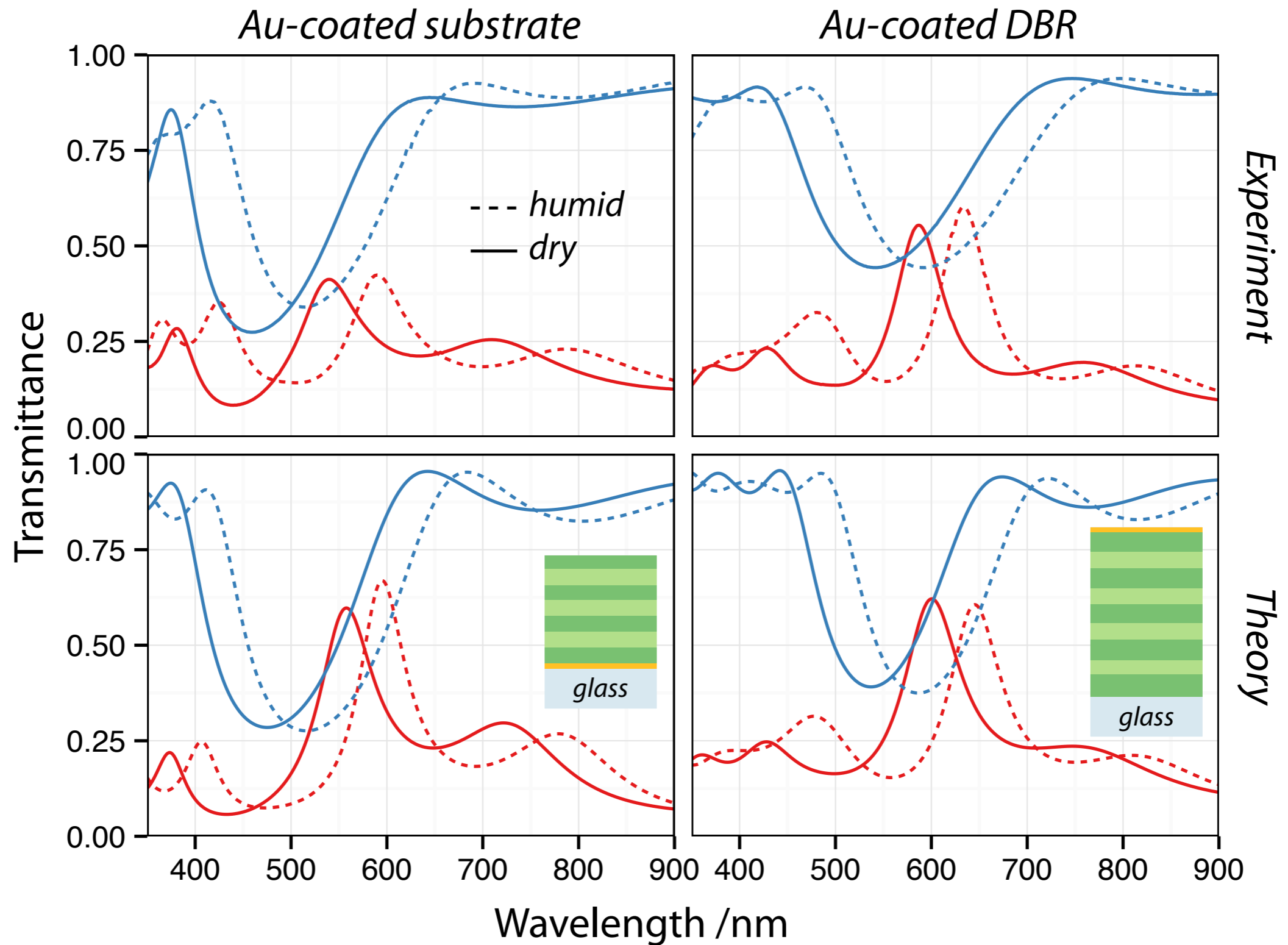


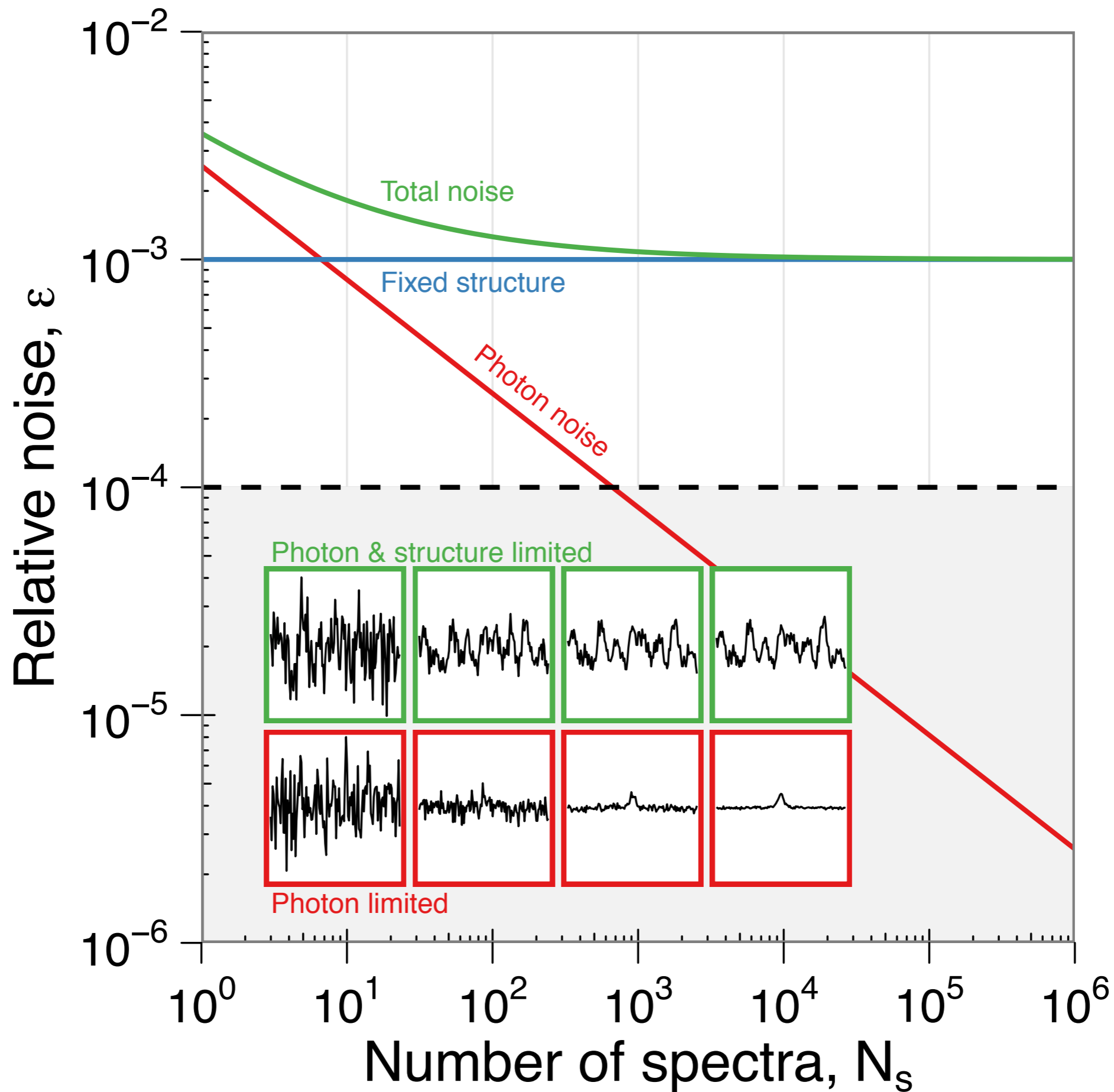
Tree

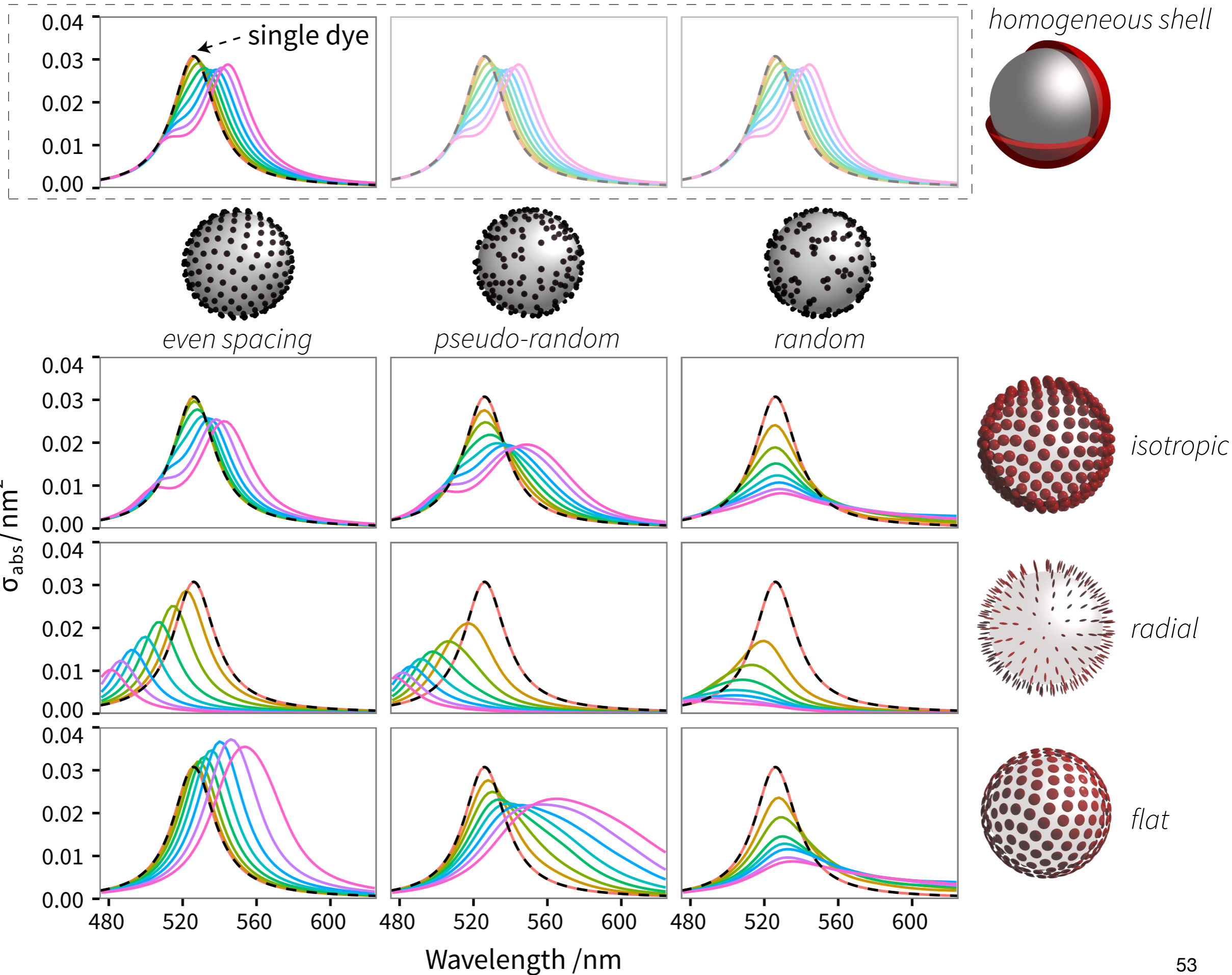
- 4
- 2
- 5
- 1
- 3



SMALL MULTIPLES REVISITED

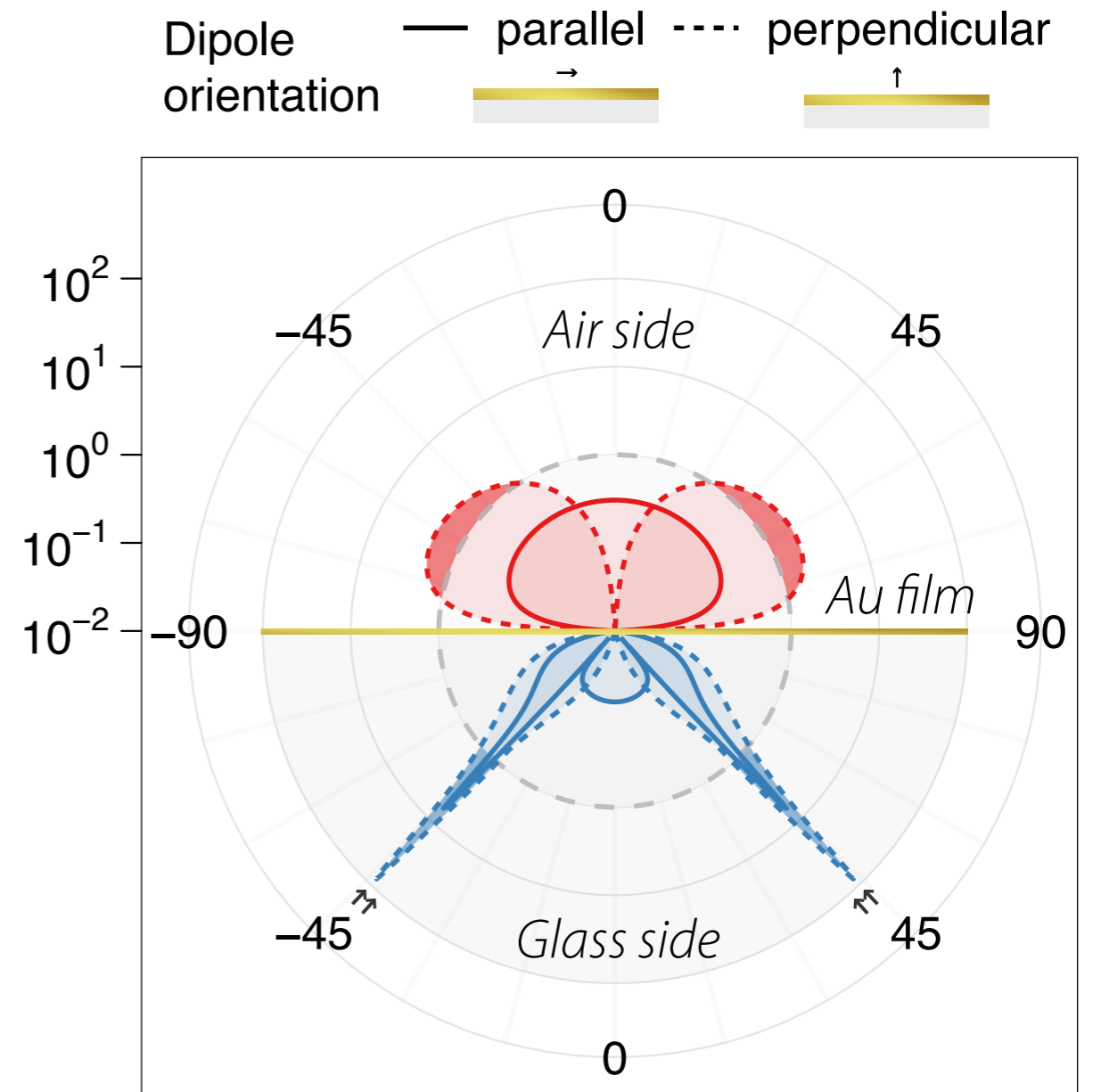




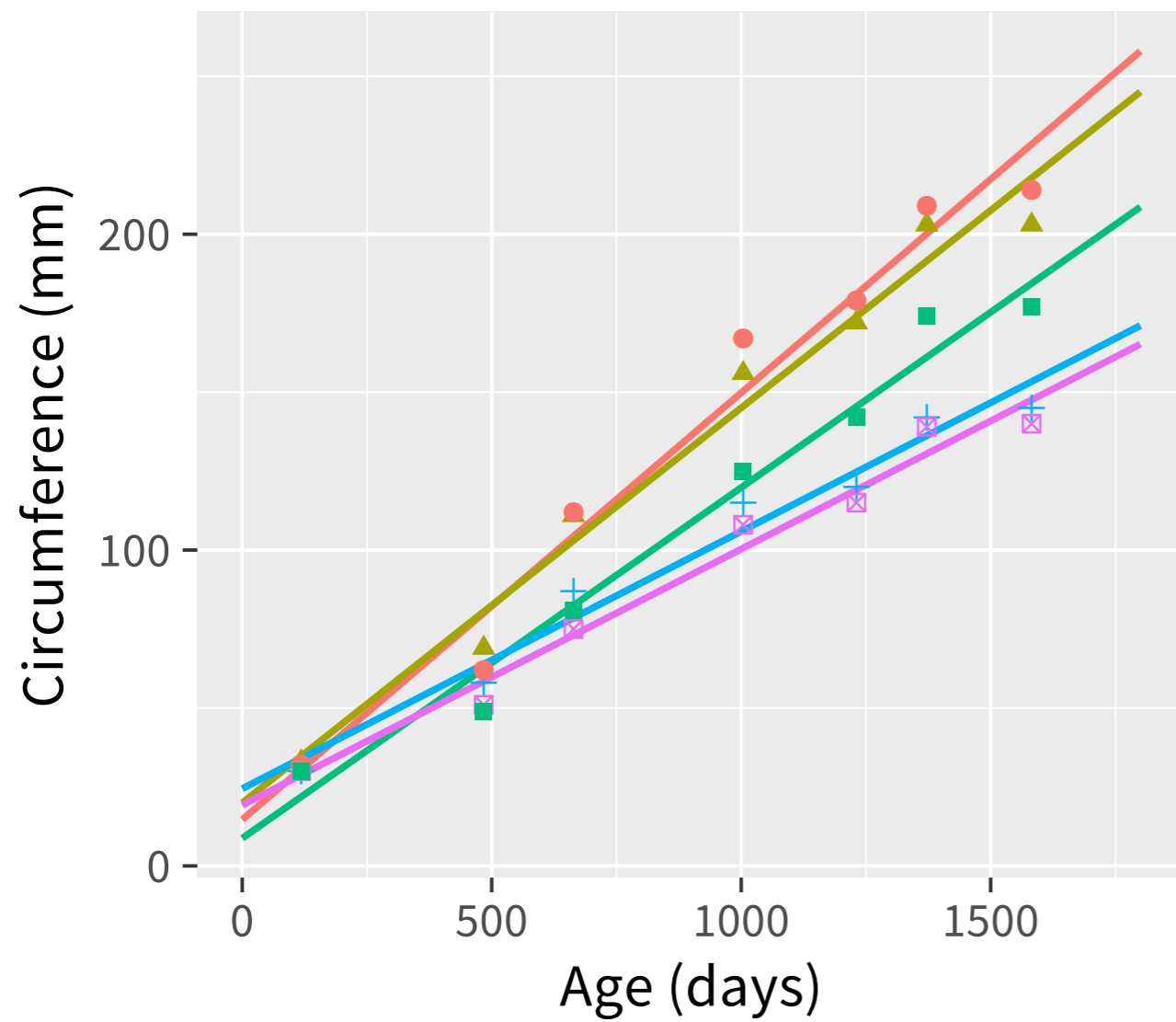


COORDINATE TRANSFORMATIONS

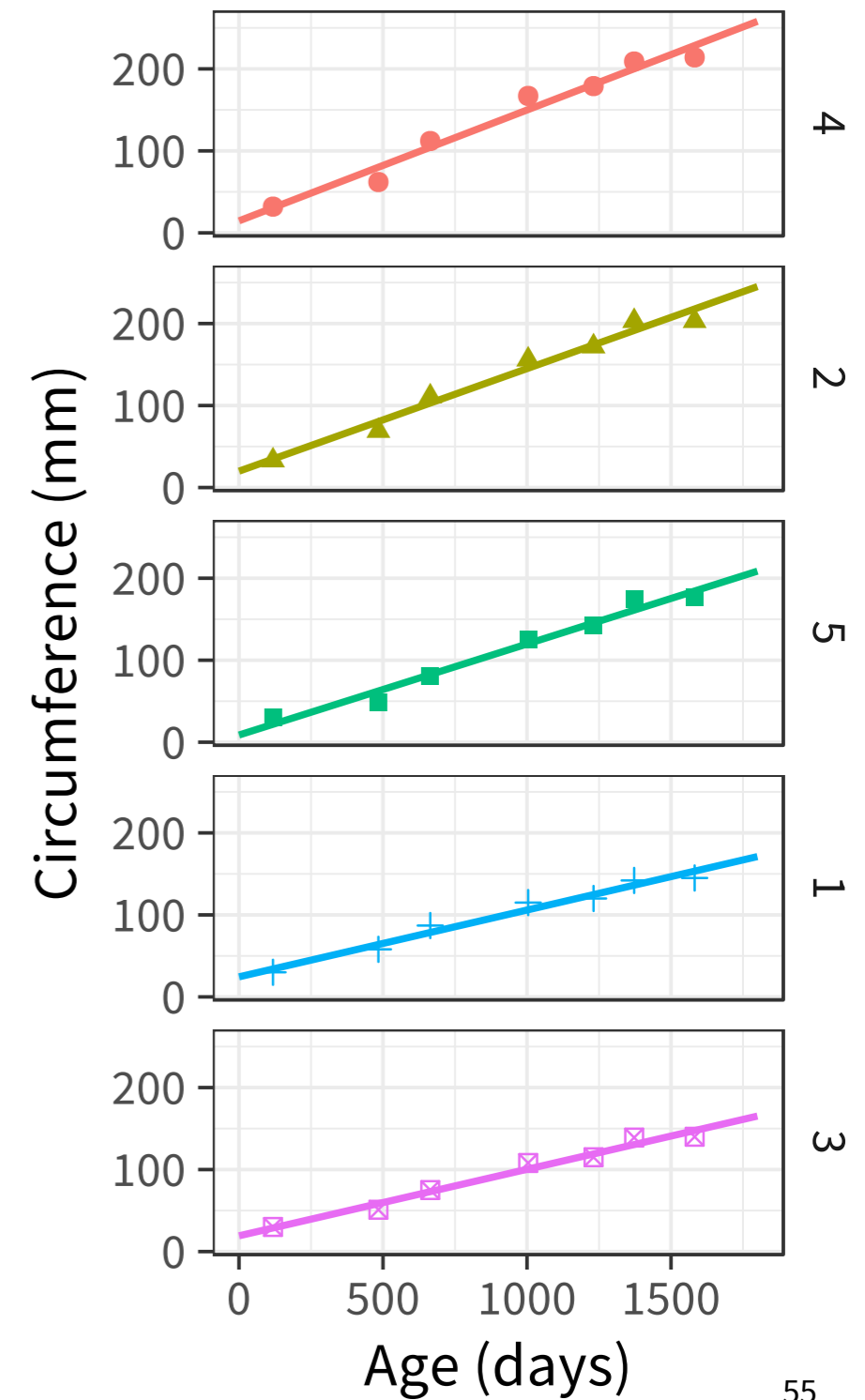
```
plot(data, map(x, y)) +  
  layer(line, map(linetype = t)) +  
  coord_polar(theta = x) +  
  . . .
```



D.R.Y. PRINCIPLE



Tree
4
2
5
1
3



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

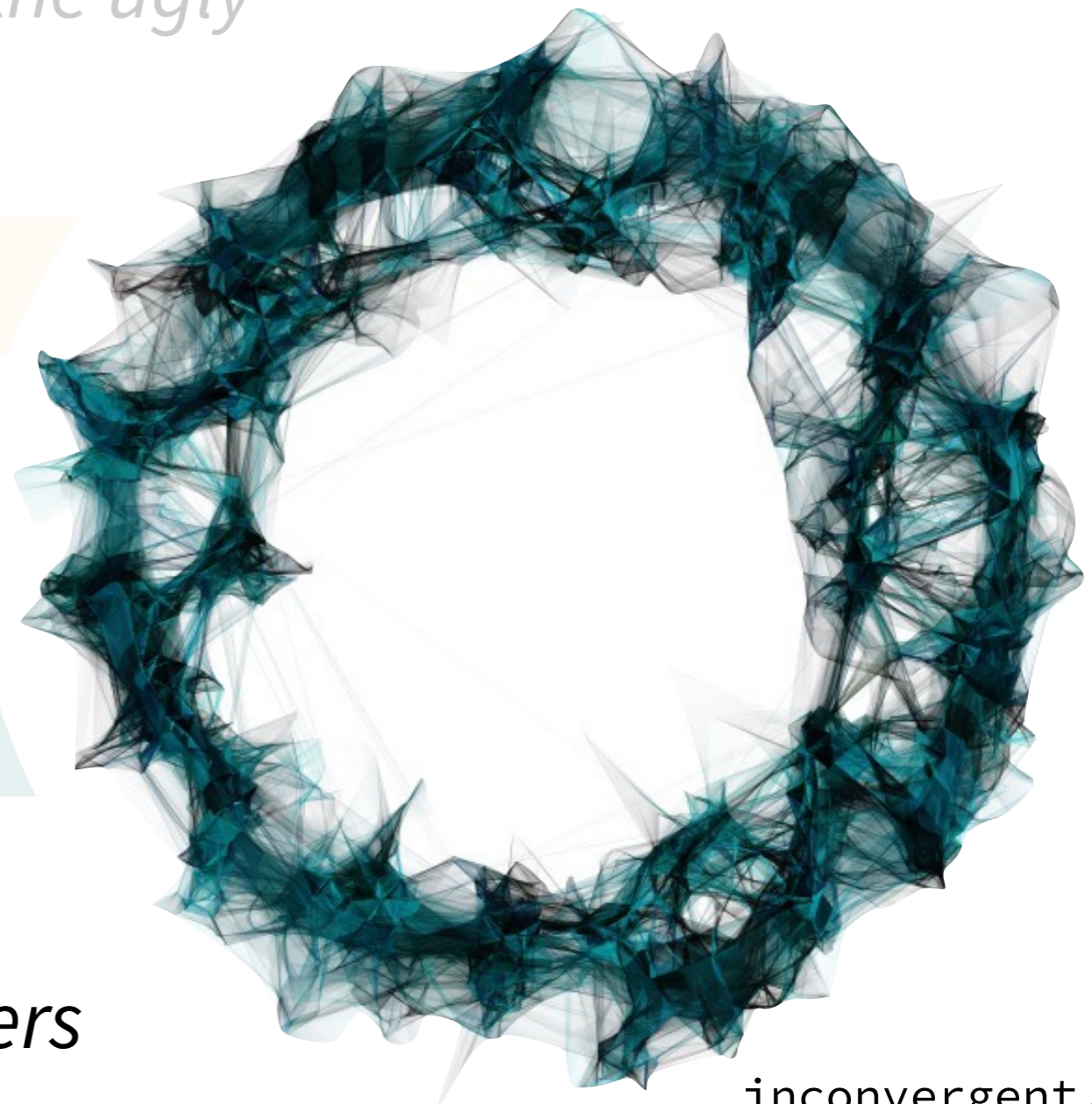
- *The good, the bad, and the ugly*
- *Tips and guidelines*

▶ A GRAMMAR OF GRAPHICS

- *Elements of theory*
- *Glimpse of the future*

▶ A VISION FOR GRAPHICS

- *Aesthetics and impact*
- *TOC figures, slides, posters*



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

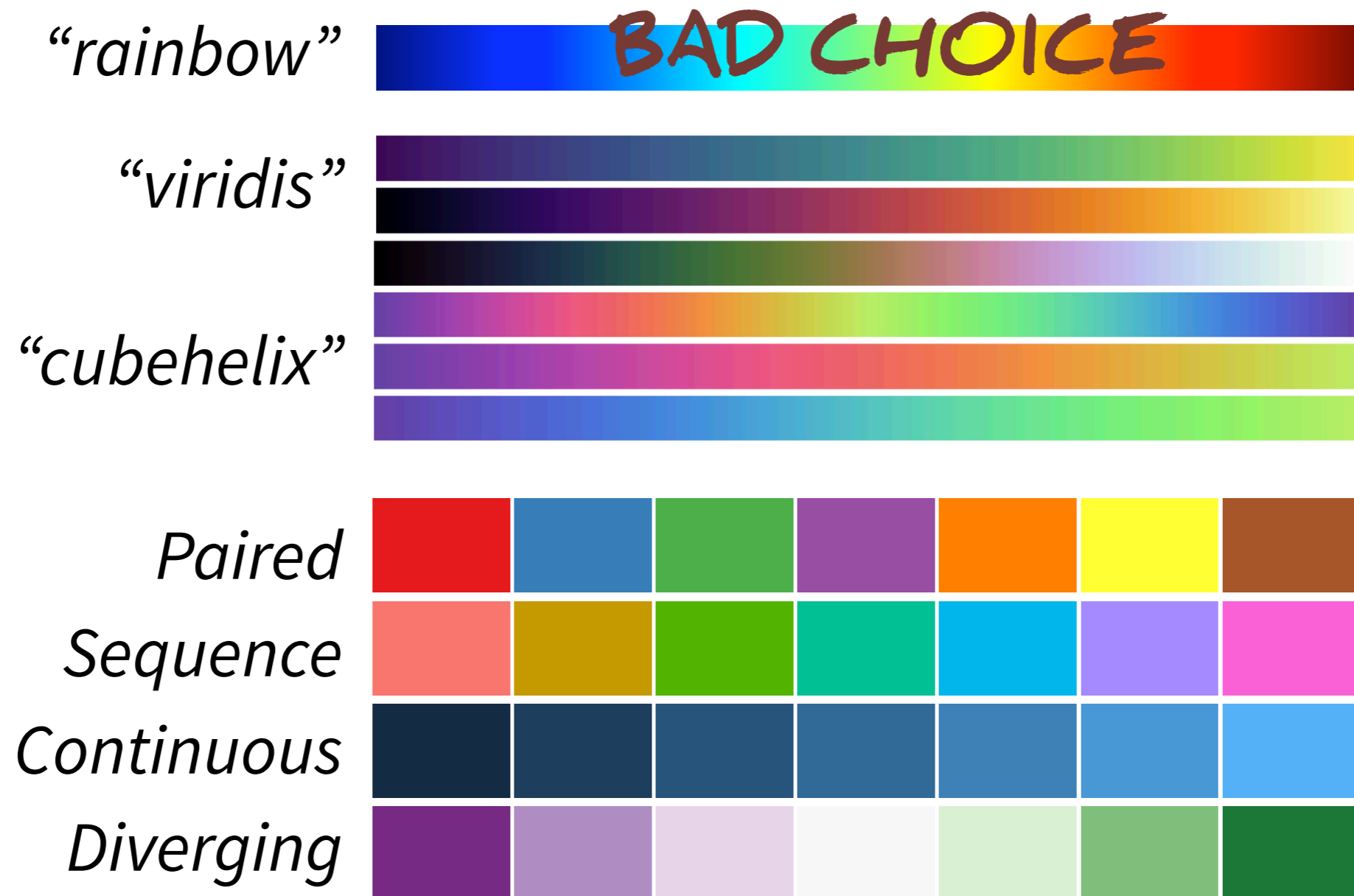
- ▶ **USE COLOUR TO PRIORITISE INFORMATION**

Smaller areas brighter, larger areas lighter

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

Be consistent

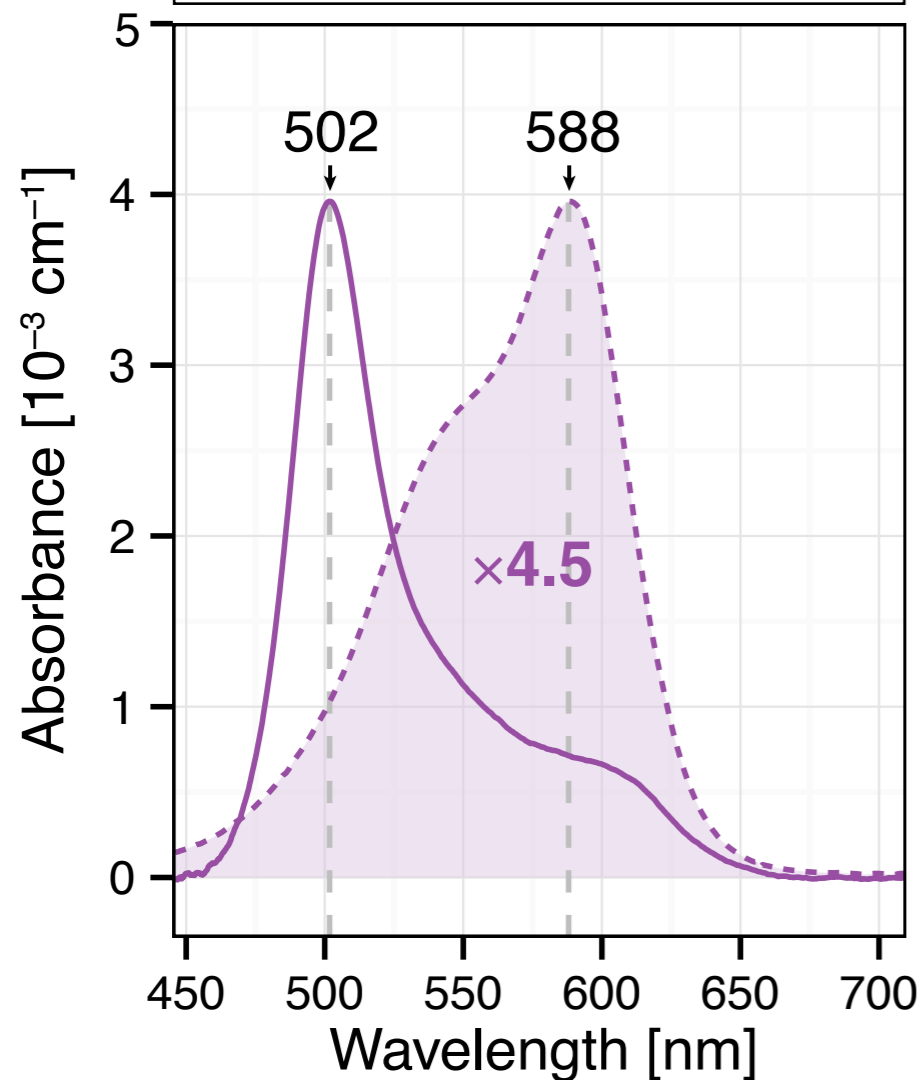
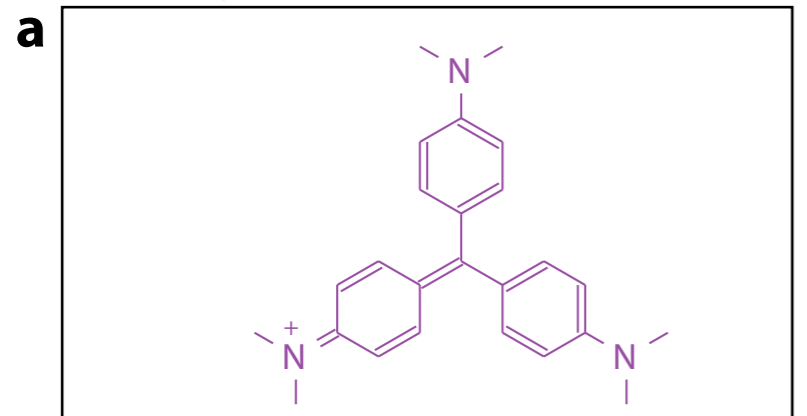
CHOOSING COLOUR PALETTES



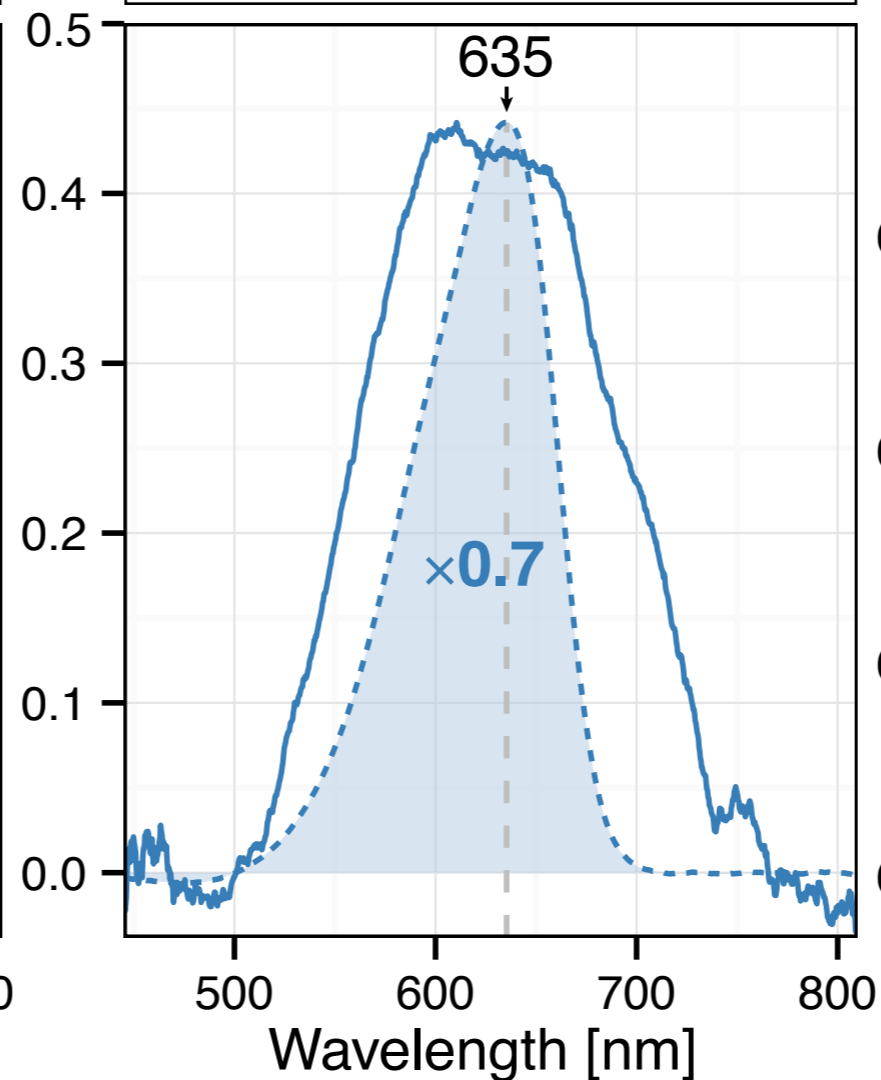
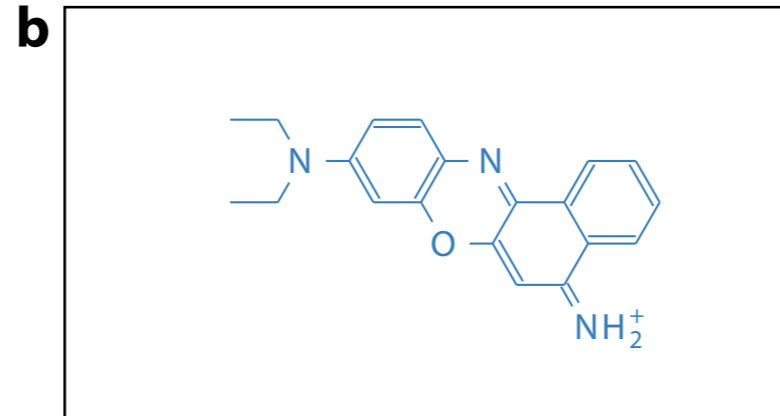
Note: ~8% of males, 0.5% of females, are **colour blind**

COLOUR AND CONTEXT

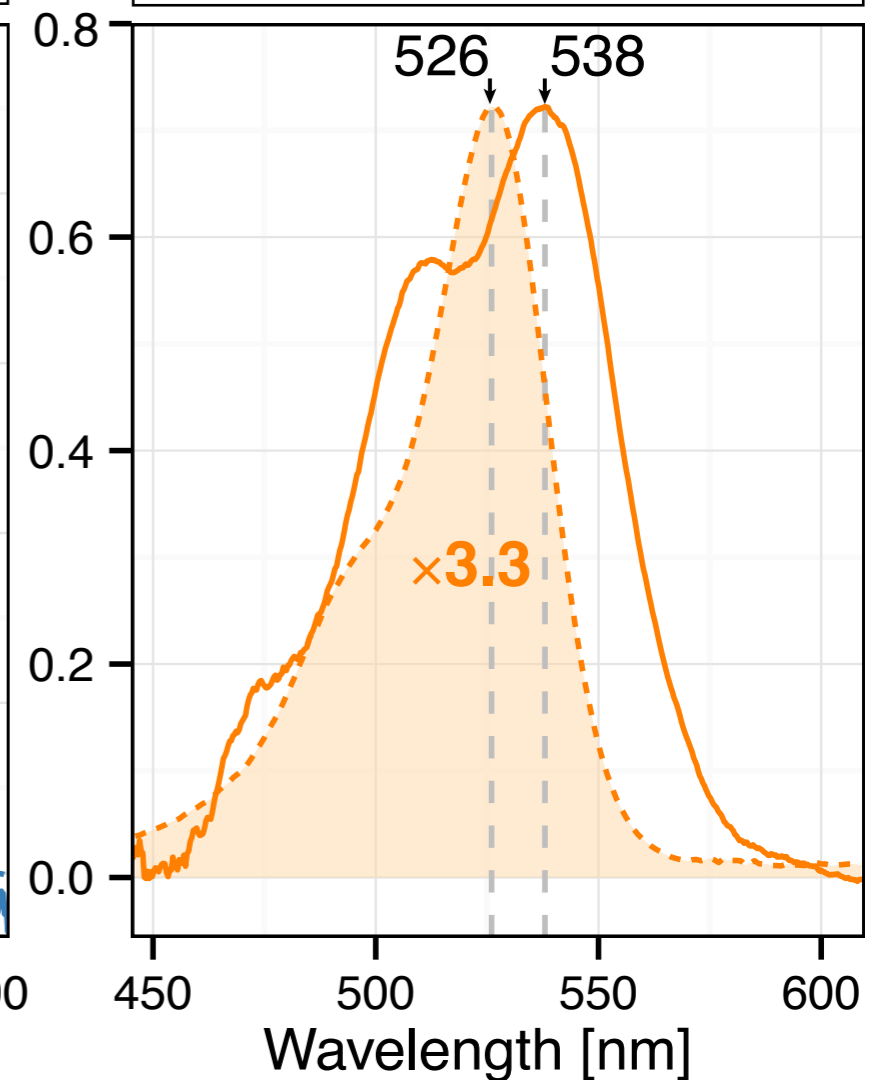
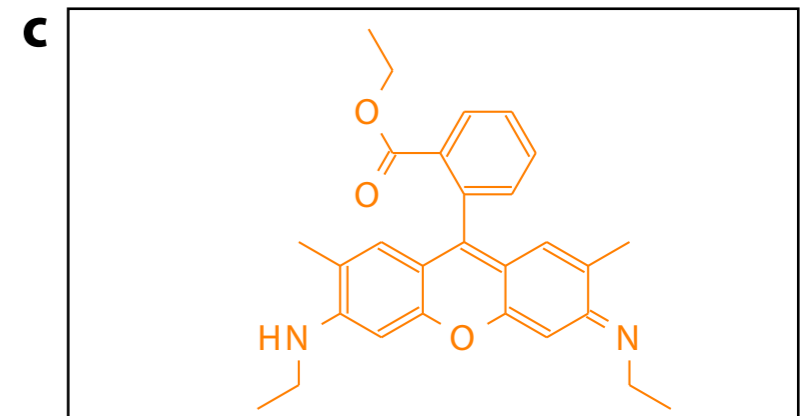
Crystal Violet (10nM)

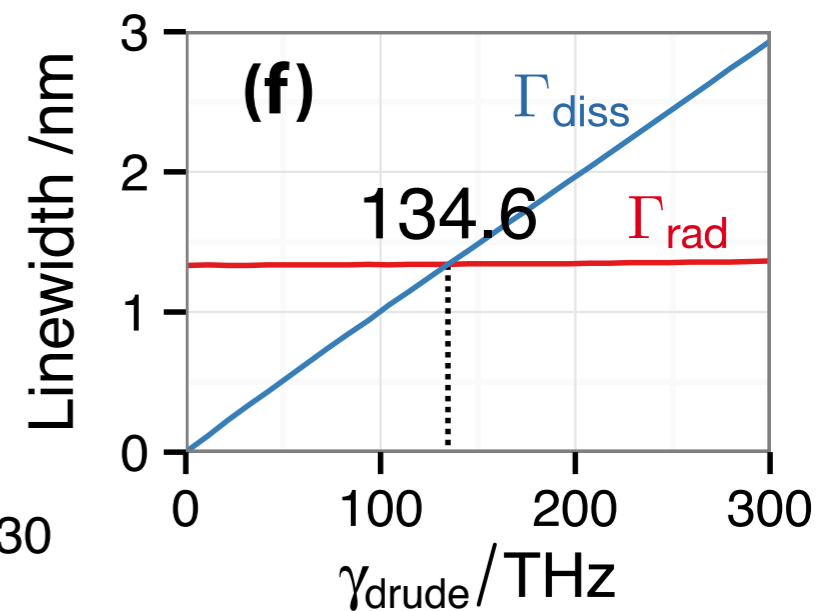
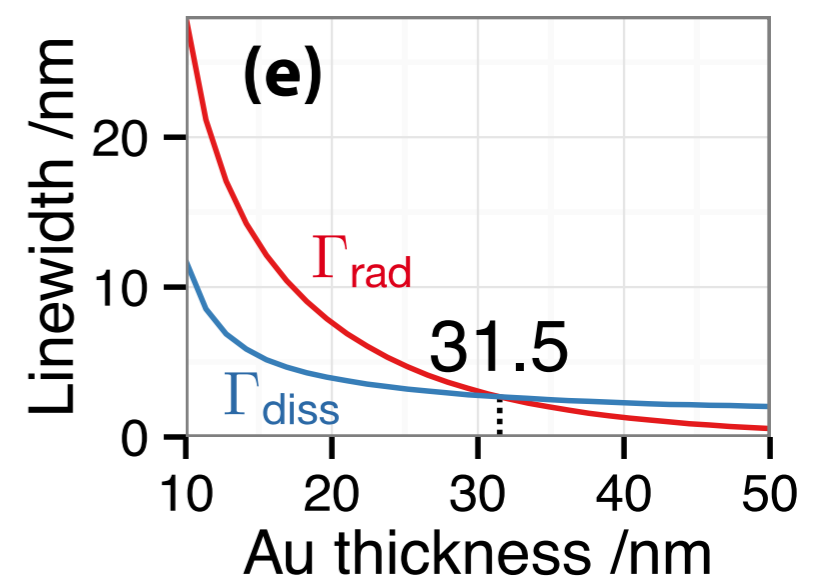
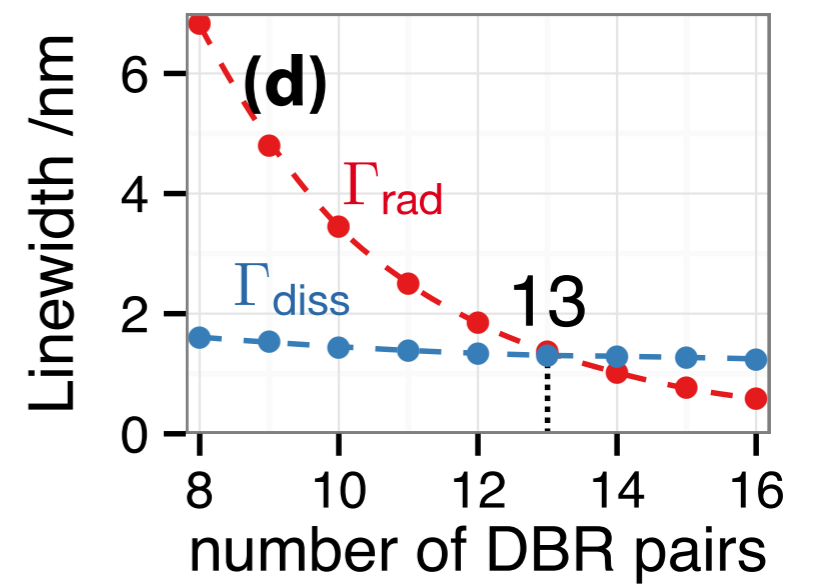
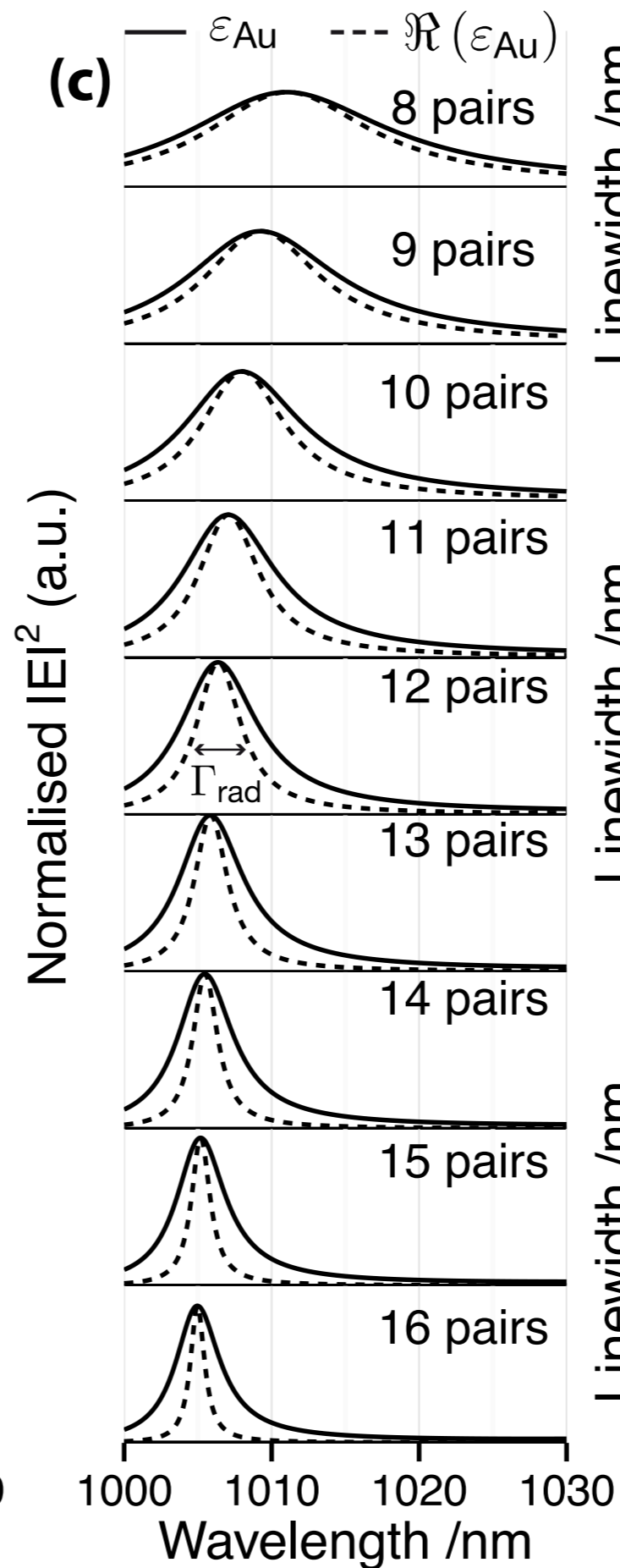
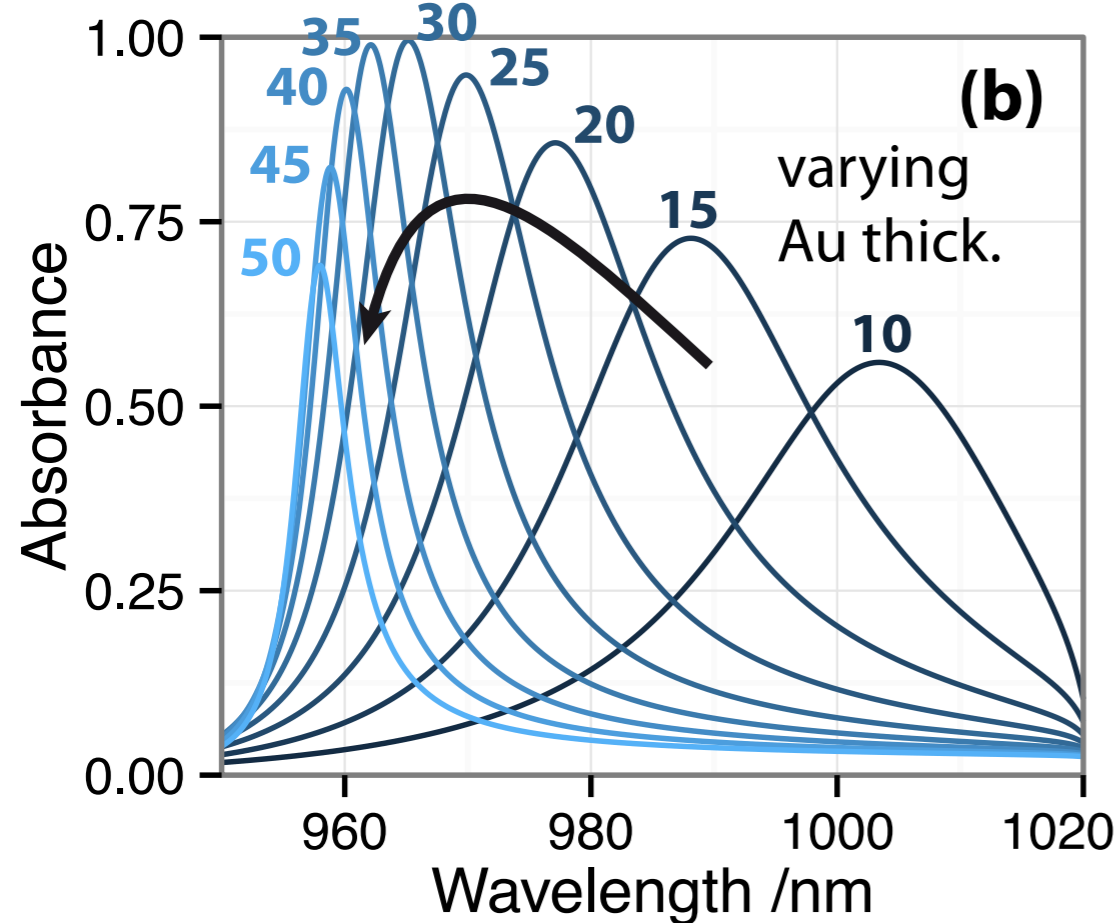
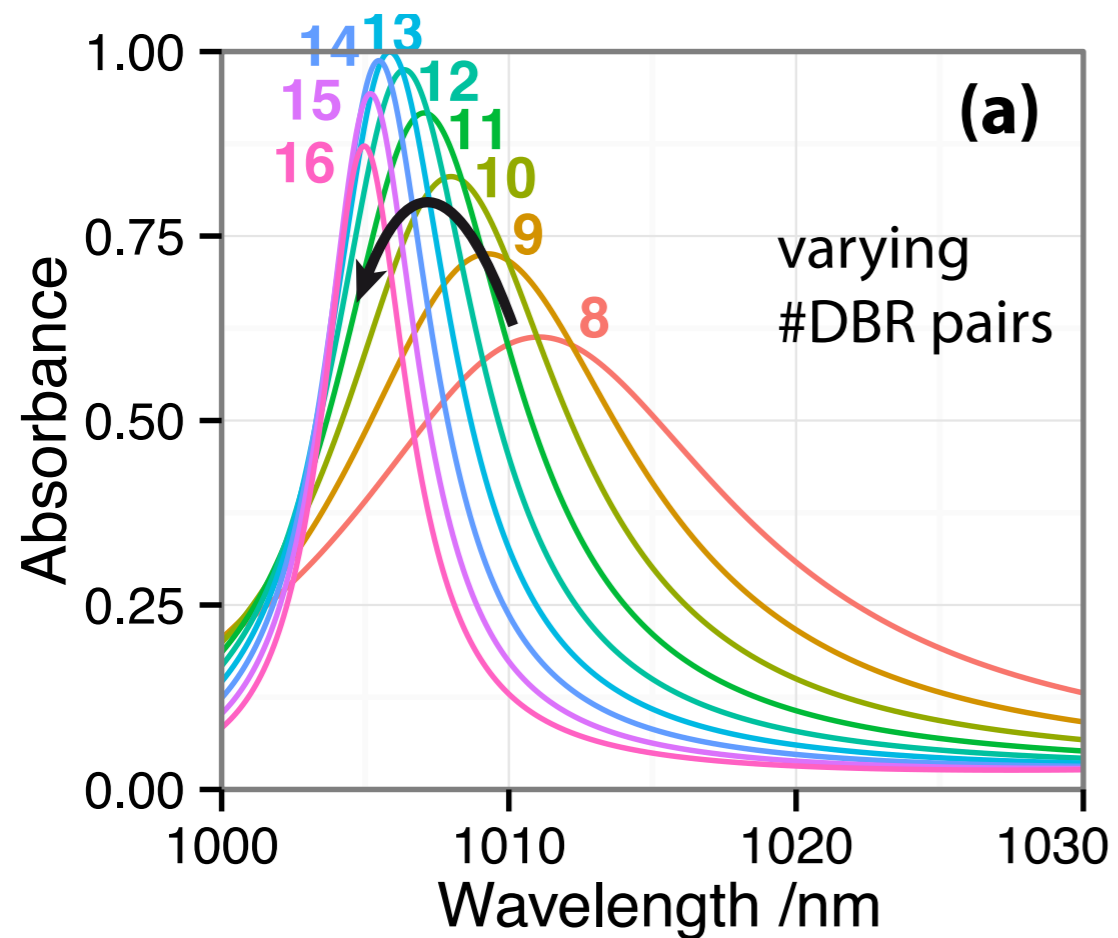


Nile Blue A (10nM)



Rhodamine 6G (2.5nM)





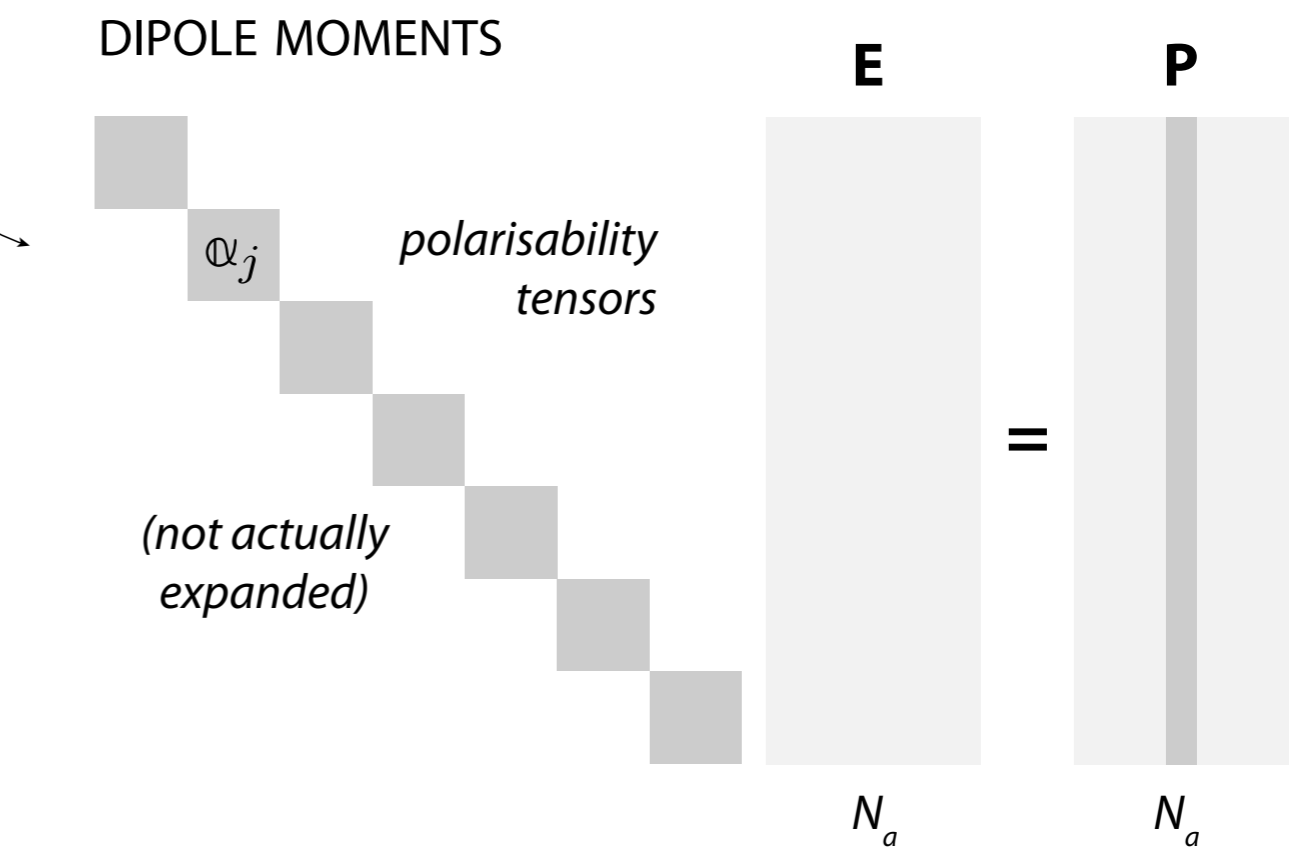
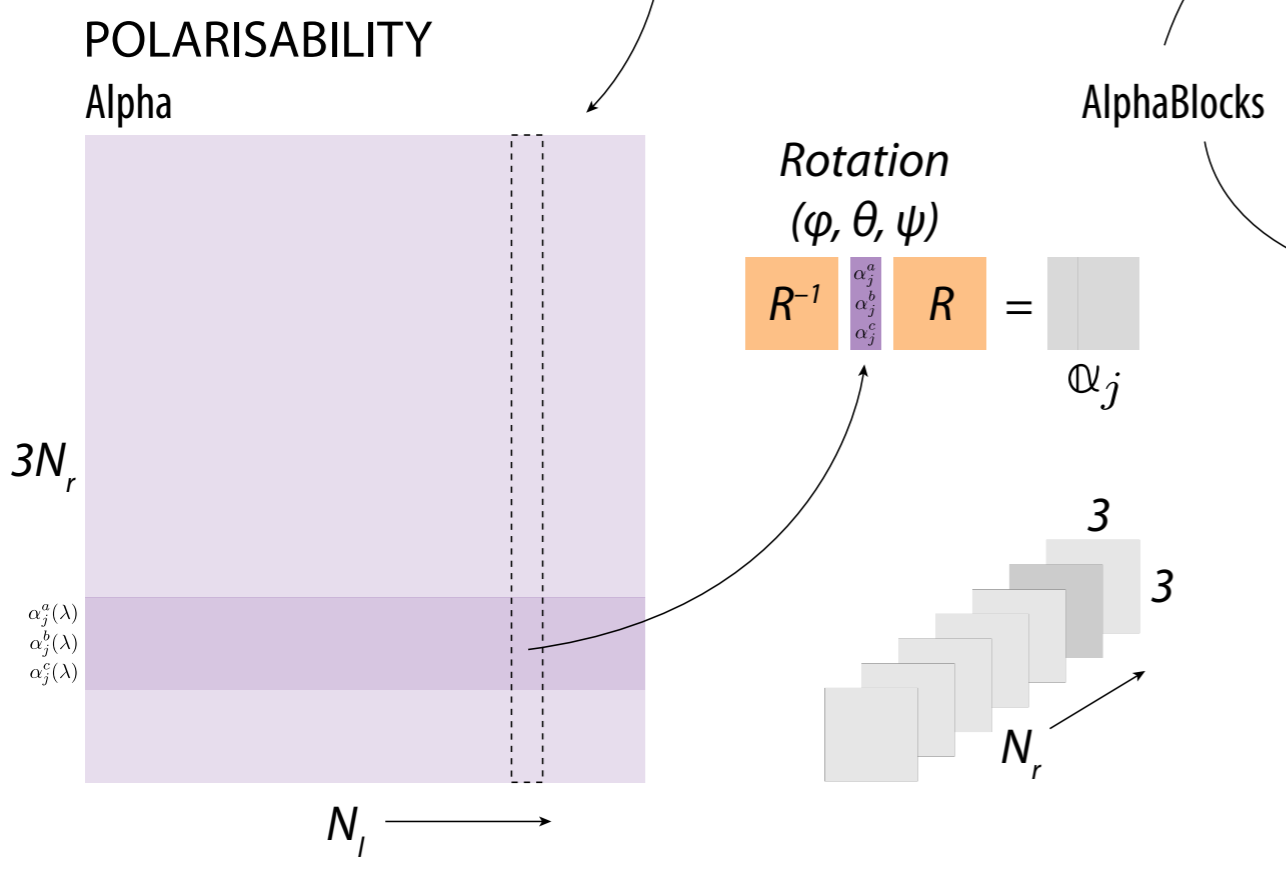
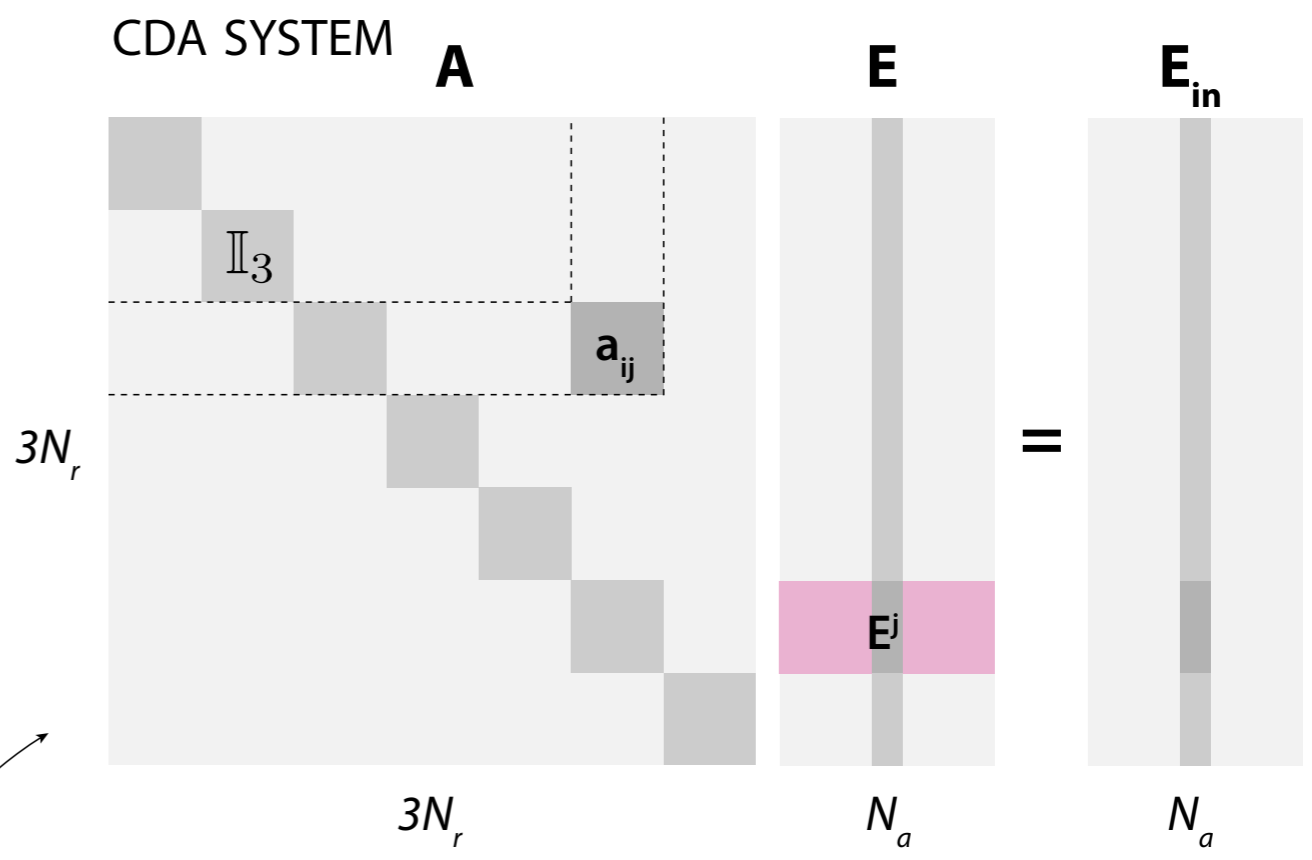
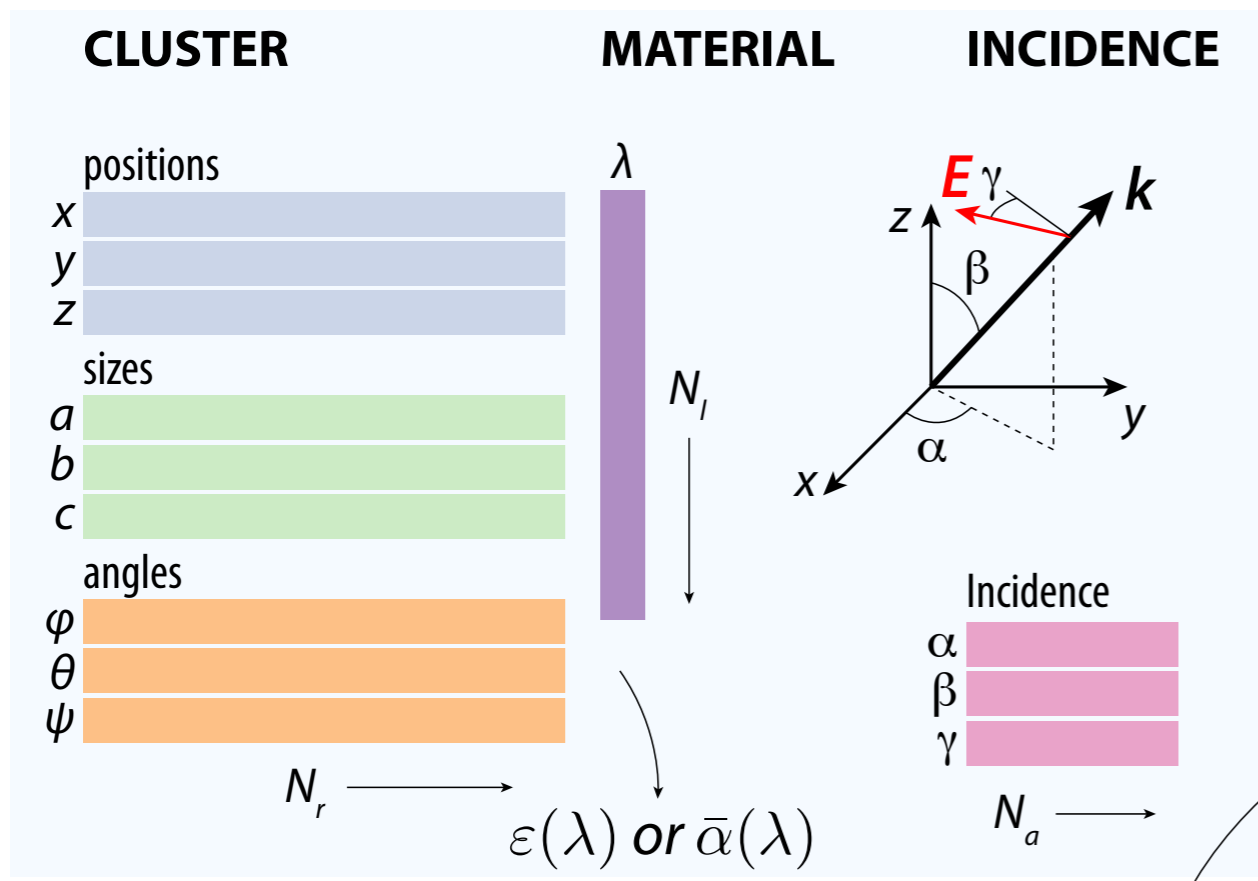
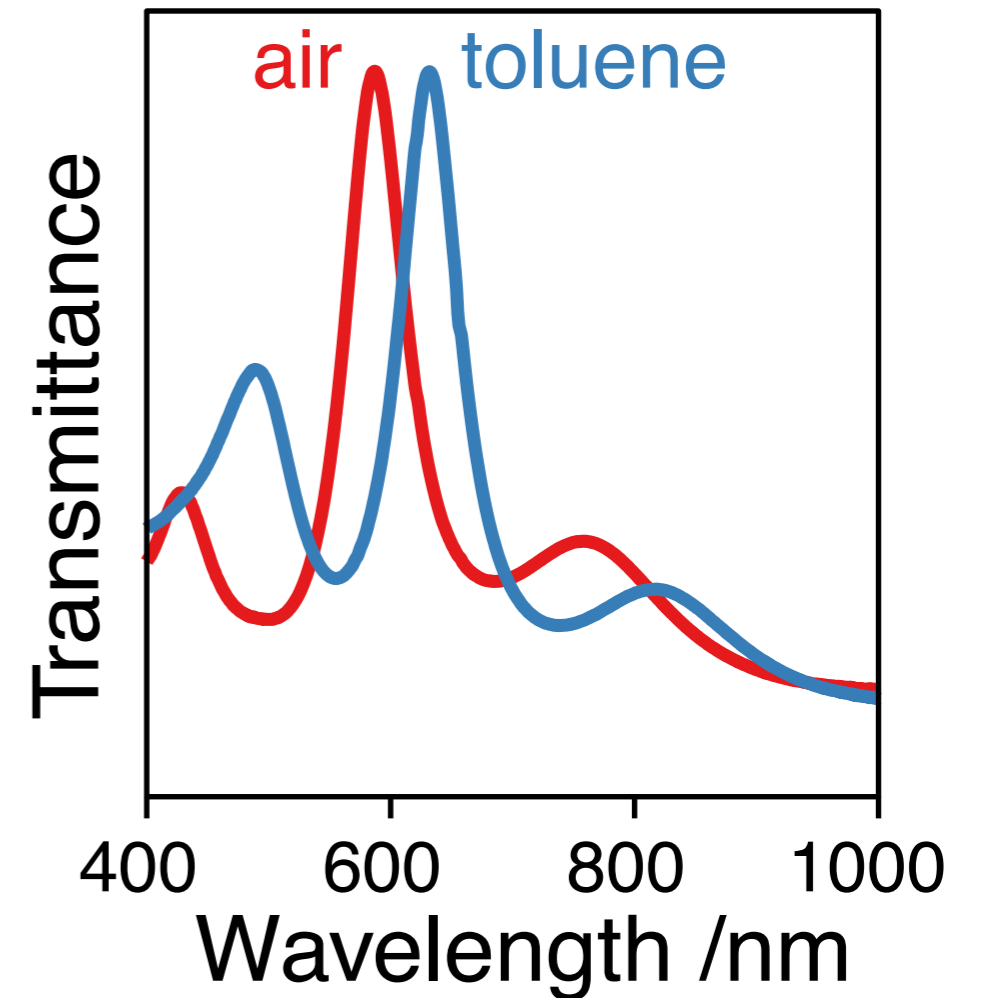
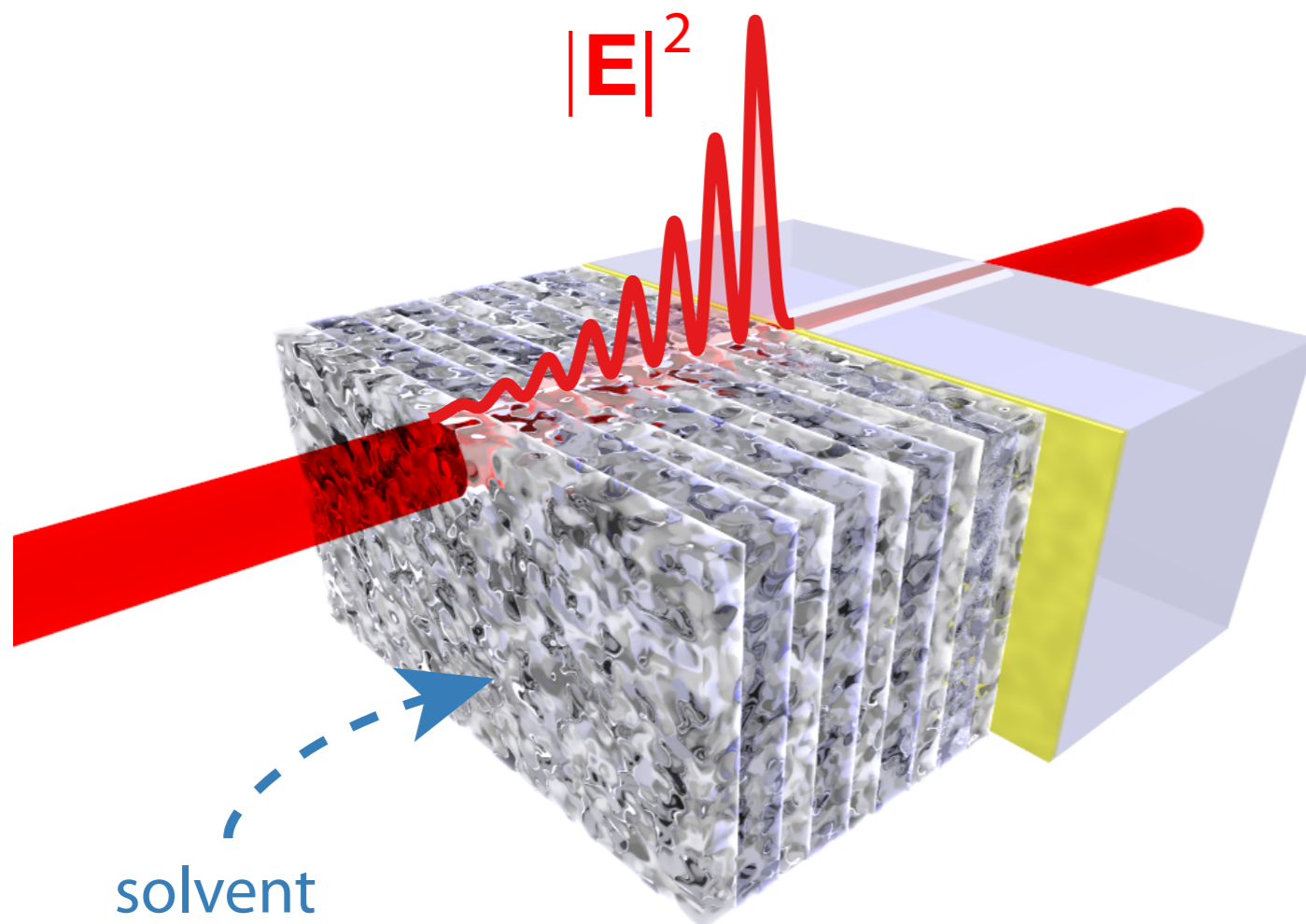
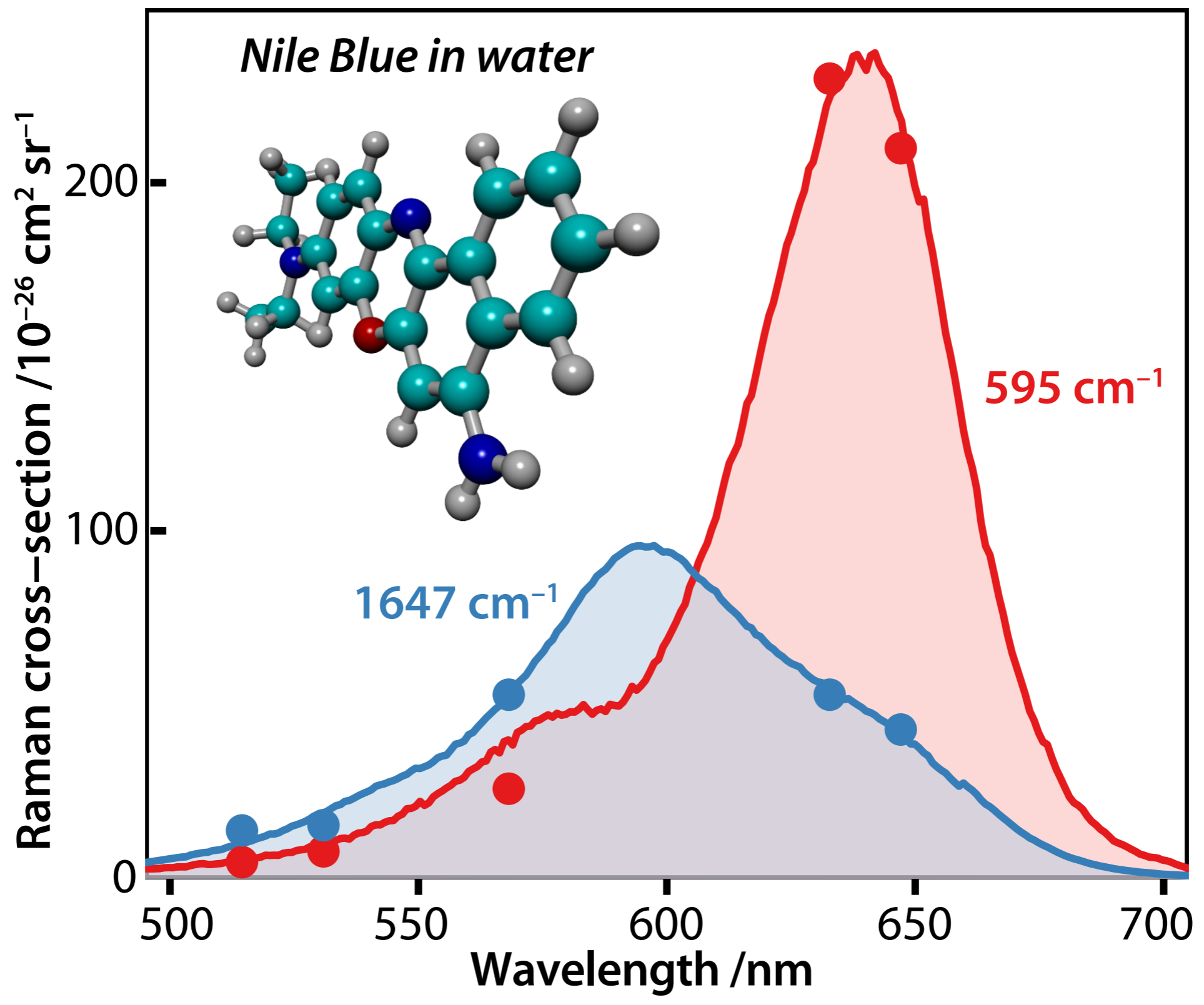
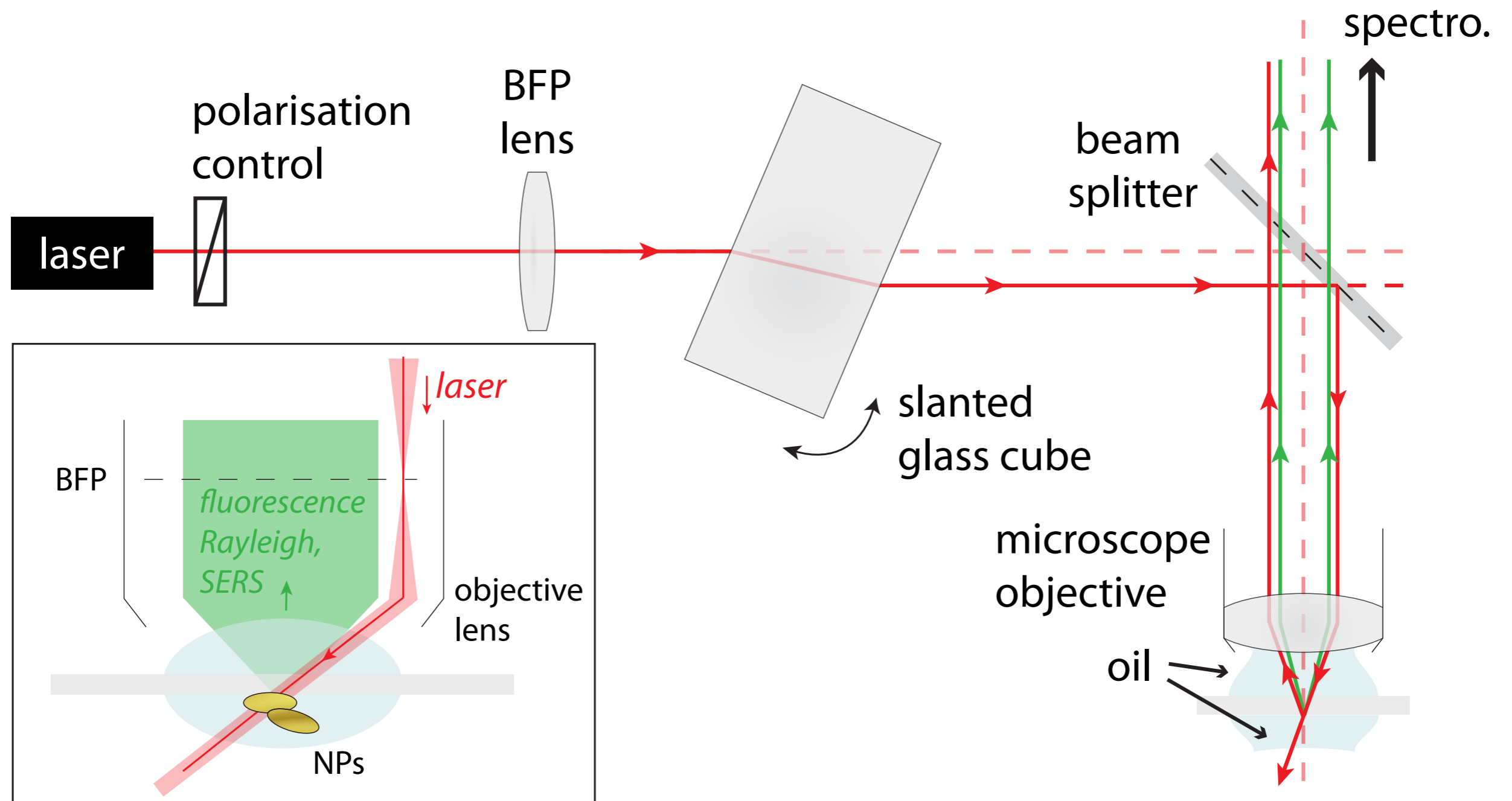


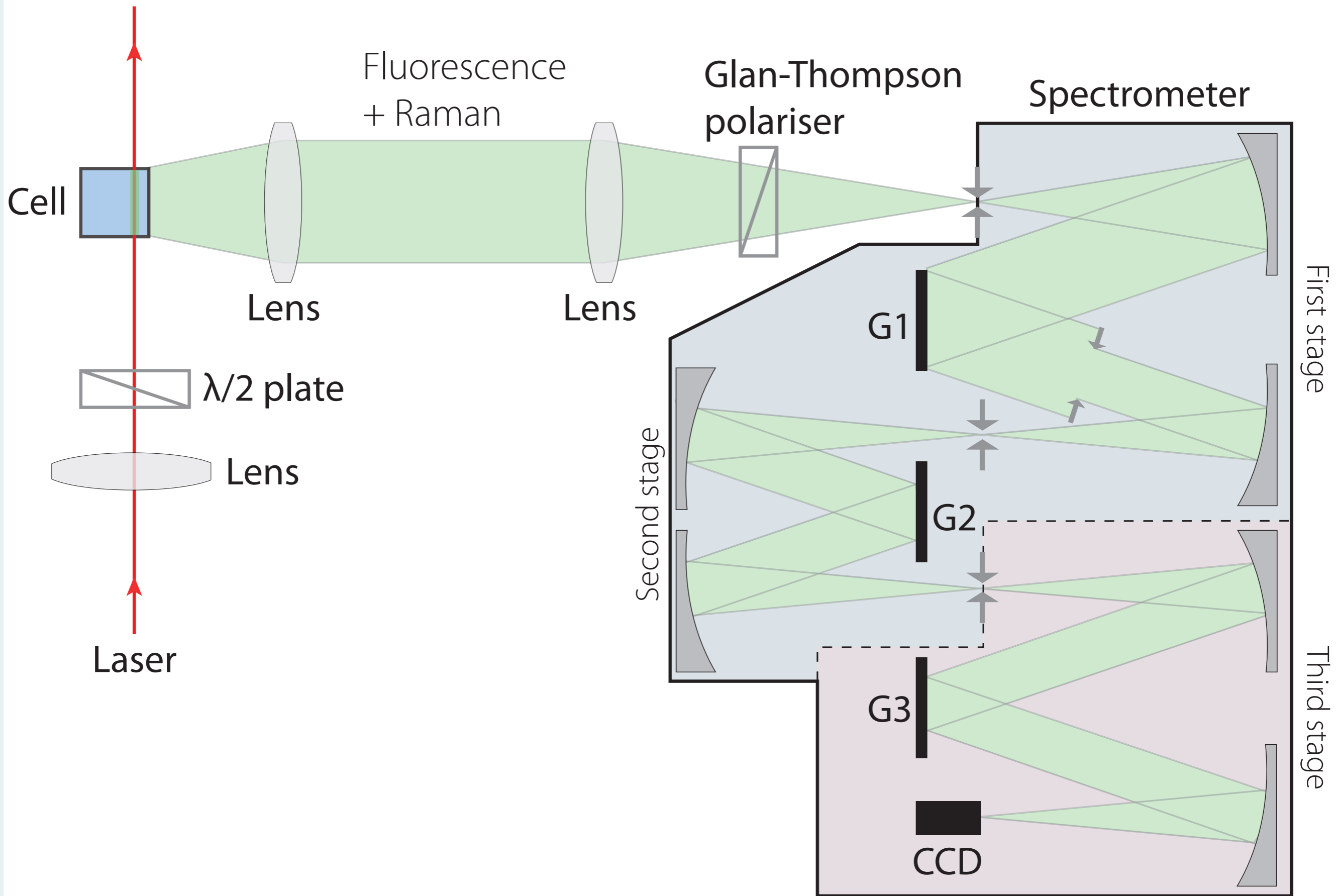
TABLE OF CONTENTS ARTWORK

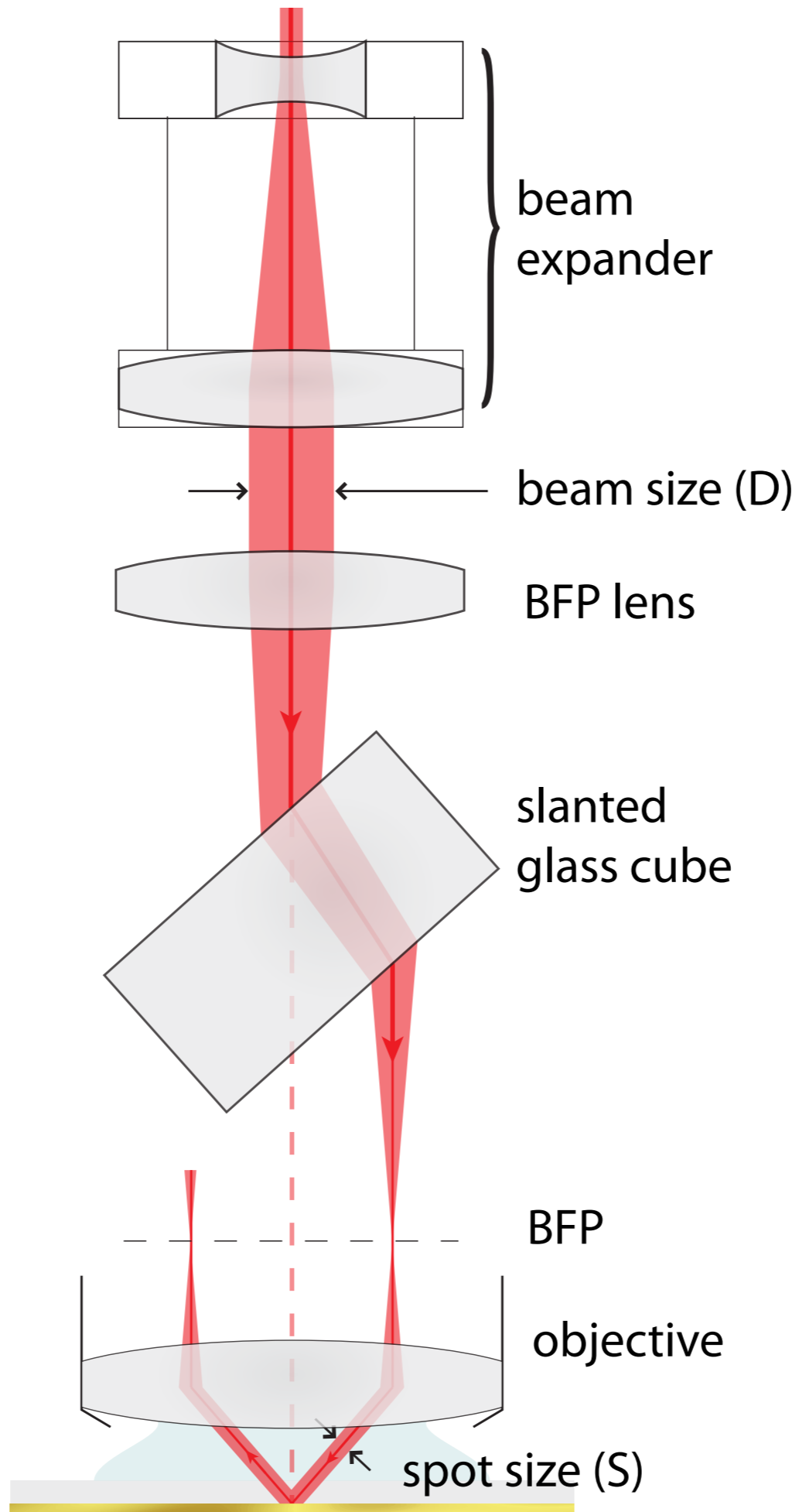




SCHEMATICS: MINIMAL & ANNOTATED

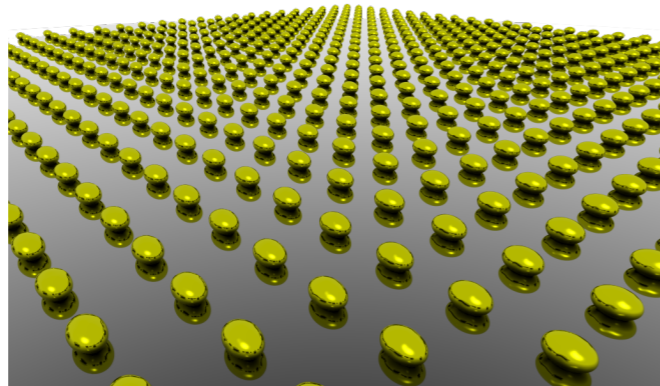






GRAPHICS FOR PRESENTATION SLIDES

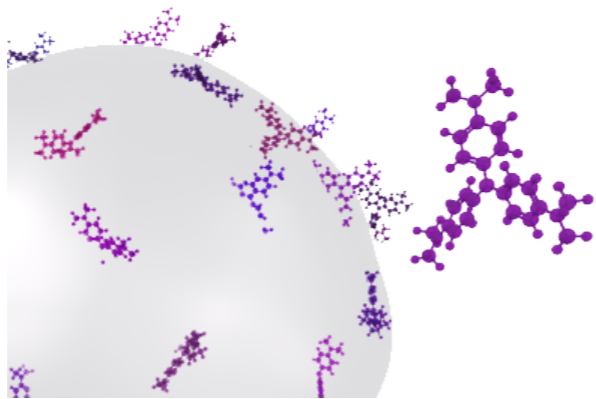
PARTICLE ARRAYS



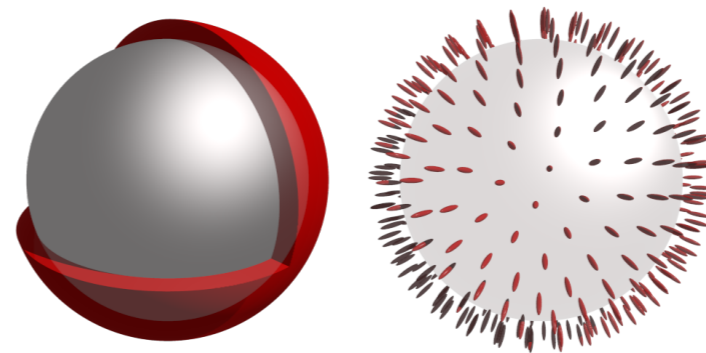
CHIRAL NANO-STRUCTURE



MOLECULES ON COLLOIDS

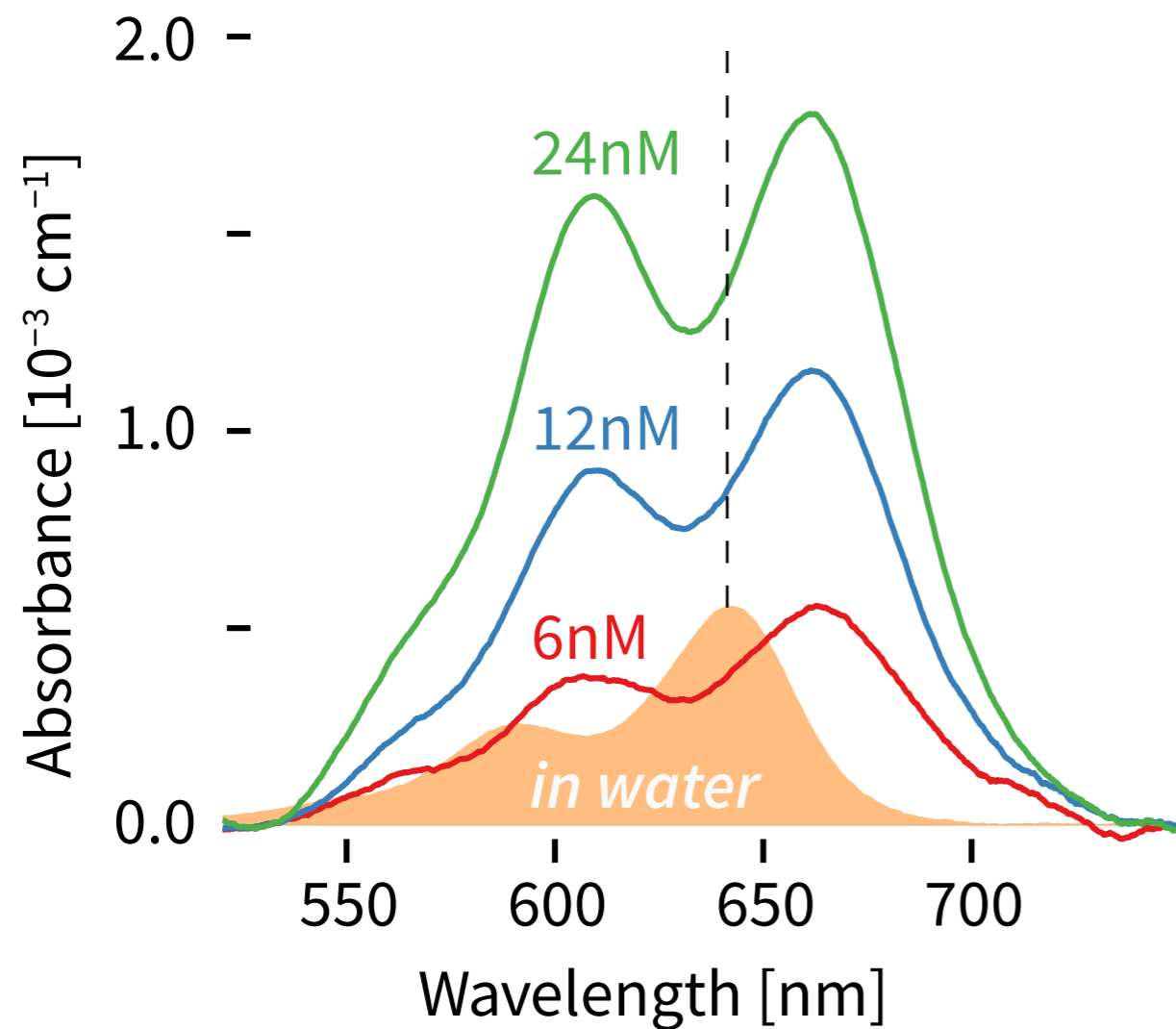


SHELLS OF INTERACTING DYES



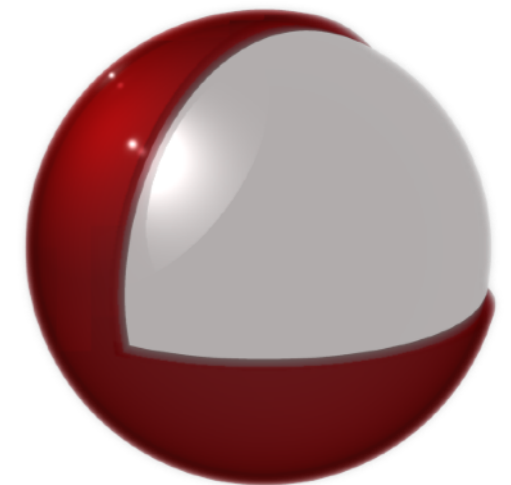
GRAPHICS FOR SLIDES – MINIMALIST

EXPERIMENTS

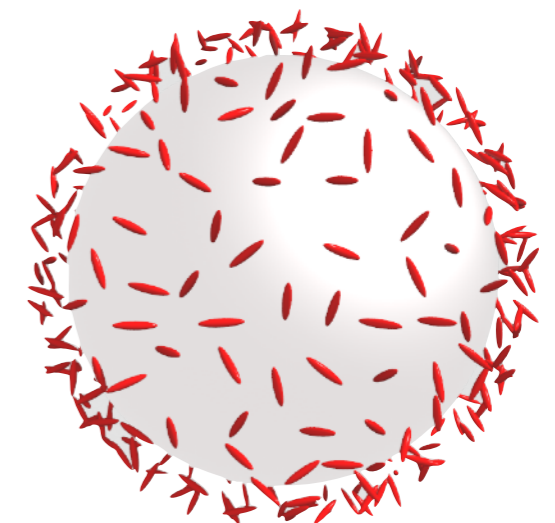


THEORY

continous shell
(Mie theory)

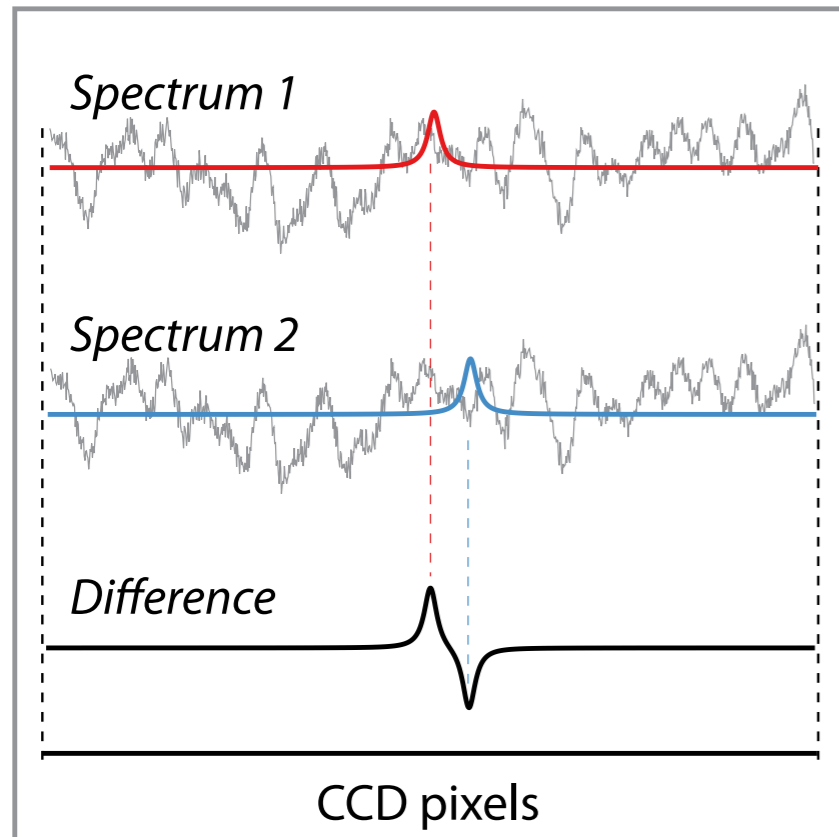


dipoles
&
Mie theory

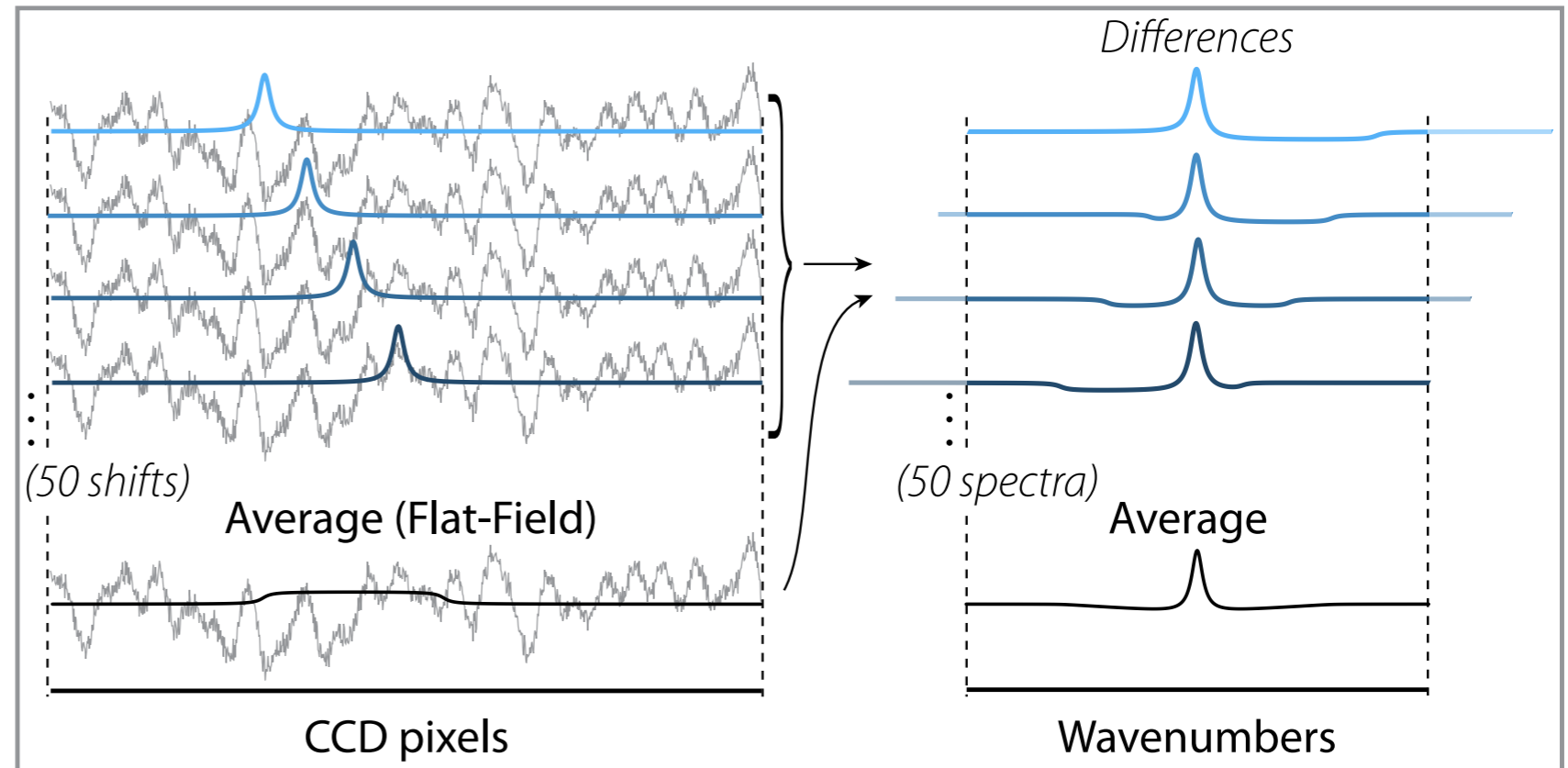


SLIDES – MINIMALIST

Subtracted-Shifted RS



flat-field-corrected Continuously-Shifted RS



Transition Matrix

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

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

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



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

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 DUVAL MARTIN SHEEN 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 Screenplay by MICHAEL HERR
 Co-Produced by FRED ROOS, GRAY FREDERICKSON and TOM STERNBERG
 Director of Photography VITTORIO STORARO Production Designer DEAN TAVOLARIS Editor RICHARD MARKS
 Sound Design by WALTER MURCH Music by CARMINE COPPOLA and FRANCIS COPPOLA
 R PARENTAL STRONG LANGUAGE, DRUGS, AND SOME SMOKING
 TECHNOLOGY DOLBY DIGITAL UNITED ARTISTS AN OMNI ZOEITROPE 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

Paramount Pictures presents a Steve Tisch/Wendy Finerman production a Robert Zemeckis film Tom Hanks Forrest Gump Robin Wright Gary Sinise Mykelti Williamson
 and Sally Field and Charles Newman and Joanne Johnston and Alan Silvestri and Joel Sil and Arthur Schmidt and Rick Carter and Don Burgess and Winston Green and Eric Roth
 and Wendy Finerman Steve Tisch Steve Starkey and Robert Zemeckis
 A Paramount Communications Company
 READ THE PAPERBACK BOOK SPECIAL VISUAL EFFECTS BY INDUSTRIAL LIGHT & MAGIC
 LANGUAGE AVAILABLE ON THE SOUNDTRACK

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 Auguie (†) [†: ba208@ex.ac.uk](mailto:ba208@ex.ac.uk)
 Andy Murray
 Bill Barnes
 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

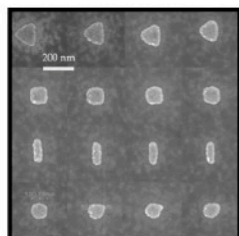
Optimizing the particle shape, size, and configuration,

- 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)

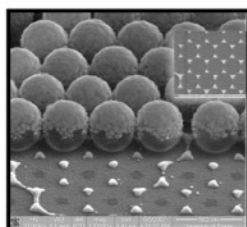


- a 10 nm fabrication resolution is easily achieved using EBL
- by changing the particle shape and size, we tune the resonance to favorable spectral regions.
- polycrystalline nature is the main limitation, both in terms of reproducibility and material properties: surface roughness and grain boundaries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

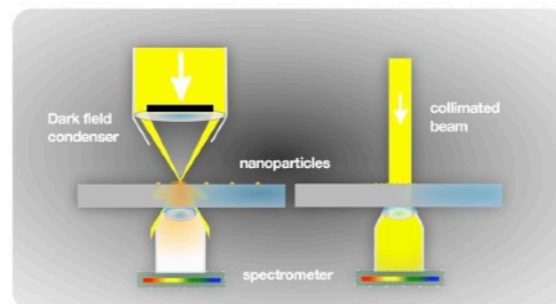
Producing large areas

- 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

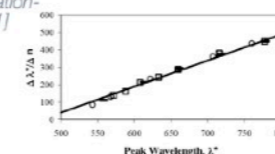
Aspect ratio and spectral position

- 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)

Many particles: collective response

Additional freedom in design

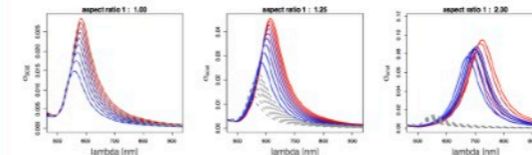
Building upon the knowledge of single particles response, new challenges and opportunities arise from the interaction of a collection of particles

- 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

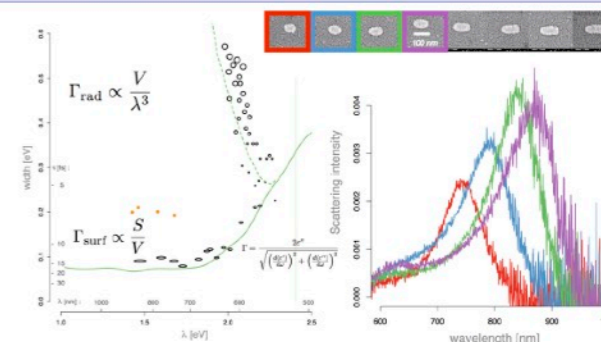
Modelling

Several numerical schemes have been used

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



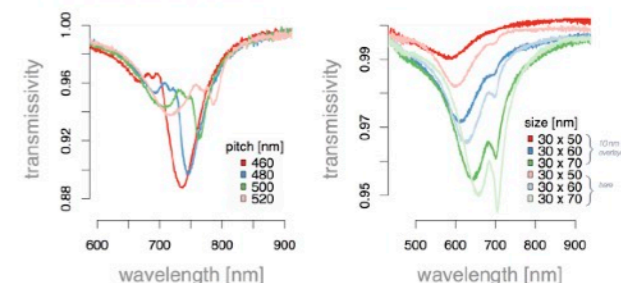
T-matrix calculations of the scattering cross-section for gold ellipsoids coated by a thin layer ($n=1.5$) of increasing thickness (step 5nm), for three different aspect ratio. The surrounding medium is water. Grey curves are for incident polarisation along the short axis, colored curves are for the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



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, $n=1.44$).

Future directions

Investigate ordered and disordered arrays

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

References

- Plasmonic Nanoparticles: Factors Controlling Refractive Index Sensitivity. PhD thesis. M. Miller, 2007
- Sonnishen et al. "Drastic Reduction of Plasmon Damping in Gold Nanorods". Phys. Rev. Lett., 88(7):077402, Jan 2002.
- 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 Auguie



Universidade de Vigo

Co-workers:

Química Física

Andrés Guerrero-Martínez

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.



~1 nm

Atomic cluster
Absorption bands



~10 nm

Nanoparticle
Plasmonic response

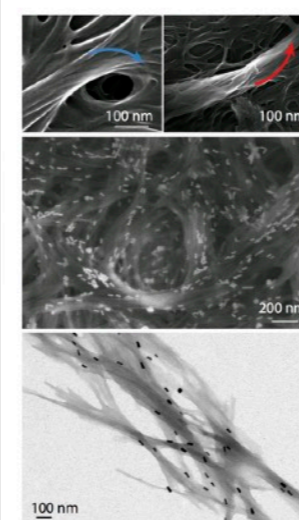


~100 nm

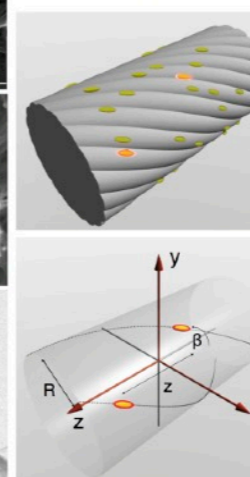
Collection of NPs
Plasmon hybridisation

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

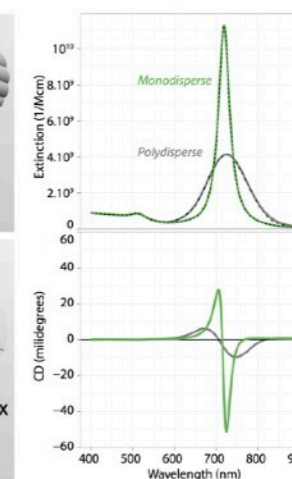
EXPERIMENTAL RESULTS



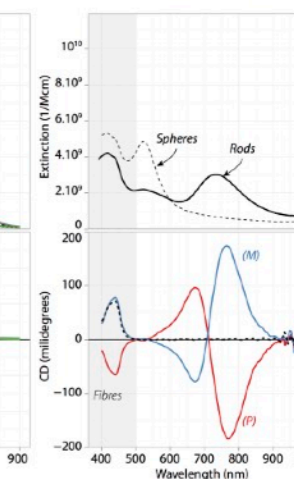
Minimal CD model



Calculated spectra



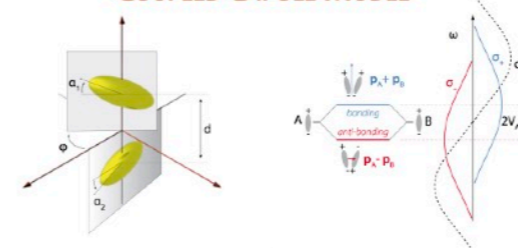
Experimental spectra



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



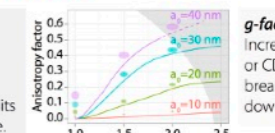
Chiral dimer of nanorods
Minimal model of plasmonic optical activity [2–4]. Coupling between the plasmon modes + chirality.

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)LS* / 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-Martínez *et al.* *Angew. Chem.* 50 (2011)
[2] B. Auguie *et al.* *J. Phys. Chem. Lett.* 2 (2011)
[3] A. Guerrero-Martínez *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

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School of Chemical and Physical Sciences
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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 $P_{\text{ext}} = \frac{1}{2}\omega \text{Im}(\alpha_0) |E_{\text{inc}}|^2$
- 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

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

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

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

— 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*: $\mathbf{S} = \mathbf{I} + 2\mathbf{T}$

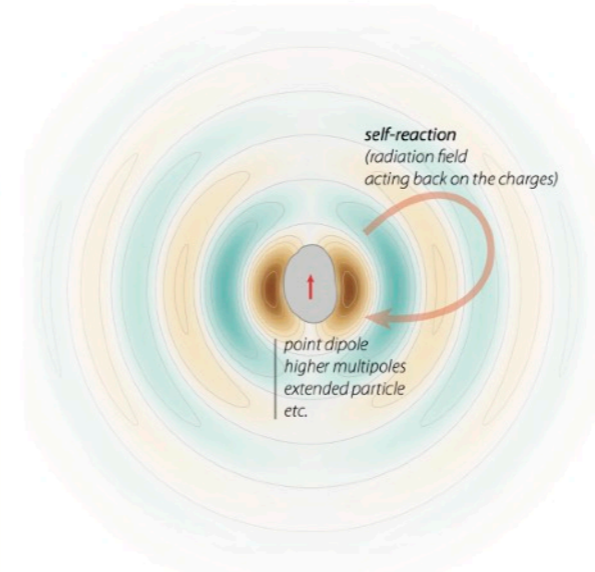
Cayleigh transform

We define a *reactance matrix*, \mathbf{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: $i\mathbf{K} - i\mathbf{K}^{\dagger}$ is Hermitian positive semi-definite (\mathbf{K} is *dissipative*) (generalizes $\text{Im}(\mathbf{K}) \geq 0$ for a response function \mathbf{K} , to matrices)
- Given an (truncated, approximate...) expression for \mathbf{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, $K_d^{(0)} = -iT_d^{(0)} = \frac{k^3 \alpha_0}{6\pi\epsilon_0\epsilon_1}$

We justify

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

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 —

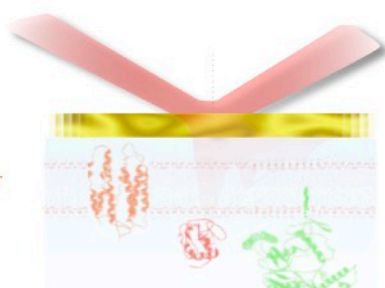
- [1] P. de Vries *et al*, Rev. Mod. Phys. **70**, 447 (1998)
- [2] A. Wokaun *et al*, Phys. Rev. Lett. **48**, 957 (1982)
- [3] M. I. Mishchenko, L. D. Travis, and A. A. Lacis, *Scattering, absorption and emission of light by small particles*, 3rd ed. (Cambridge Univ. Press, 2002)
- [4] R. G. Newton, *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)

Surface Plasmon-Polaritons in Biosensing

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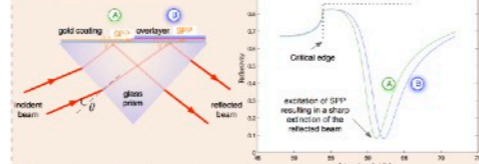


What is a SPP?

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

SPPs have a shorter wavelength than light in free space at the same frequency. Because of that, direct optical excitation of SPPs is not possible. Using the electric field of a laser beam to excite SPPs requires a special setup, for example using a glass prism as shown below.



A laser beam hits the surface, and undergoes total internal reflection when the incident angle is above a critical angle. If we go further in angle, we may match the resonance condition with SPPs propagating at the metal/air interface. This results in a sharp dip in reflectivity for this particular angle. Here we plot reflectivity curves for two different schemes, (A) bare metal coating, (B) adding an overlayer on the surface. A shift in the resonance position is characteristic of the change in refractive index close to the surface.

Interest in biosensing

- optical probing → non-intrusive method
- can achieve great sensitivity; any change in refractive index in the few hundreds of nanometers to the surface leads to a huge change in the excitation of these waves (resonance condition).

To go further

- differential technique: increase signal to noise ratio giving two orders of magnitude greater sensitivity (see 'Differential SPR ellipsometry')
- two channel fluid cell, to subtract the noise due to thermal fluctuations, pressure, ...
- reducing the sensing volume, using localised plasmon resonance in nanoparticle arrays (see 'Particle Plasmons')

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<http://projects.ex.ac.uk/atto/>

Attogram Sensitivity

The Attogram project, in collaboration with the University of Nottingham, intends to find the most sensitive technique to detect optically a few biological molecules in solution. Classical methods make use of Attenuated Total Reflection (ATR) 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.

Attogram Sensitivity Project

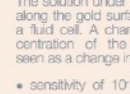
The Attogram project, in collaboration between the Universities of Nottingham and Exeter intends to find the most sensitive technique to detect optically a few biological molecules in solution. Classical methods make use of Attenuated Total Reflection of light as a very sensitive probe of any change 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

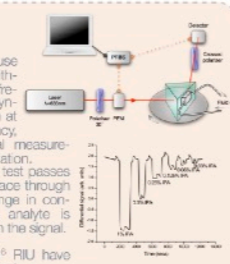
Looking at intensity reflected from a planar surface as a function of incident angle is not the most accurate technique one can use. Indeed, it has been shown that a polarization-sensitive differential technique can improve sensitivity by two orders of magnitude [1]. This technique consists in comparing the phase shift of two different states of polarization, only one of them being affected by the plasmon resonance.

Polarization of a wave describes the direction of oscillation of the electric field:

- generally rotates in time, drawing an ellipse
- two eigenstates: s and p. Only p-polarized light may couple to SPPs, the other state remains unaffected
- the azimuth Ψ is characteristic of the phase difference between the two orthogonal states of polarization p and s.



The setup makes use of a polarization dithering at a given frequency, and a synchronous detection at the same frequency, giving a differential measurement of azimuth rotation. The solution under test passes along the gold surface through a fluid cell. A change in concentration of the analyte is seen as a change in the signal.



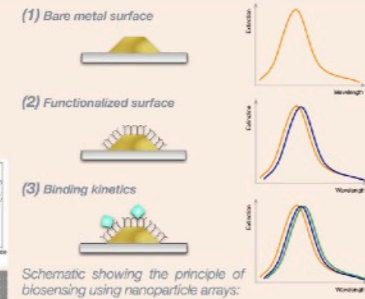
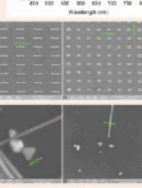
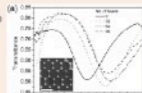
Particle Plasmons

When making noble metal particles at a nanometer scale, SPPs become localised and the structure exhibits a resonant oscillation of the conduction electrons. This results in dramatic changes in extinction of light (absorption and scattering being strongly related to the particle size, spacing, and surrounding medium). The sensing volume is reduced down to a few tens of nanometers, around some 'very sensitive' hot spots.

Different methods are being used to make these particles, such as,

- Nanosphere lithography**
 - an array of nanospheres acting as a mask
 - metal deposition
 - lift-off, leaving triangular particles in an hexagonal array

- e-beam lithography**
 - exposing a photoresist
 - developing, coating, and lift-off
 - large variety of shapes and sizes
- Colloidal particles**
 - growth in solution
 - single crystals



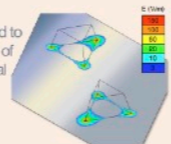
Schematic showing the principle of biosensing using nanoparticle arrays:

- (1) a bare gold particle is characterized (e.g. measuring extinction spectrum)
- (2) receptor molecules are added, carefully distributed on the nanoparticles. This layer causes a change in extinction spectrum, due to a change in refractive index.
- (3) finally, in the actual sensing process, some target molecules would interact with the receptors, seen as a minor change in the extinction spectrum.

Future work

✓ Theoretical modeling is being held to improve our understanding of LSPR, and design the optimal setup:

- shape of the particles
- array pitch
- materials
- wavelength, ...



Distribution of the electric field for triangular nanoparticles (coloured with a false colour map). Note the strong enhancement of the field at the tips ('hot spots').

✓ Observation techniques

- dark field spectroscopy
- fluorescence
- reflection and transmission
- ...

✓ Experiments on biology,

- BSA (Bovine Serum albumin) binding on gold
- protein folding (Ca^{2+} / calmodulin)
- gene expression monitored by RNA loading

✓ Automation for pharmaceutical industry, via an array printer to label thousands of molecules in a row.

Conclusions

SPPs have been proved to provide an efficient technique for sensing. Here we intend to further increase sensitivity, and probe biological processes in real time. Different techniques are being explored,

Differential SPR ellipsometry

By looking at polarisation changes rather than intensity, and using a differential technique, one can increase sensitivity by a factor of 2 at least. A two channel system is being developed to normalized out for thermal and pressure variations.

Localised SPPs

With many different production techniques available, and a wide variety of sizes and shapes, particle plasmons give us the opportunity to carry out many experiments and modeling. Good sensitivity is expected as a result of a much smaller sensing volume.

References

- [1] "Sensing using differential surface plasmon ellipsometry" Hooper, I. R., Sambles, J. R. *Journal of Applied Physics* 96, pp. 3004-3011 (2004).
- [2] "Overlayers on silver nano-triangles: field confinement and spectral position of Localised Surface Plasmon Resonances". Murray W. A., Suckling J. R., Barnes W. L., *Nano Lett.*, accepted for publication.

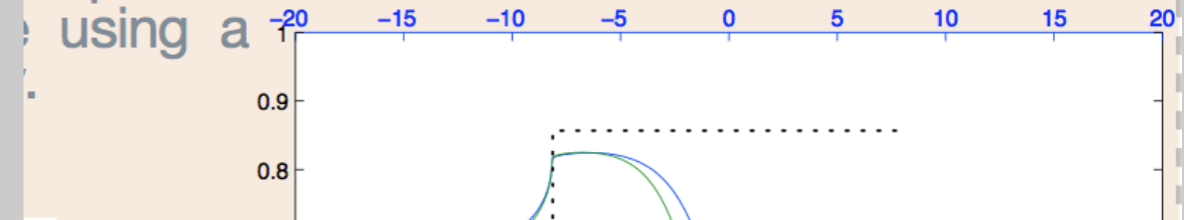
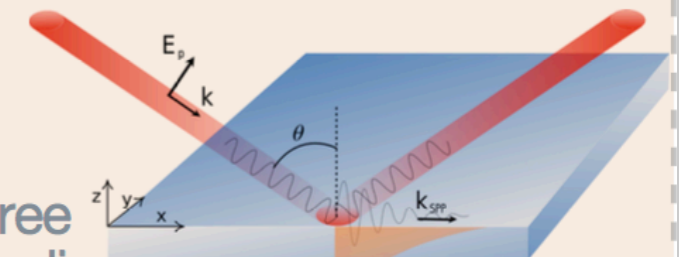
Acknowledgements

Engineering and Physical Sciences Research Council (EPSRC)
Dr. Andy Murray, Dr. Ian Hooper and Dr. James Suckling from Exeter for data and comments.

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.

Ps

length than light in free space at the same frequency. Because of that, direct optical excitation of SPPs is not possible. Using the electric field of a laser beam to excite SPPs requires a special setup, for example using a glass prism as shown below.



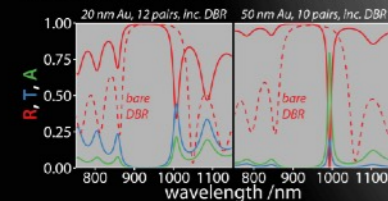
CRITICAL COUPLING OF LIGHT to Tamm SURFACE-PLASMONS



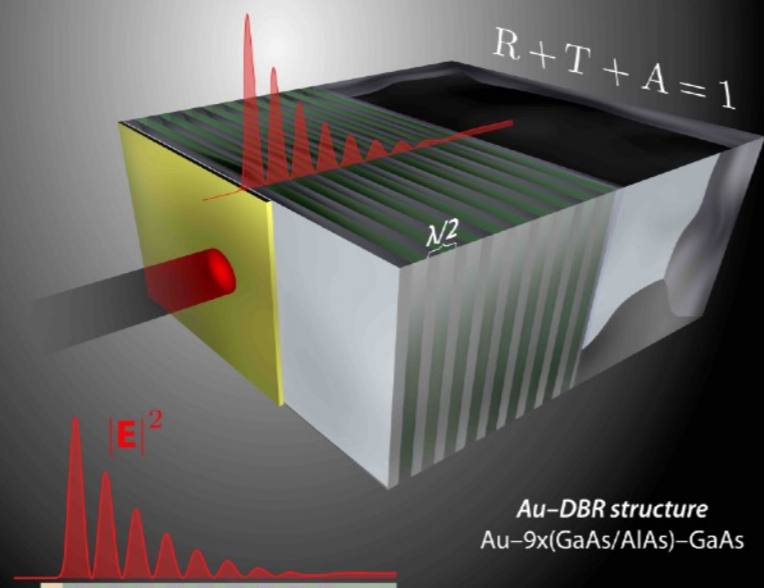
Baptiste Auguie, Viviana Villafaña, Axel Bruchhausen, Alejandro Fainstein
 Centro Atómico Bariloche e Instituto Balseiro, San Carlos de Bariloche, 8400 Río Negro, Argentina

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].



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



Au-DBR structure
 Au-9x(GaAs/AlAs)-GaAs

Critical coupling

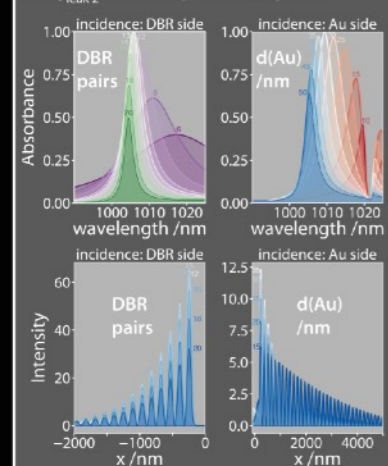
» **transparency**, $T=1$, only in a *dissipationless symmetric resonator*

$$R = \frac{(Q_{\text{diss}}^{-1} - Q_{\text{leak}1}^{-1} + Q_{\text{leak}2}^{-1})^2}{(Q_{\text{diss}}^{-1} + Q_{\text{leak}2}^{-1} + Q_{\text{leak}1}^{-1})^2}$$

» $R=0$ (**critical coupling**) when

$$Q_{\text{diss}}^{-1} = Q_{\text{leak}1}^{-1}$$

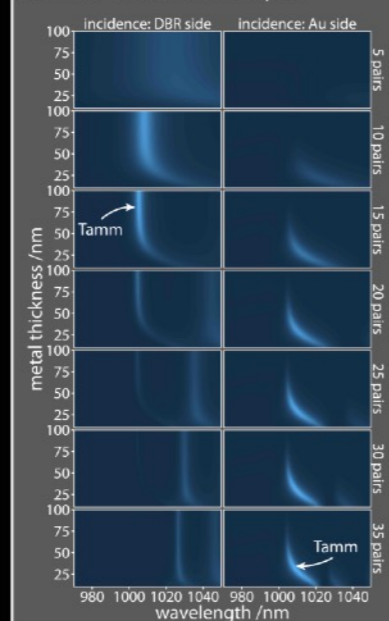
» if $Q_{\text{leak}2}^{-1} = 0$: **complete absorption**



» optimal TP excitation requires different parameters for either side

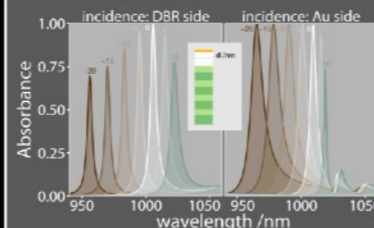
» from DBR: ~13 pairs, and thick Au layer

» from Au: ~35nm, and ∞ DBR pairs



Tuning

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



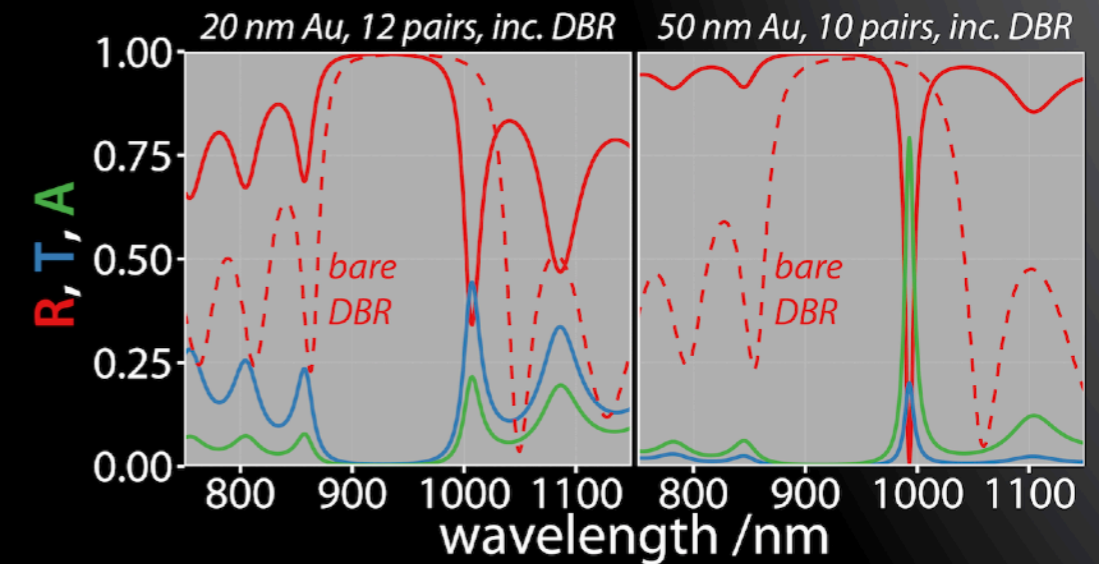
Conclusions

- » 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.

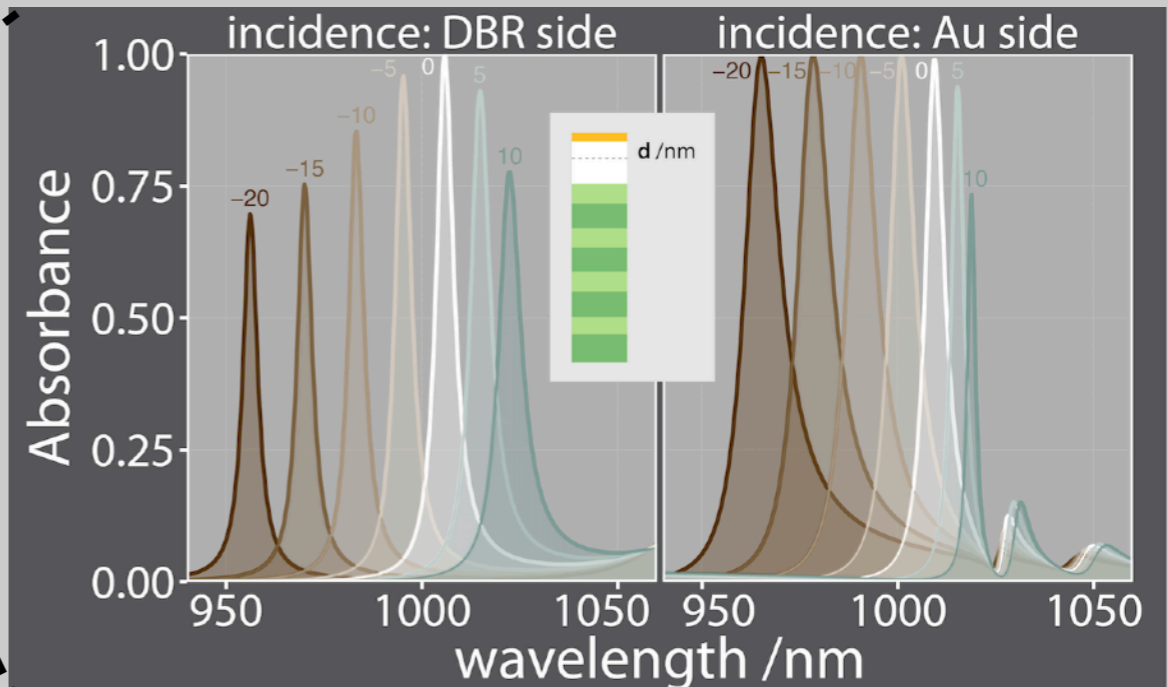
References

- [1] Phys Rev B 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



CSRS — CONTINUOUSLY-SHIFTED RAMAN SPECTROSCOPY

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

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

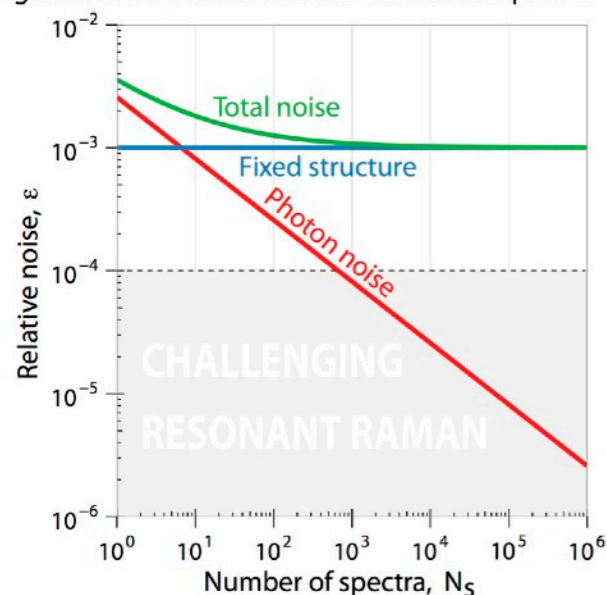
The MacDiarmid Institute for Nanotechnology
School of Chemical and Physical Sciences
Victoria University, Wellington, New Zealand



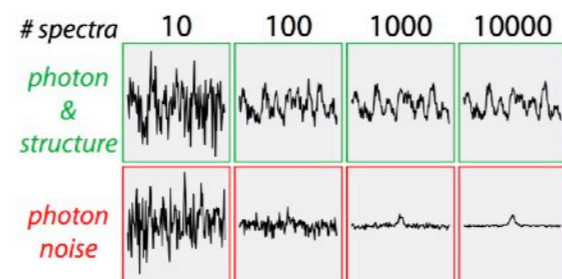
MOTIVATION

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 spectro-

scopic 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.



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,



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} .

whereby the relative rms noise, and therefore the detectable Raman-to-fluorescence ratio, can reach $\epsilon \sim 10^{-5}$.

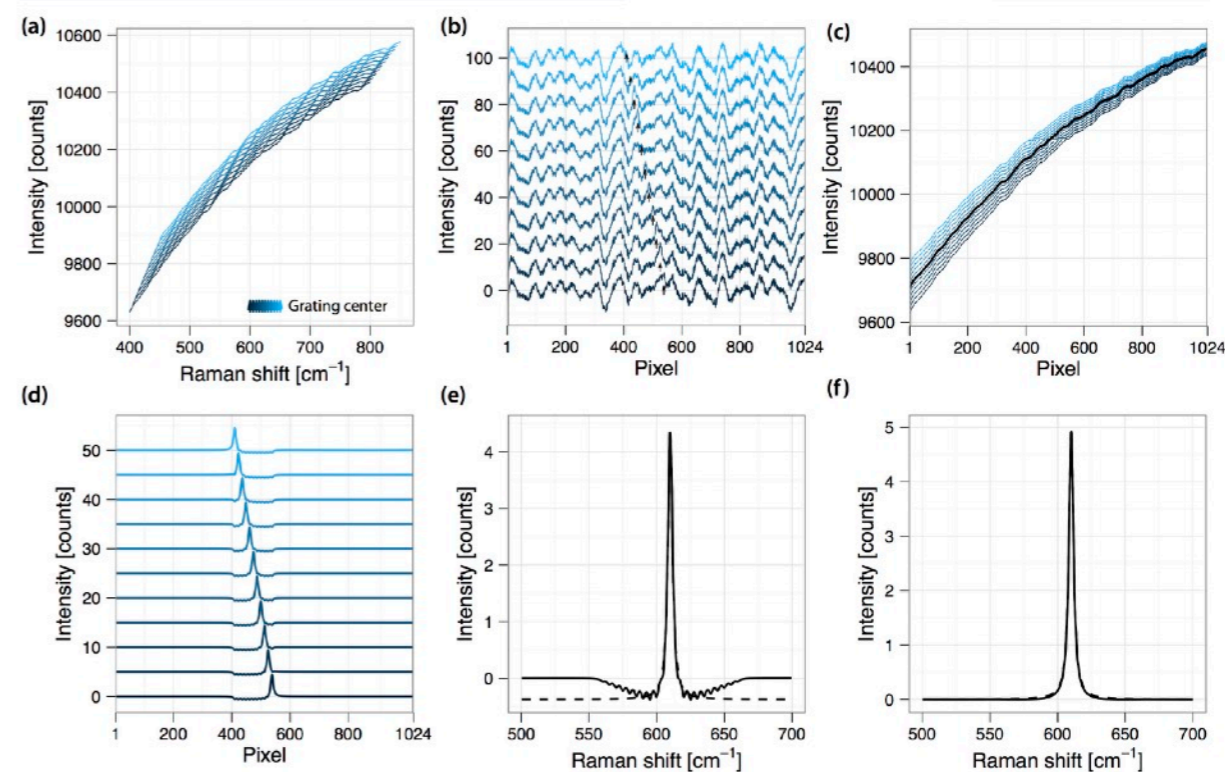
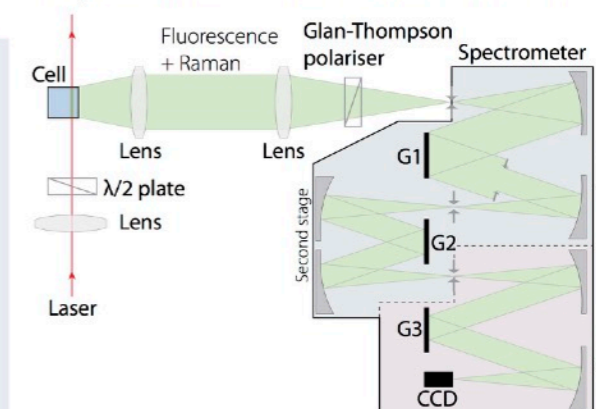
METHODOLOGY

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 90° 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 $\lambda/2$ -waveplate.

In a typical experiment, multiple spectra are acquired for ~ 50 positions of the gratings, each totalling $\sim 10^4$ 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), plot-

ted 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)