INSTITUTO FEDERAL
São Paulo
Câmpus Matão

Advanced School on
QUANTUM MODELLING
of Materials with CRYSTAL

Design principles applied to scientific communication

Prof. Dr. Filipe Camargo Dalmatti Alves Lima

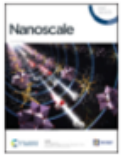
Why there is no layout in the slides
if this is design applied to scientific communication?

Figures are about focus

Figures are about storytelling.

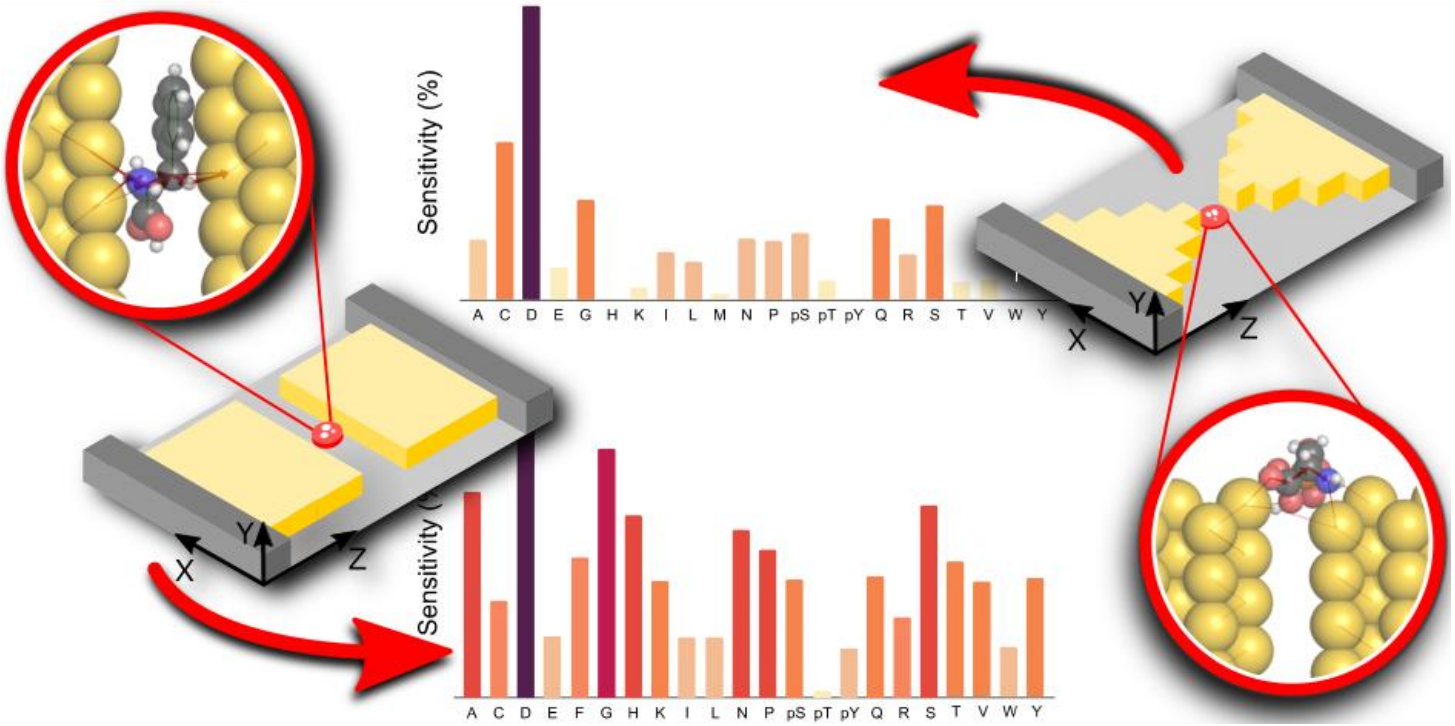
Figures are about design principles

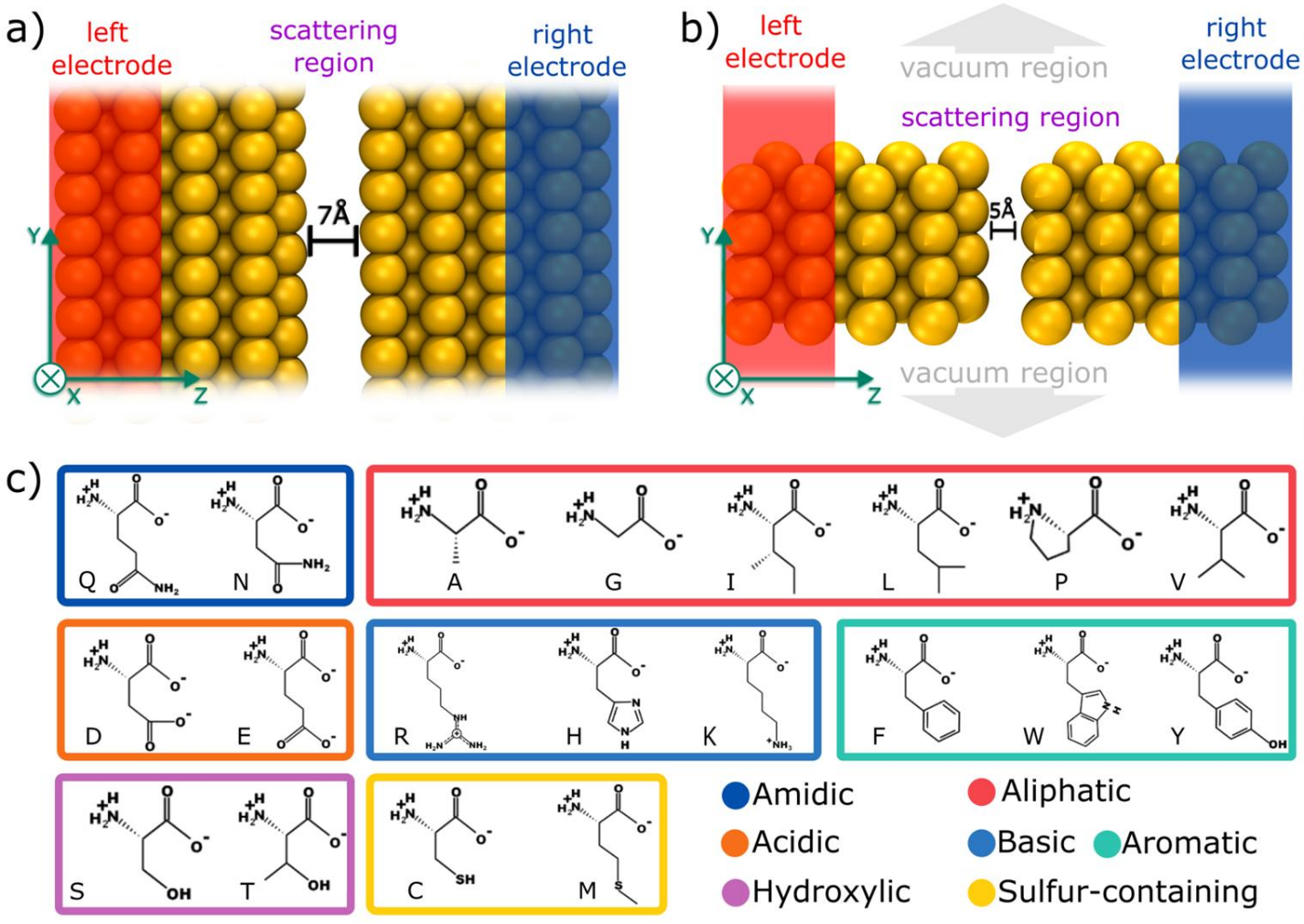
now let me show you what this looks like in practice…



From the journal:
Nanoscale

Detection and distinction of amino acids and post-translational modifications with gold nanojunctions




a)
left electrode
scattering region
right electrode
7Å
Y
X
Z
b)
left electrode
vacuum region
right electrode
scattering region
5Å
vacuum region
Y
X
Z
c)
Q
N
A
G
I
L
P
V
D
E
R
H
K
F
W
Y
S
T
C
M
Amidic
Aliphatic
Acidic
Basic
Aromatic
Hydroxylic
Sulfur-containing

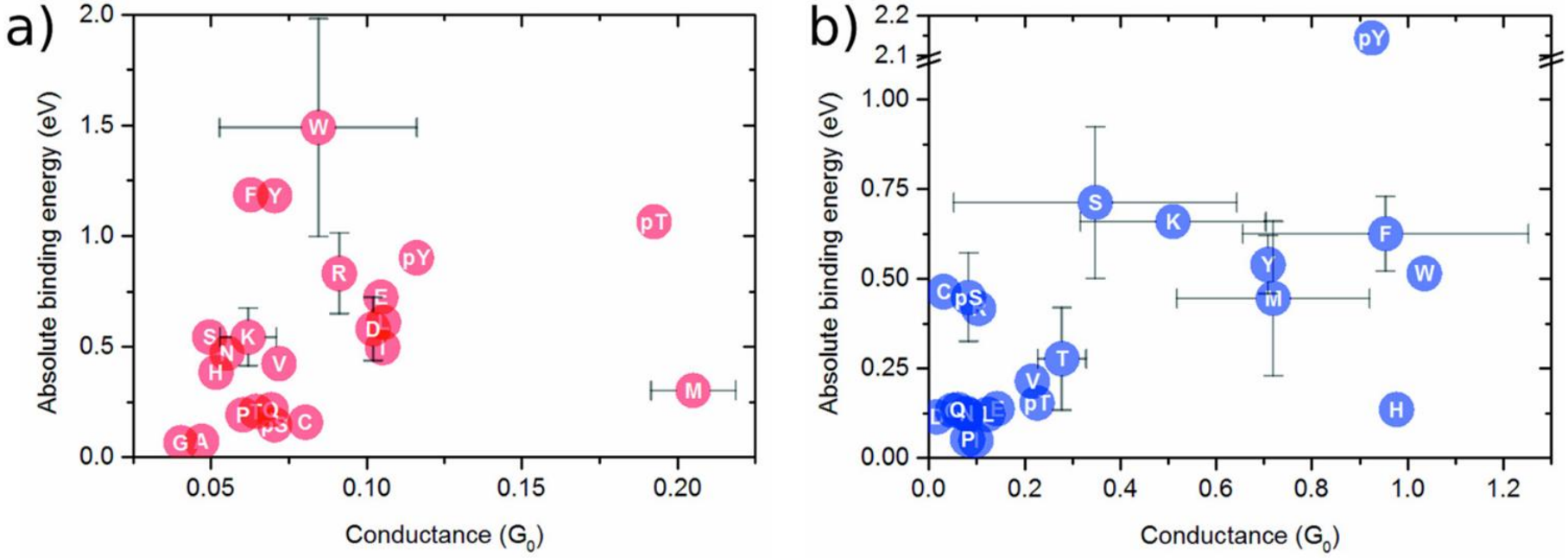
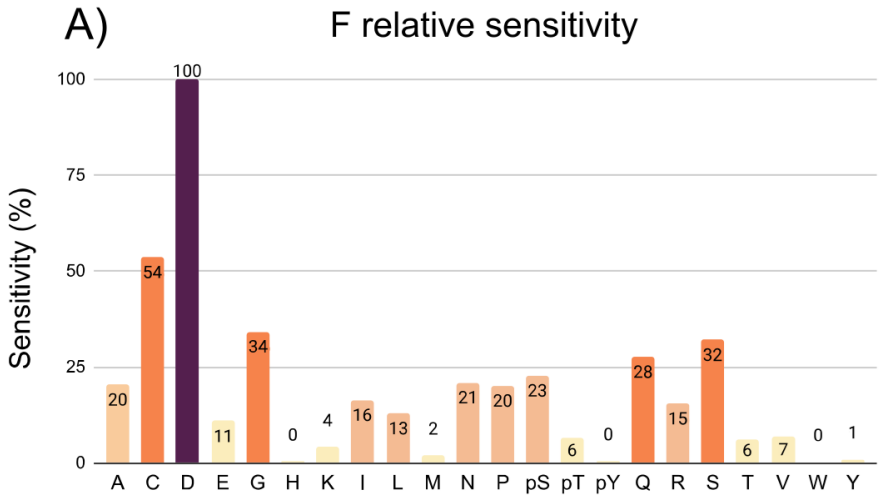


Fig. 2 Binding energy as a function of the conductance (at Fermi level) for (a) capacitor of 7.0 Å nanogap; (b) 5.0 Å nanojunction.



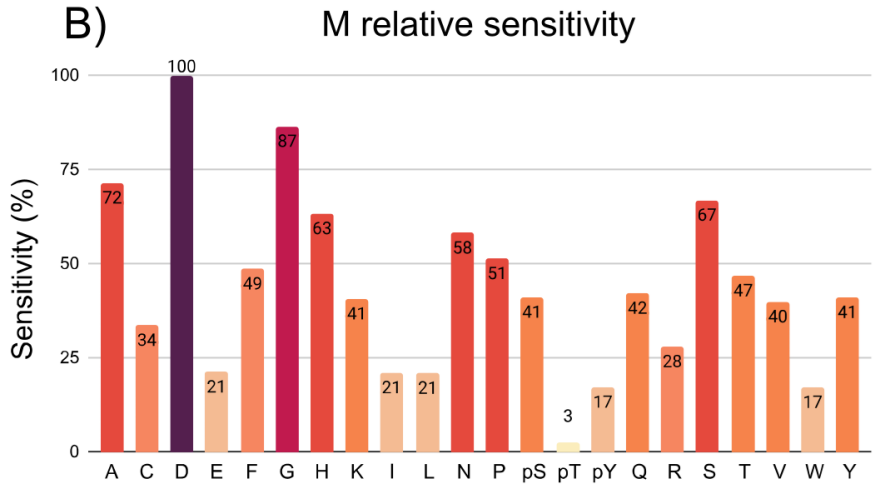
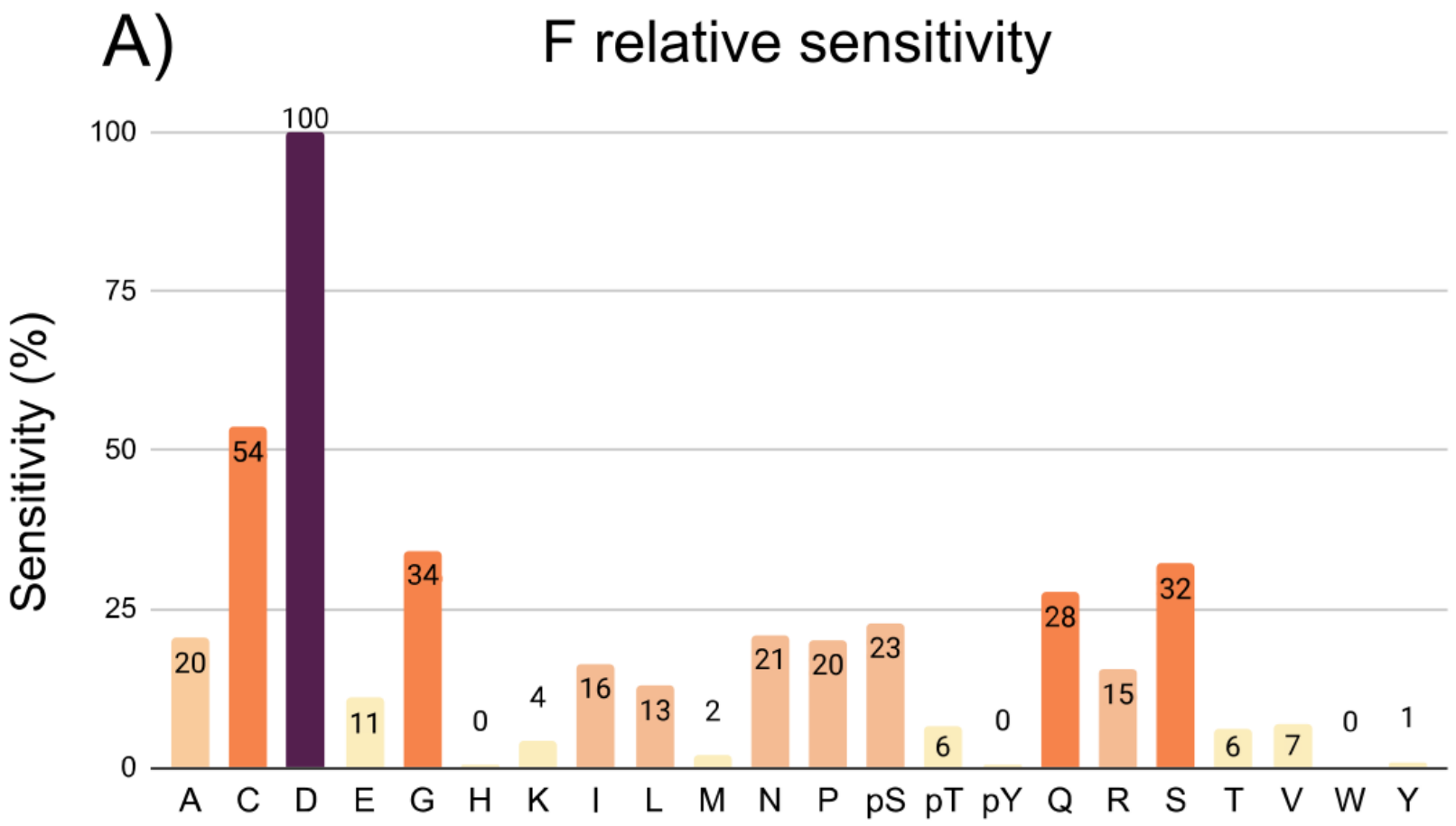
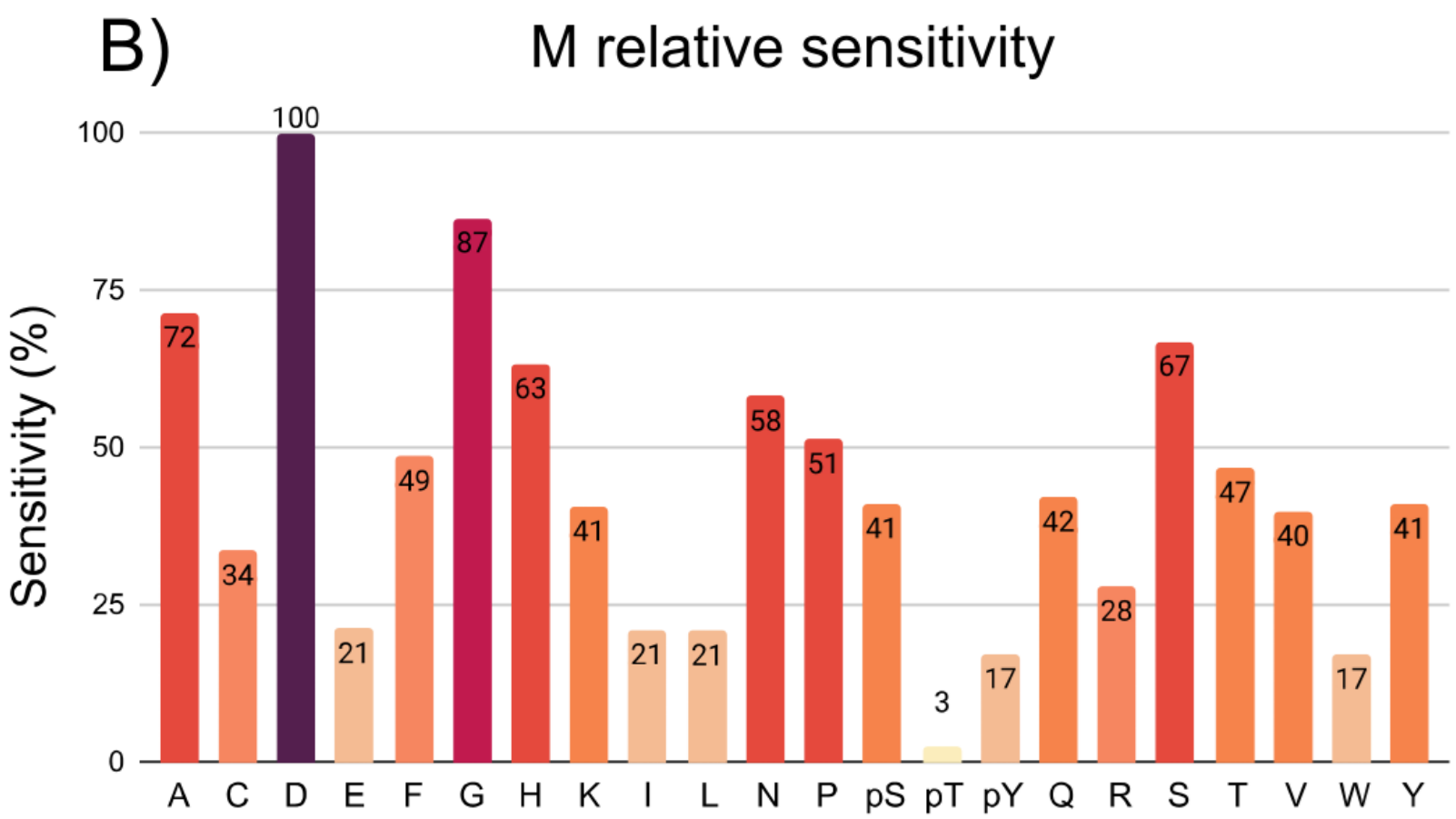


Fig. 3 Graphical representation depicting the sensitivity (%) of the following devices: (a) 7.0 Å infinite capacitor; (b) 5.0 Å nanojunction.


A)
F relative sensitivity
Sensitivity (%)
100
75
50
25
0
A C D E G H K I L M N P pS pT pY Q R S T V W Y
20 54 100 11 34 0 4 16 13 2 21 20 23 6 0 28 15 32 6 7 0 1


B)
M relative sensitivity
Sensitivity (%)
100
75
50
25
0
72
34
100
21
49
87
63
41
21
21
58
51
41
3
17
42
28
67
47
40
17
41
A
C
D
E
F
G
H
K
I
L
N
P
pS
pT
pY
Q
R
S
T
V
W
Y

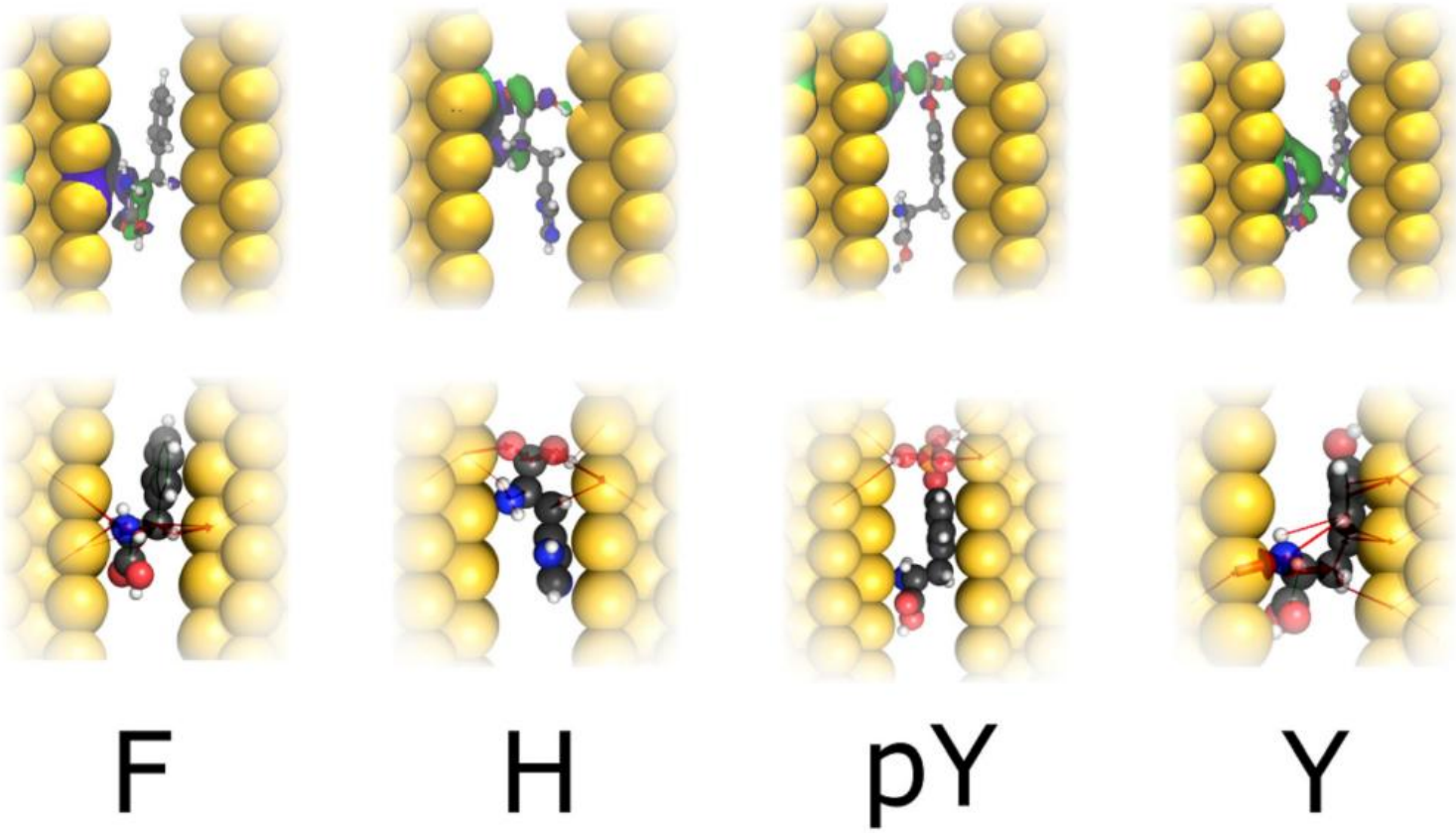


Fig. 4 Top row: WF corresponding to an energy of $E - E_F = 0.0$ eV; bottom row: respective LC for Phe(F), His(H) Tyr modified (pY) and Tyr (Y) in the infinite capacitor device (7.0 Å between the gold layers). Atomic color: yellow (Au), gray (C), red (O), blue (N), orange (P) and white (H); purple spheroids (positive WF portion); green spheroids (negative WF portion).

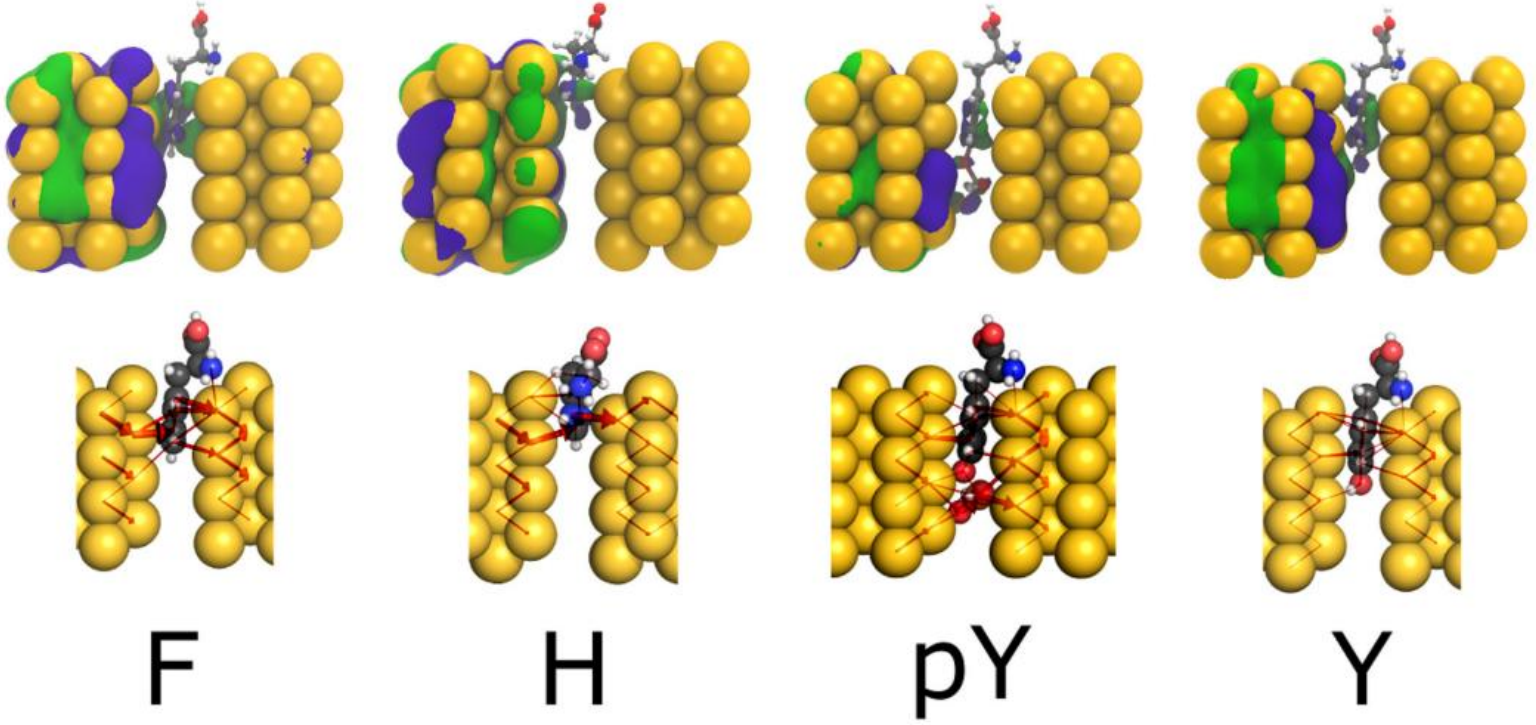


Fig. 5 Top row: WF corresponding to an energy of $E - E_F = 0$ eV; bottom row: respective local currents (LC) for Phe(F), His(H), Tyr modified (pY), and Tyr (Y) amino in the tip 5.0 Å. Atomic color: yellow (Au), gray (C), red (O), blue (N), orange (P) and white (H); purple spheroids (positive WF portion); green spheroids(negative WF portion). 5 Å nanojunction device.

Design is a …


CONTRAST
REPETITION
ALIGNMENT
PROXIMITY
CRAP!

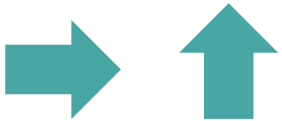
CONTRAST

COLOR

TONE/VALUE

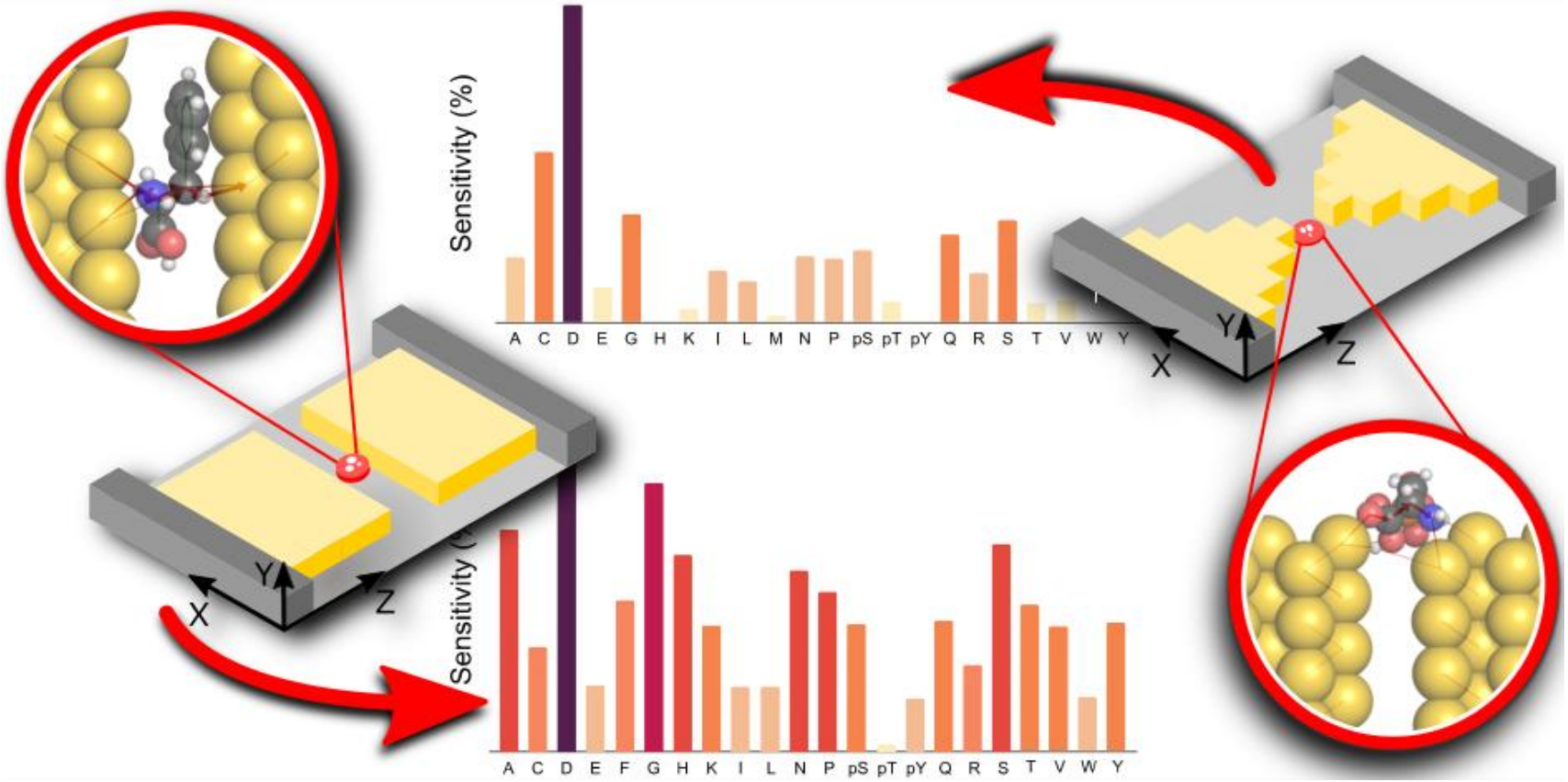
SIZE/SHAPE

DIRECTION

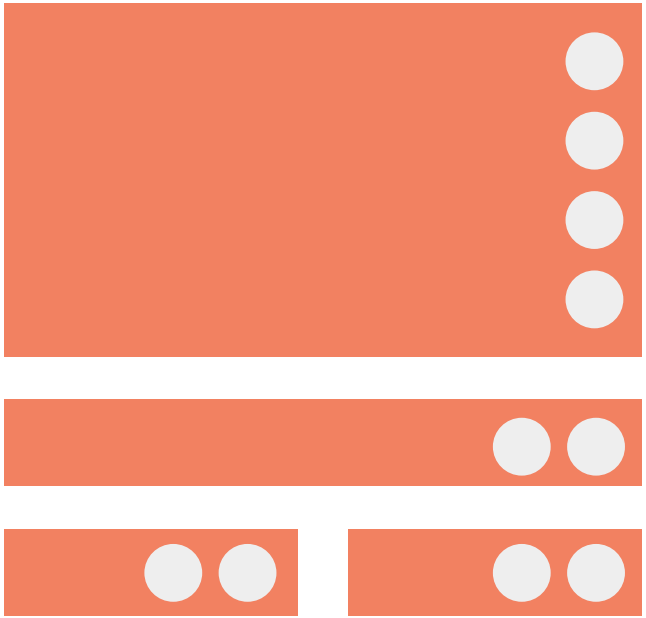


Unique elements in a design should stand apart from one another. One way to do this is to use contrast. Good contrast in a design – which can be achieved using elements like color, tone, size, and more – allows the viewer's eye to flow naturally.

To the left, you can see 4 ways to create contrast in your design.


Sensitivity (%)
A C D E G H K I L M N P pS pT pY Q R S T V W Y
Y
X
Z
Sensitivity (%)
A C D E F G H K I L N P pS pT pY Q R S T V W Y
Y
X
Z

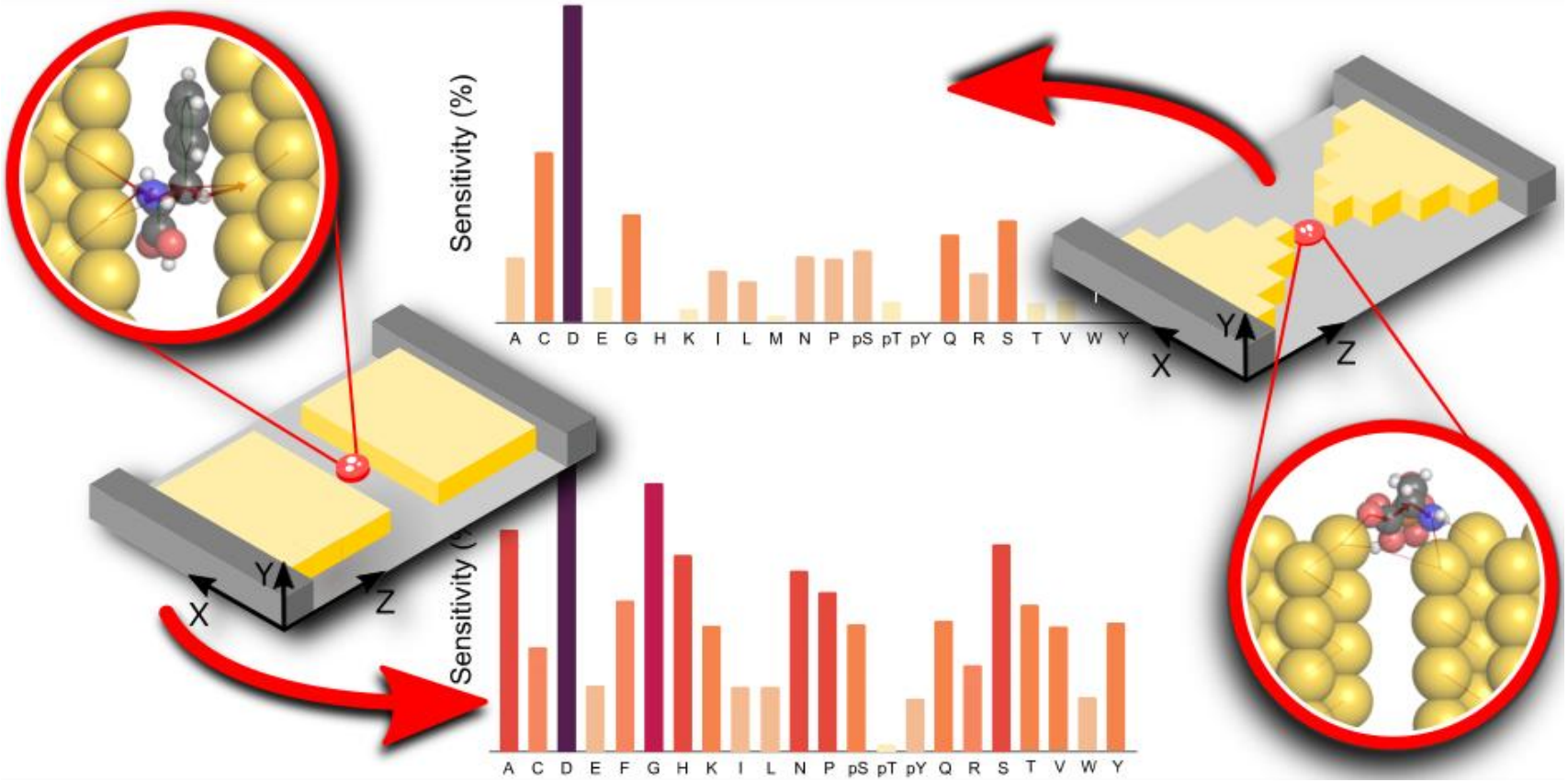
REPETITION



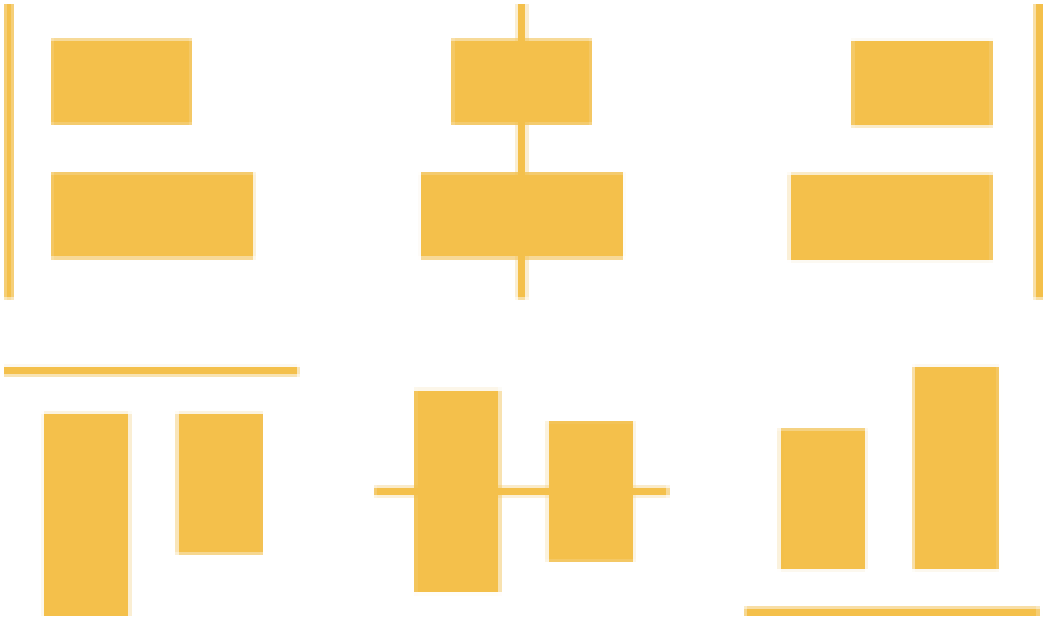
Repetition breeds cohesiveness in a design. Once a design pattern has been established – for example, a dotted border or a specific typographic styling – repeat this pattern to establish consistency.

The short version?

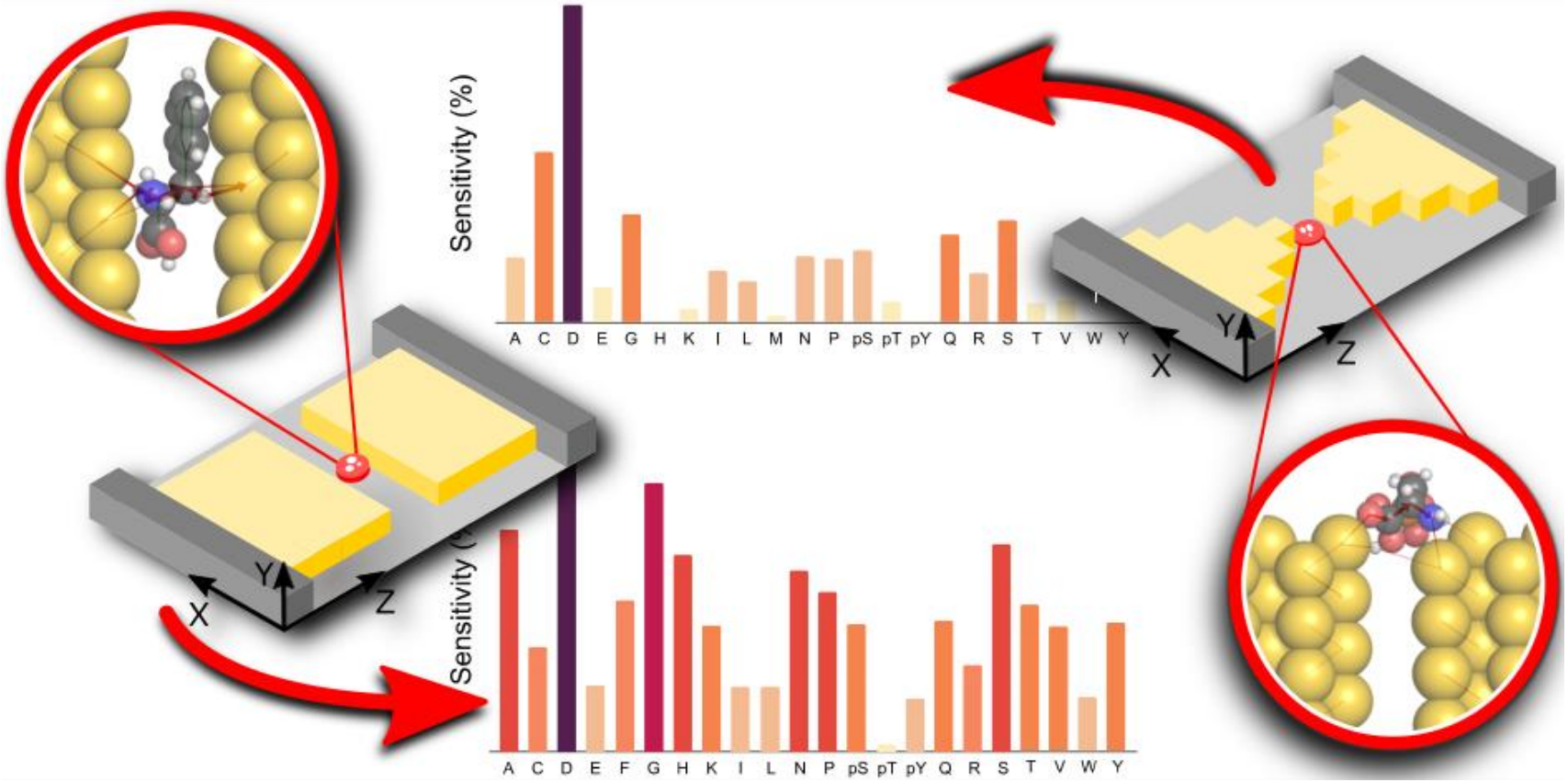
Establish a style for each element in a design and use it on similar elements.


Sensitivity (%)
A C D E G H K I L M N P pS pT pY Q R S T V W Y
Y
X
Z
Sensitivity (%)
A C D E F G H K I L N P pS pT pY Q R S T V W Y
Y
X
Z

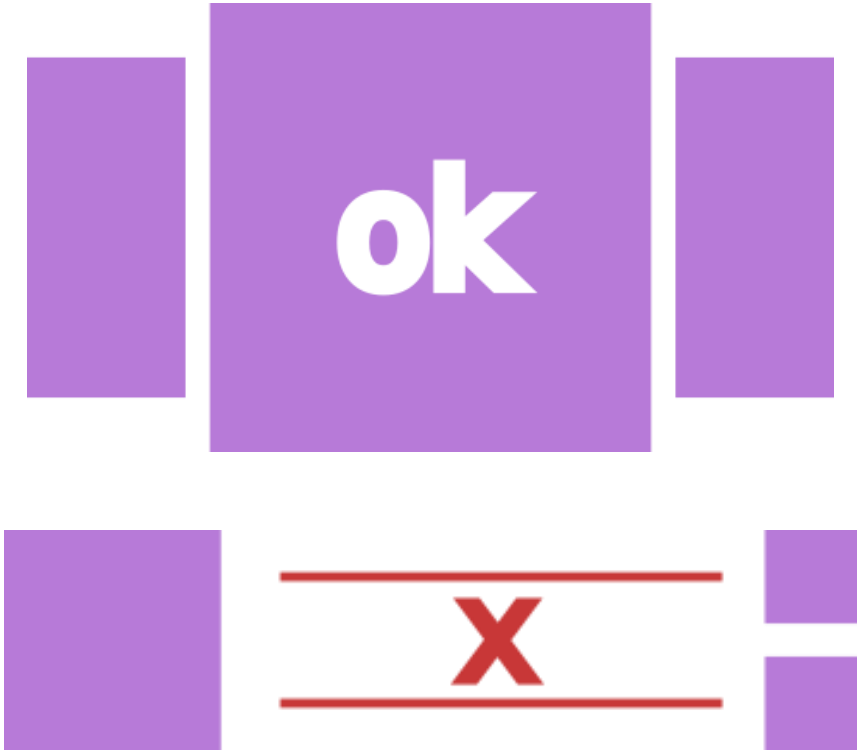
ALIGNMENT



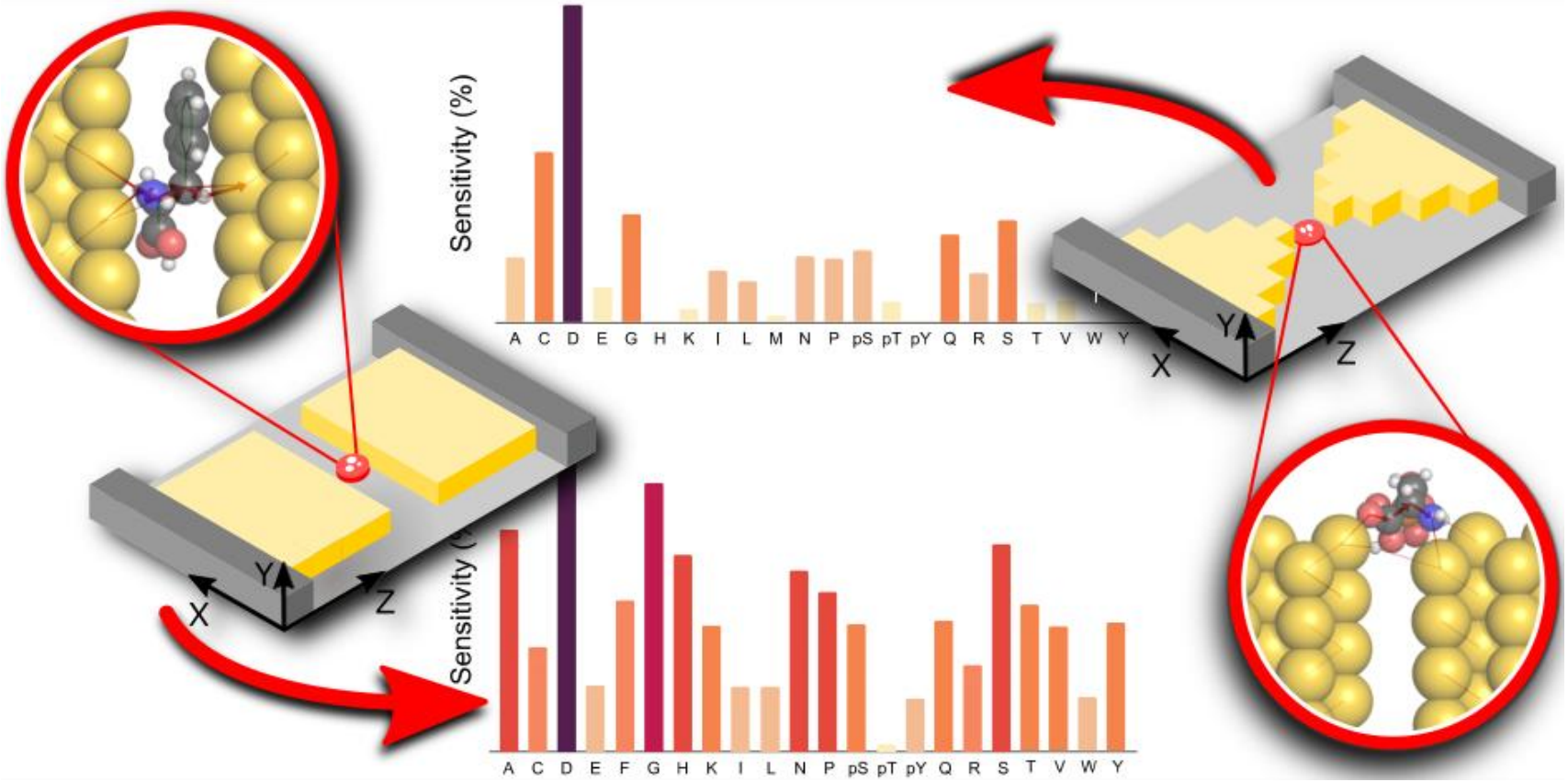
Proper alignment in a design means that every element in it is visually connected to another element. Alignment allows for cohesiveness; nothing feels out of place or disconnected when alignment has been handled well.

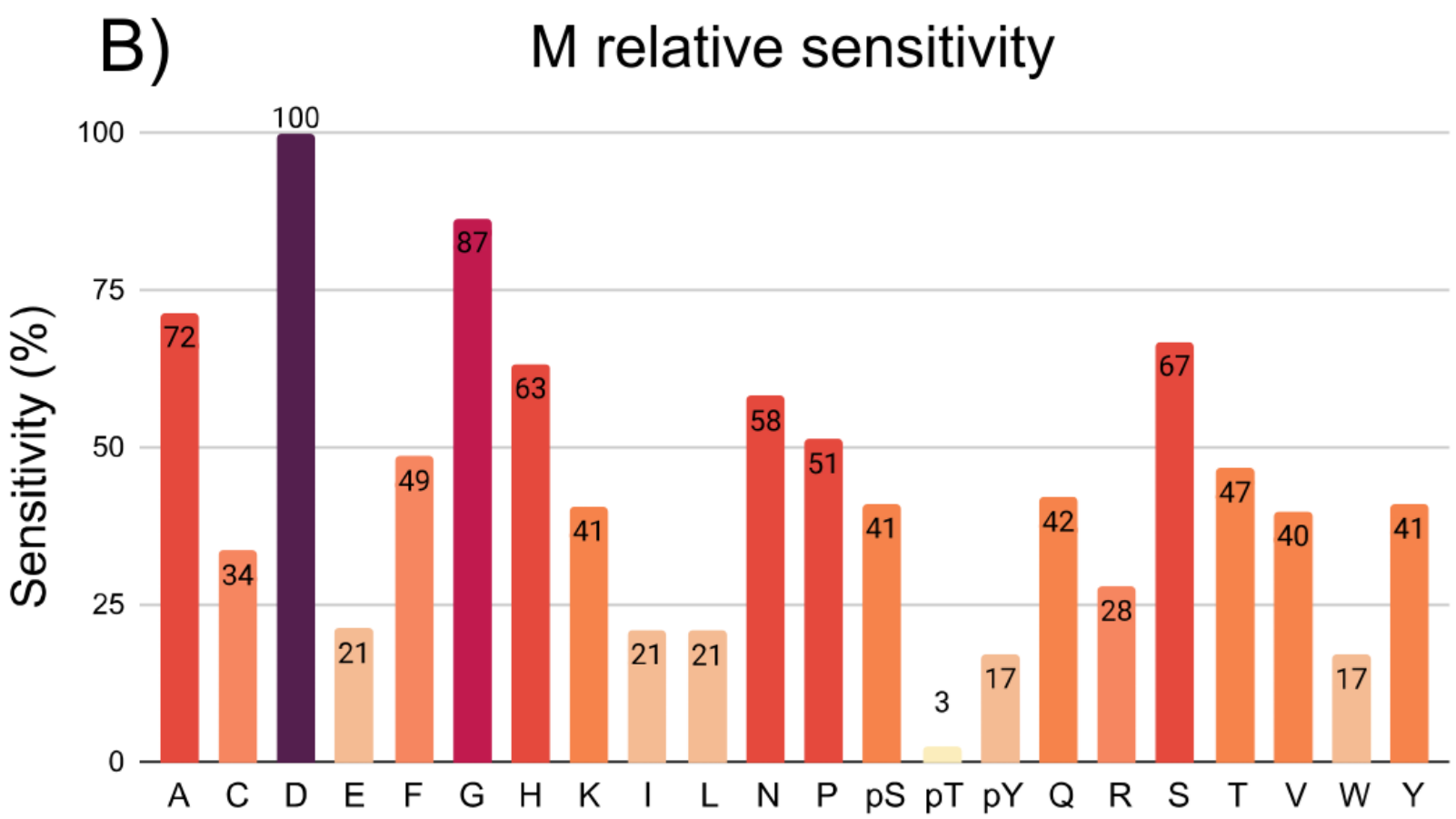

Sensitivity (%)
A C D E G H K I L M N P pS pT pY Q R S T V W Y
Y
X
Z
Sensitivity (%)
A C D E F G H K I L N P pS pT pY Q R S T V W Y
Y
X
Z

PROXIMITY



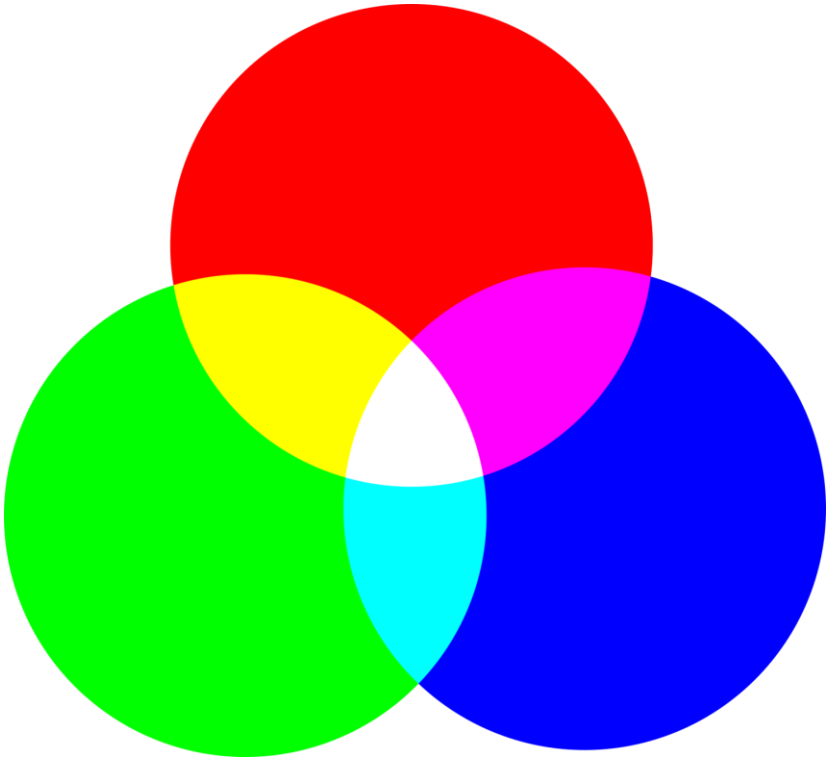
Proximity allows for visual unity in a design. If two elements are related to each other, they should be placed in close proximity to one another. Doing so minimizes visual clutter, emphasizes organization, and increases viewer comprehension.

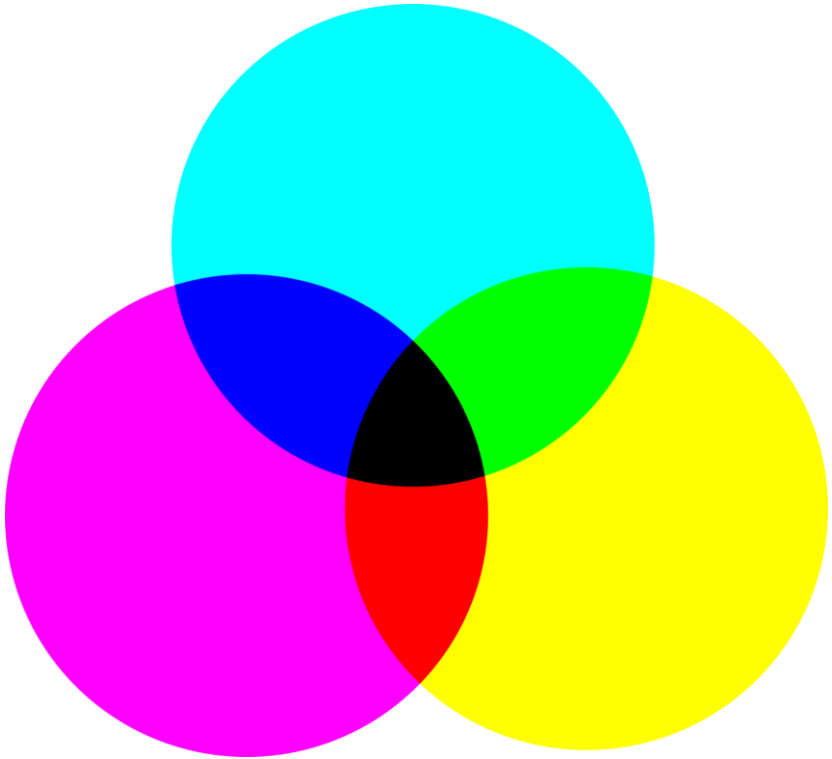

Sensitivity (%)
A C D E G H K I L M N P pS pT pY Q R S T V W Y
Y
X
Z
Sensitivity (%)
A C D E F G H K I L N P pS pT pY Q R S T V W Y
Y
X
Z


B)
M relative sensitivity
Sensitivity (%)
100
75
50
25
0
72
34
100
21
49
87
63
41
21
21
58
51
41
3
17
42
28
67
47
40
17
41
A
C
D
E
F
G
H
K
I
L
N
P
pS
pT
pY
Q
R
S
T
V
W
Y

How does color works?

RGB vs CMYK

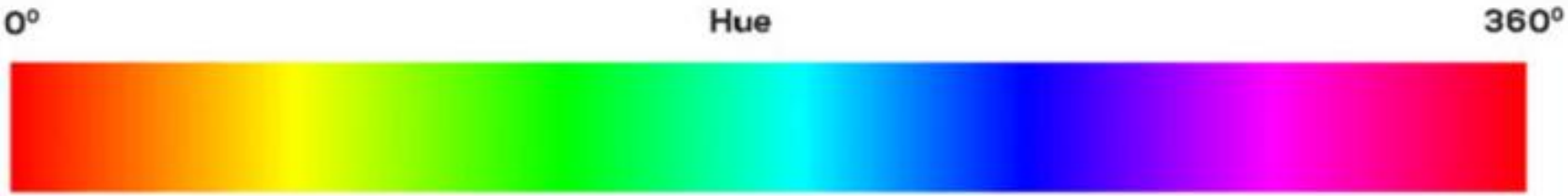




Color palettes

https://color.adobe.com/pt/create/color-wheel


Reds
Oranges
Yellows
Yellows Greens
Greens
Blue Greens
Blues
Blue Violets
Violets
Mauves
Mauve Pinks
Pinks

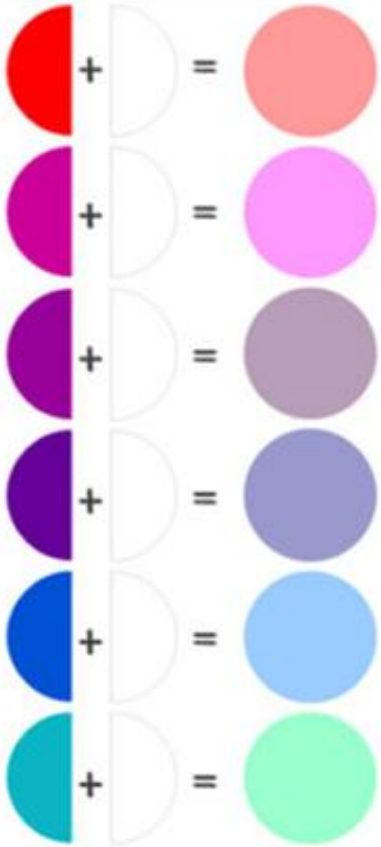

0°
Hue
360°

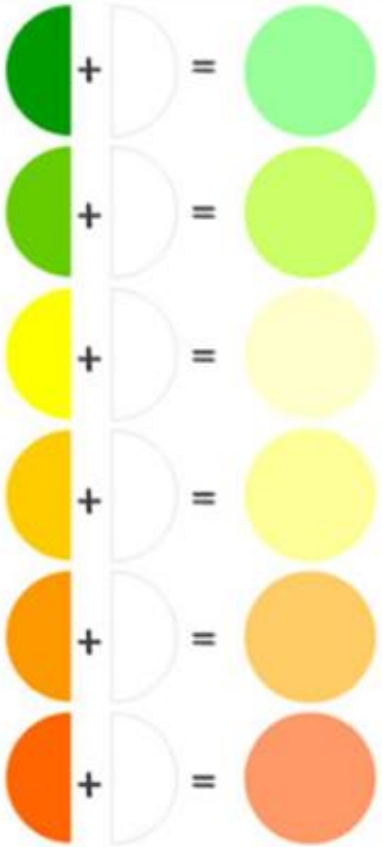
SHADE

Adding black to pure Hue

TINT

Adding White to a pure hue





TONE

Adding grey to a pure hue

Analogous Colors List

Red

Red-Orange

Orange

Yellow-Orange

Yellow

Yellow-Green

Green

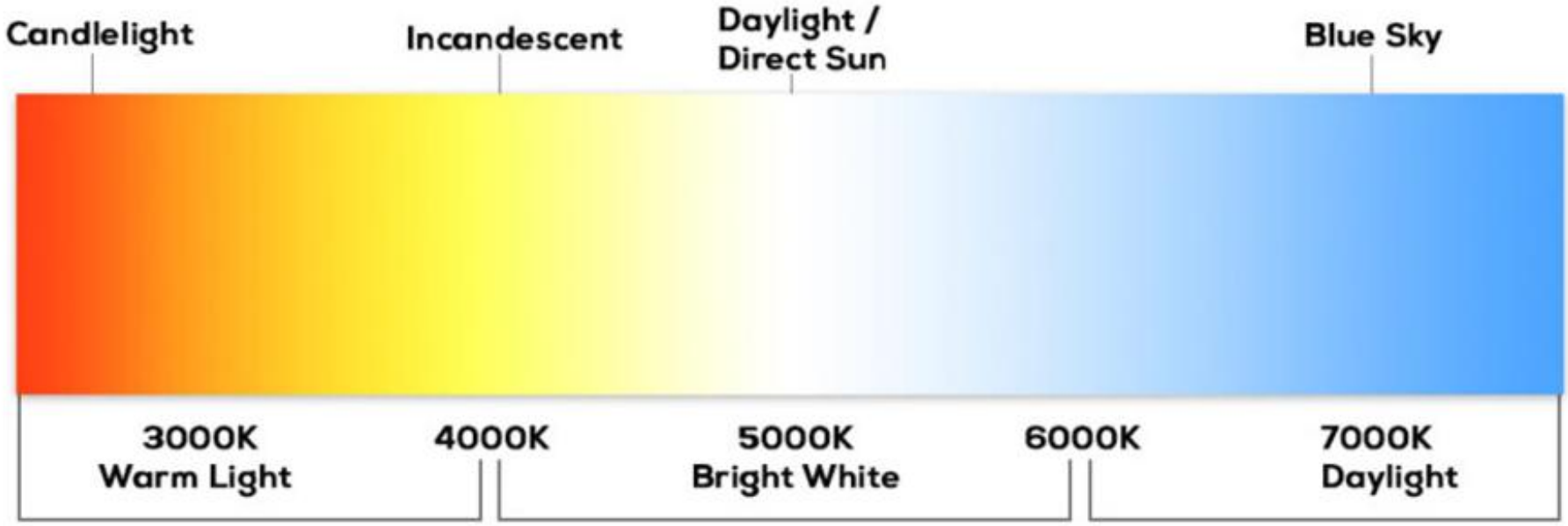
Blue-Green

Blue

Blue-Violet

Violet

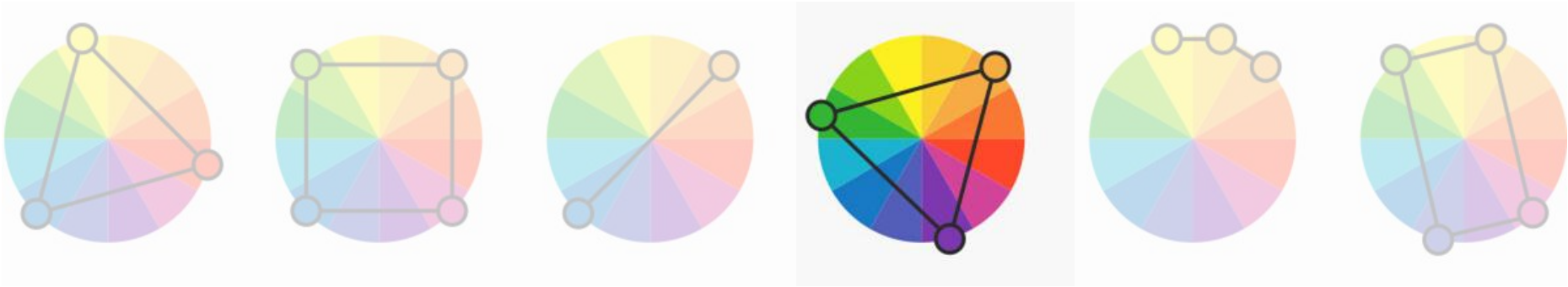
Red-Violet


Candlelight
Incandescent
Daylight /
Direct Sun
Blue Sky
3000K
Warm Light
4000K
5000K
Bright White
6000K
7000K
Daylight

“Use triadic when you have three key ideas that deserve equal attention”

“Use square when you need four balanced categories with strong visual separation.”

“Use complementary when your message is a direct comparison: A versus B.”



“Use split-complementary when you want contrast without the visual conflict.”

“Use analogous when you want harmony, flow, and a clean professional look.”

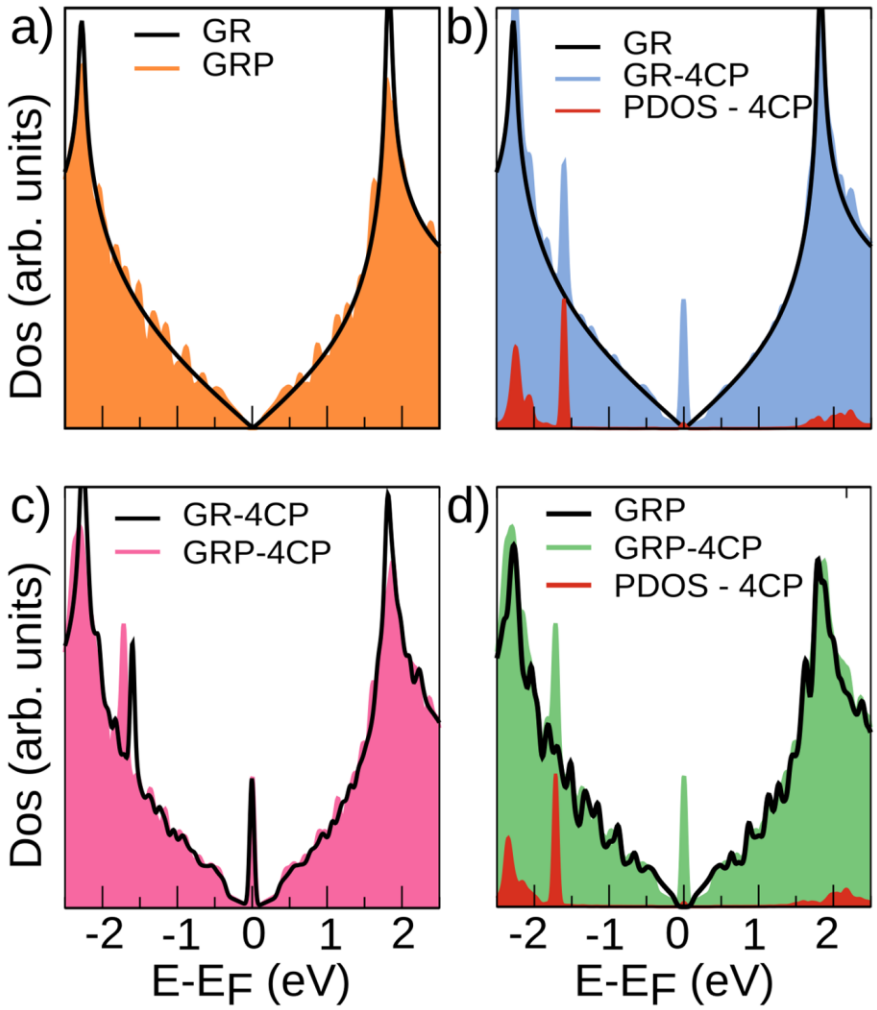
“Use rectangle when you need four balanced categories with strong visual separation.”

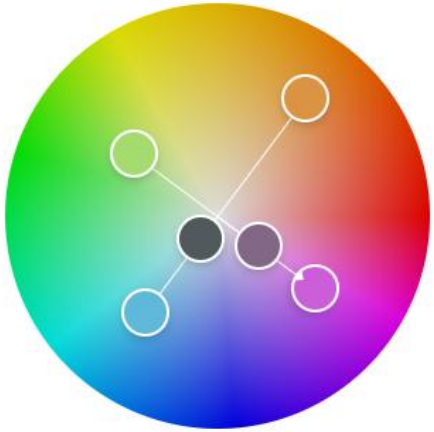
Color Palettes ready to use

https://www.canva.com/colors/color-wheel/

https://color.adobe.com/pt/trends

https://colorhunt.co/palettes/popular


a)
GR
GRP
b)
GR
GR-4CP
PDOS - 4CP
c)
GR-4CP
GRP-4CP
d)
GRP
GRP-4CP
PDOS - 4CP
Dos (arb. units)
Dos (arb. units)
-2 -1 0 1 2
E-EF (eV)
-2 -1 0 1 2
E-EF (eV)



#5EB9DB

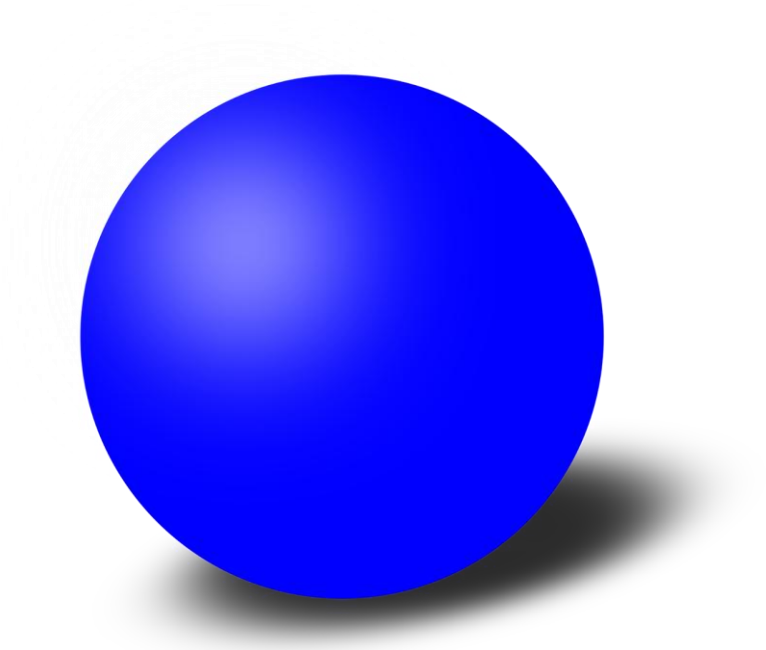
#A6DB70

#CD5EDB

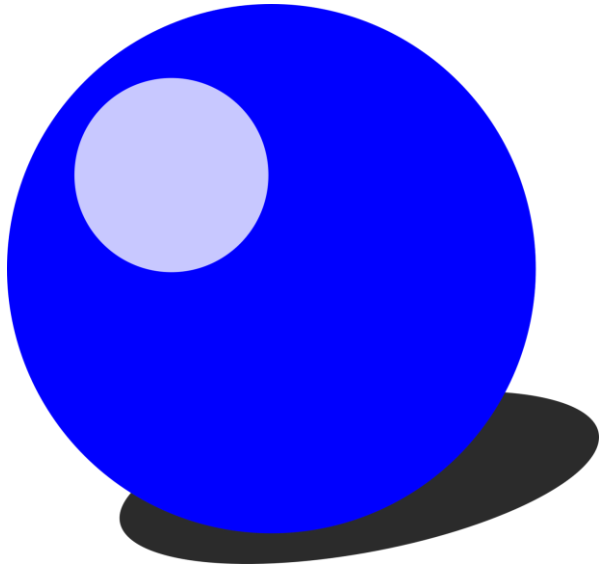
#DB9344

How about light and shadows?

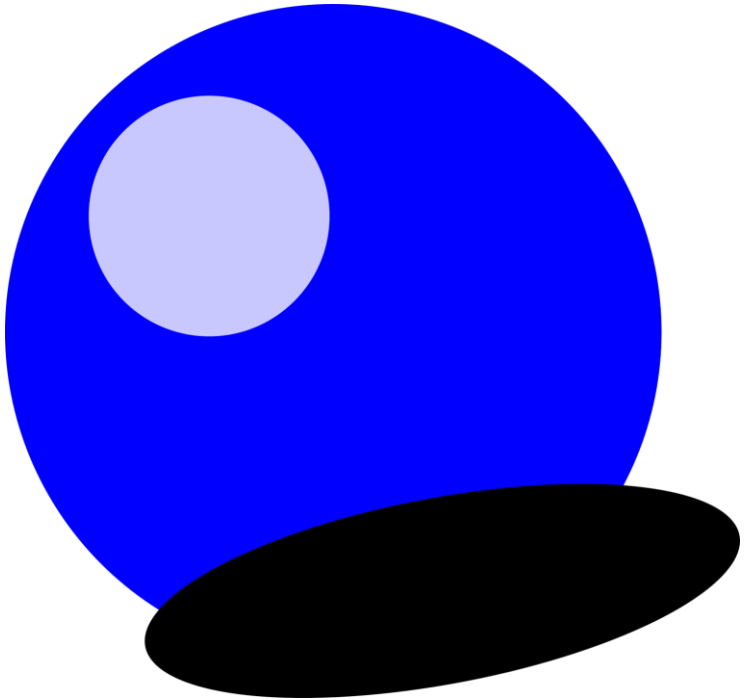
Sphere or circle?

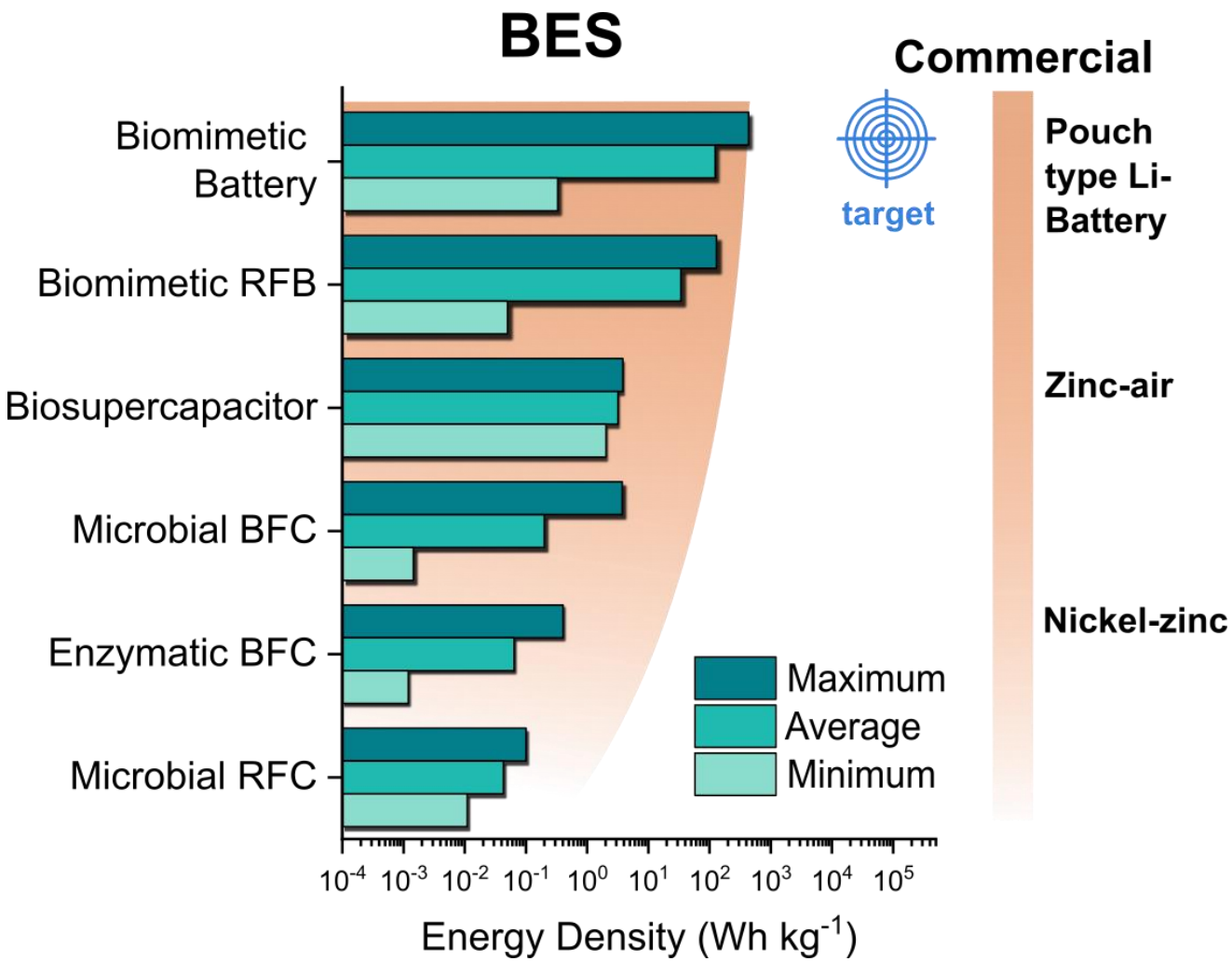


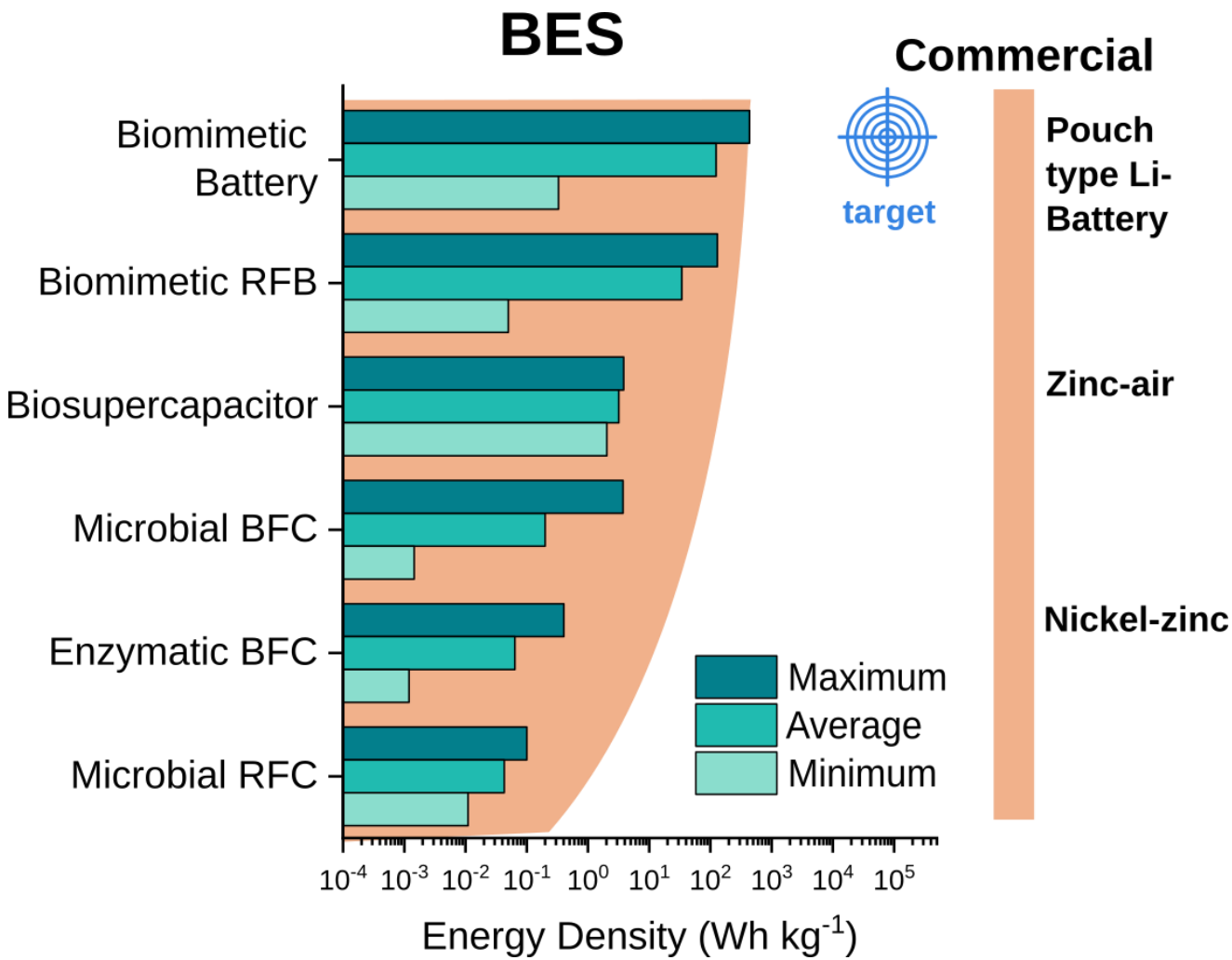
Sphere or circle?

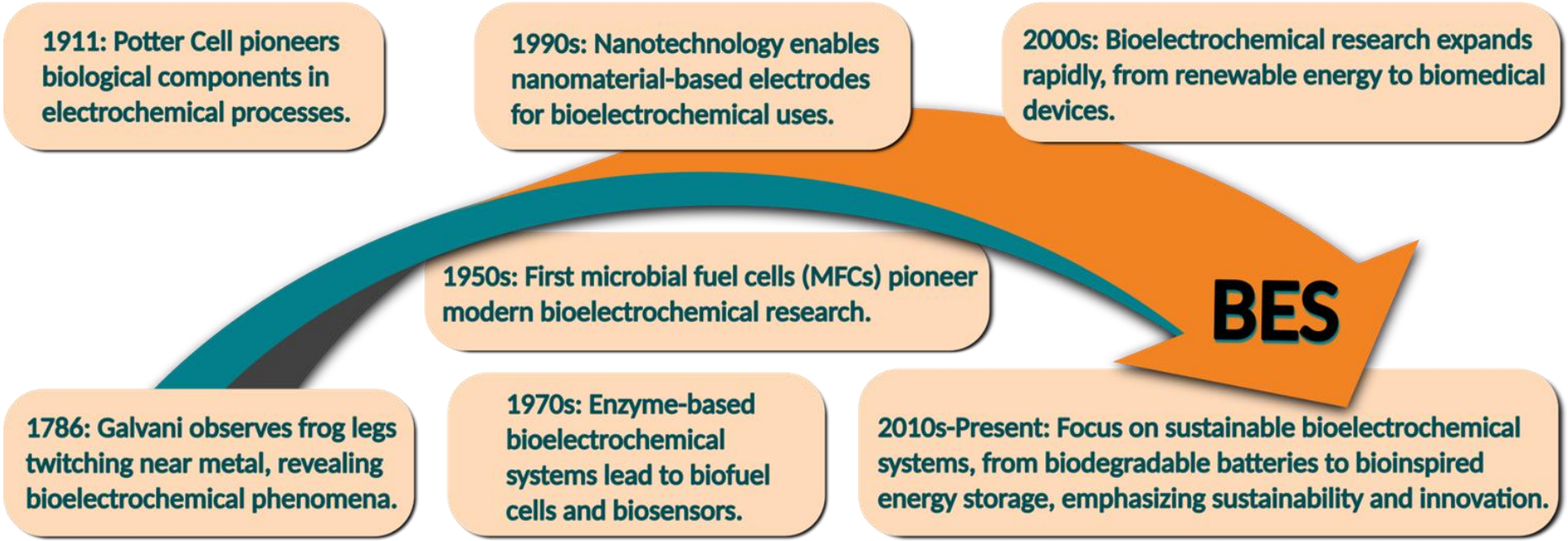


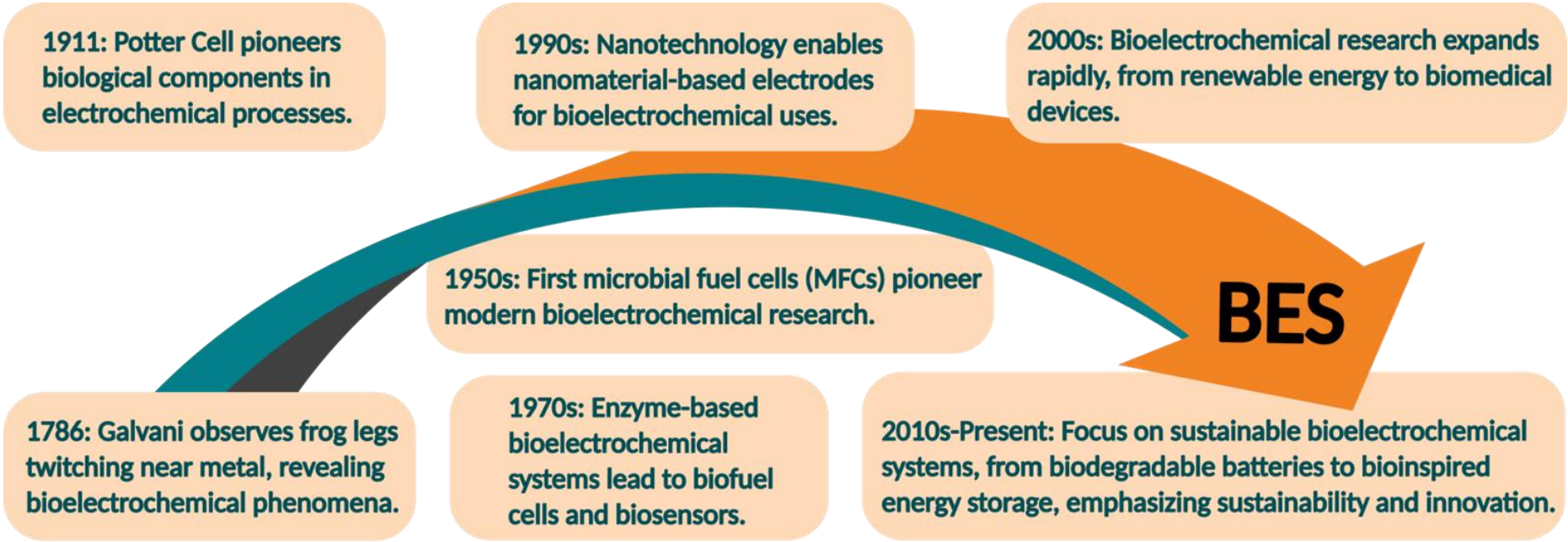
does not look right




BES
Commercial
Biomimetic Battery
Biomimetic RFB
Biosupercapacitor
Microbial BFC
Enzymatic BFC
Microbial RFC
target
Pouch type Li-Battery
Zinc-air
Nickel-zinc
Maximum
Average
Minimum
10-4 10-3 10-2 10-1 100 101 102 103 104 105
Energy Density (Wh kg-1)

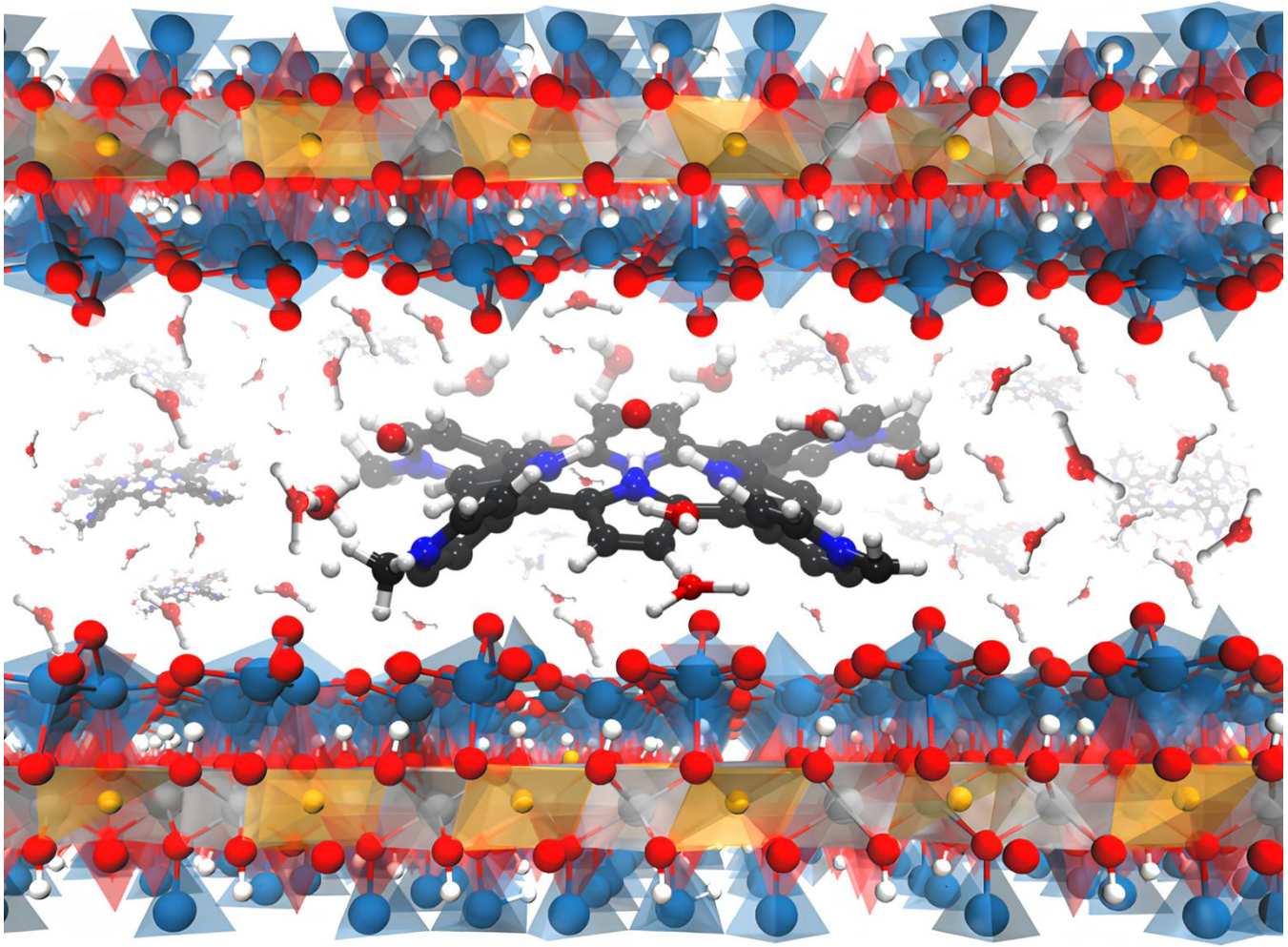

BES
Commercial
Biomimetic Battery
Biomimetic RFB
Biosupercapacitor
Microbial BFC
Enzymatic BFC
Microbial RFC
target
Pouch type Li-Battery
Zinc-air
Nickel-zinc
Maximum
Average
Minimum
10-4 10-3 10-2 10-1 100 101 102 103 104 105
Energy Density (Wh kg-1)


1911: Potter Cell pioneers biological components in electrochemical processes.
1990s: Nanotechnology enables nanomaterial-based electrodes for bioelectrochemical uses.
2000s: Bioelectrochemical research expands rapidly, from renewable energy to biomedical devices.
1950s: First microbial fuel cells (MFCs) pioneer modern bioelectrochemical research.
BES
1786: Galvani observes frog legs twitching near metal, revealing bioelectrochemical phenomena.
1970s: Enzyme-based bioelectrochemical systems lead to biofuel cells and biosensors.
2010s-Present: Focus on sustainable bioelectrochemical systems, from biodegradable batteries to bioinspired energy storage, emphasizing sustainability and innovation.


1911: Potter Cell pioneers biological components in electrochemical processes.
1990s: Nanotechnology enables nanomaterial-based electrodes for bioelectrochemical uses.
2000s: Bioelectrochemical research expands rapidly, from renewable energy to biomedical devices.
1950s: First microbial fuel cells (MFCs) pioneer modern bioelectrochemical research.
BES
1786: Galvani observes frog legs twitching near metal, revealing bioelectrochemical phenomena.
1970s: Enzyme-based bioelectrochemical systems lead to biofuel cells and biosensors.
2010s-Present: Focus on sustainable bioelectrochemical systems, from biodegradable batteries to bioinspired energy storage, emphasizing sustainability and innovation.


Reds
Oranges
Yellows
Yellows Greens
Greens
Blue Greens
Blues
Blue Violets
Violets
Mauves
Mauve Pinks
Pinks

How about figures?

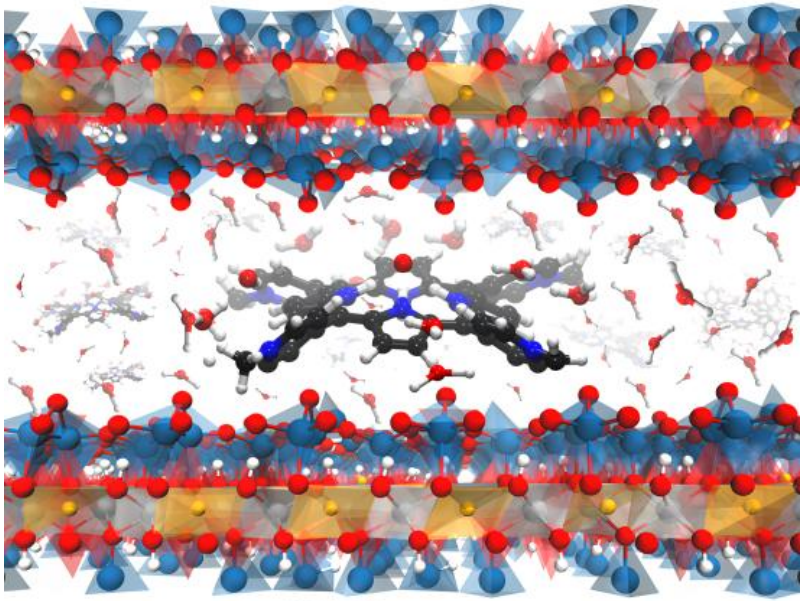


Volume NN
Number 1
N January 2025
PagesN-NNN

Dalton Transactions

An international journal of inorganic chemistry

rsc.li/dalton



ISSN7 777 7777

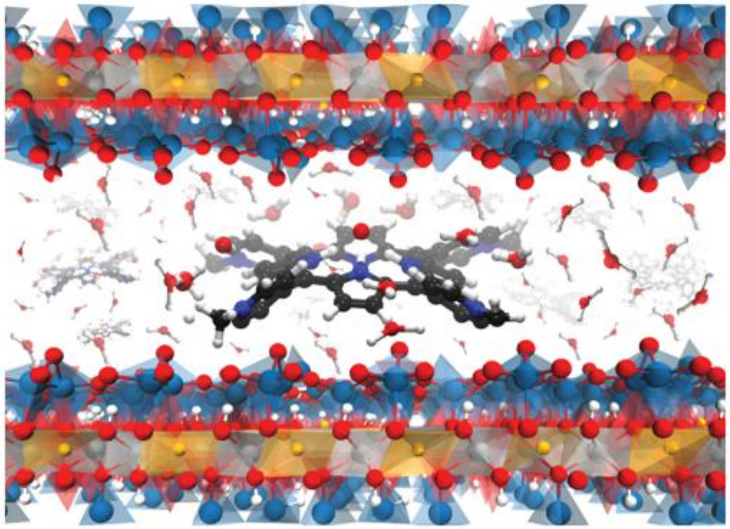
ROYAL SOCIETY OF CHEMISTRY

PAPER

Helena Maria Petrilli *et al.*

Shape-responsive host-guest chemistry: metal-free tetra cationic porphyrin nonplanarity promoted by clay mineral interactions assessed by theoretical simulations

X



Showcasing research from Professor Helena Petrilli's group, Department of Materials Physics, Institute of Physics, São Paulo University, Brazil.

Shape-responsive host–guest chemistry: metal-free tetracationic porphyrin nonplanarity promoted by clay mineral interactions assessed by theoretical simulations

DFT calculations indicate that interactions with montmorillonite lead to conformational changes in porphyrins, such as twisting of the macrocycle and rotation of the peripheral substituents. These changes increase basicity and facilitate the abstraction of protons from intercalated water. This highlights the significant role of clay microenvironments in modifying the properties of porphyrins.

As featured in:

See Vera Regina Leopoldo Constantino, Helena Maria Petrilli *et al.*, *Dalton Trans.*, 2025, **54**, 2271.

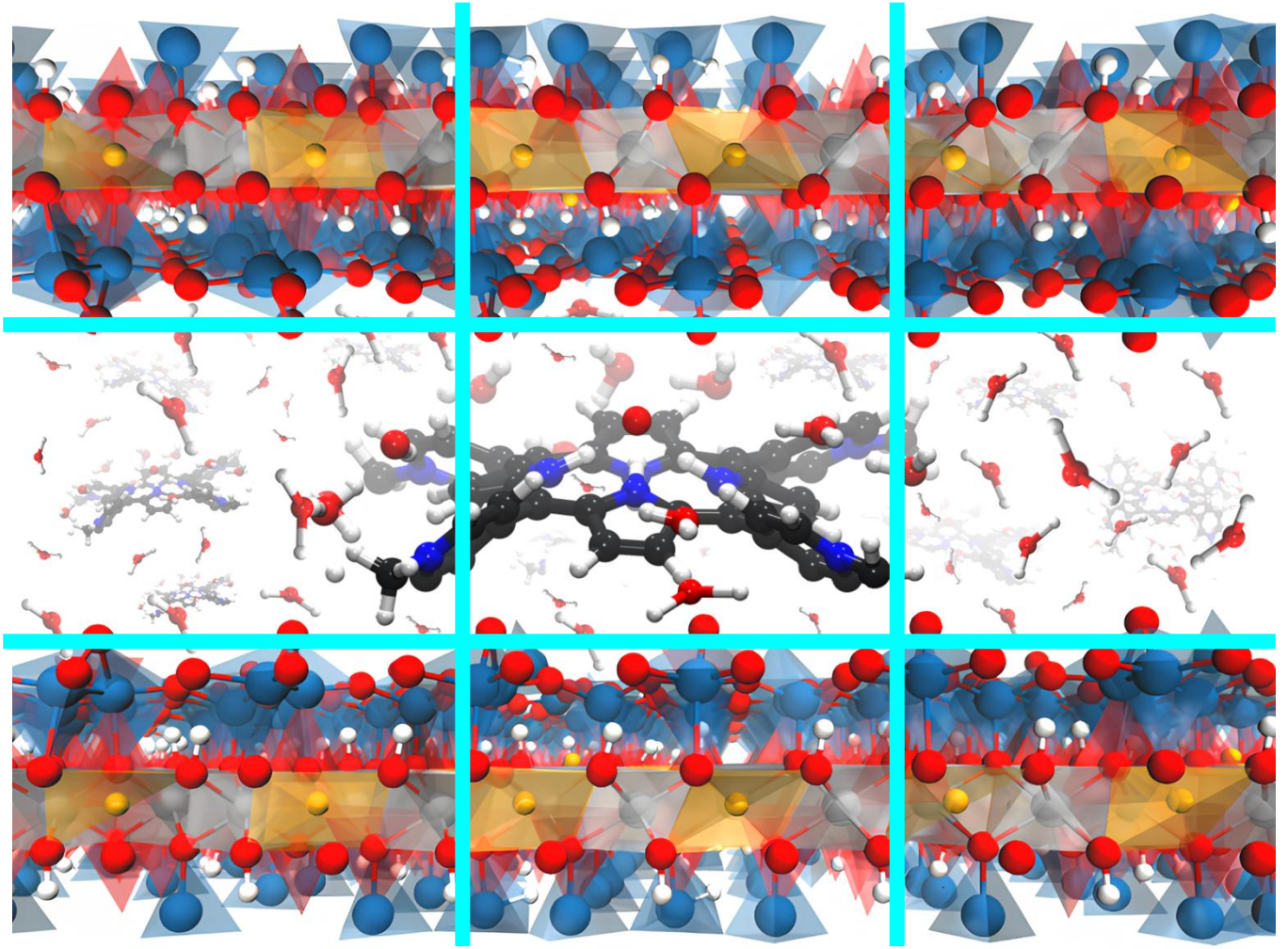
ROYAL SOCIETY OF CHEMISTRY

rsc.li/dalton

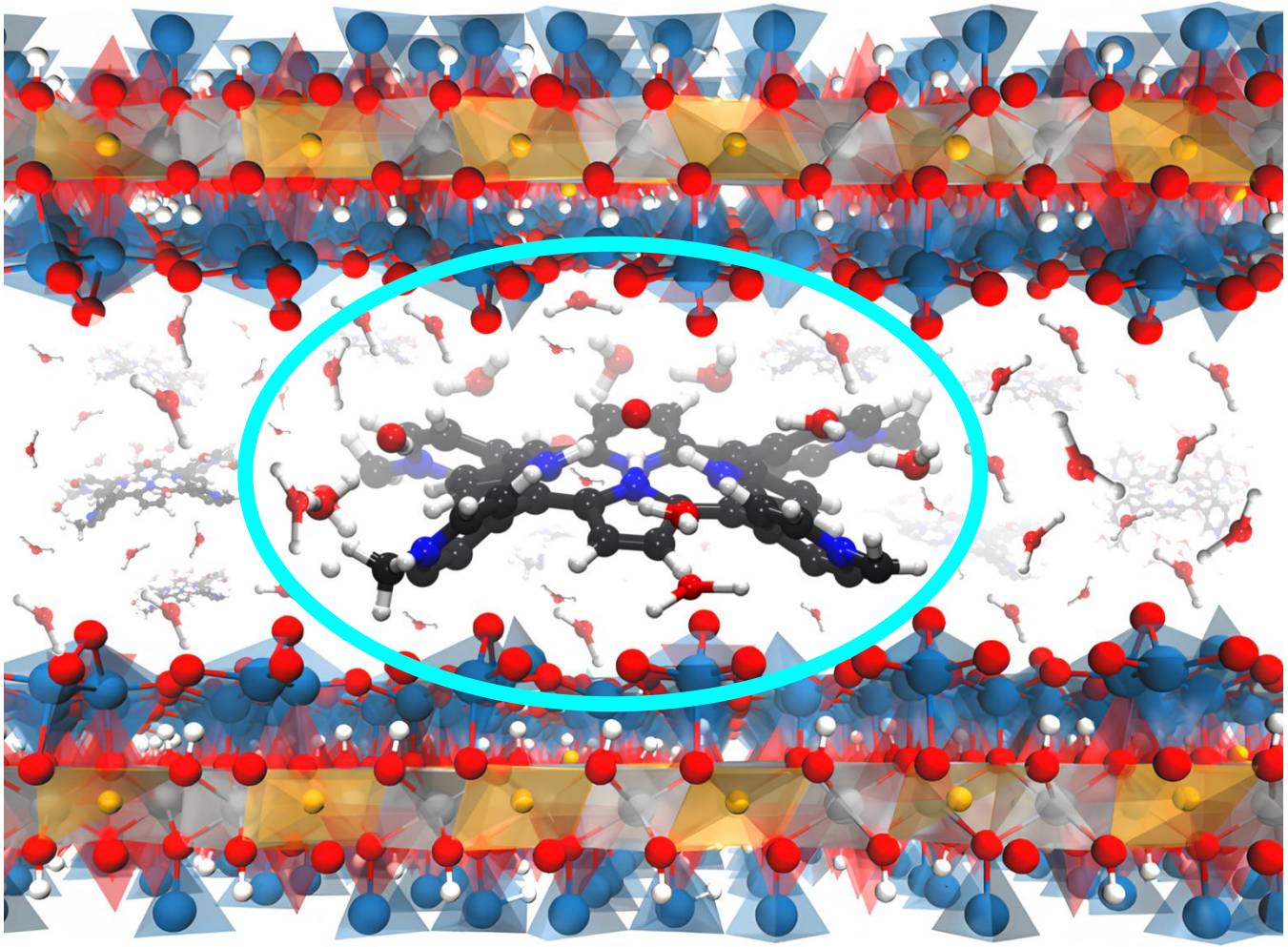
Registered charity number: 207890

What does make a good photo?

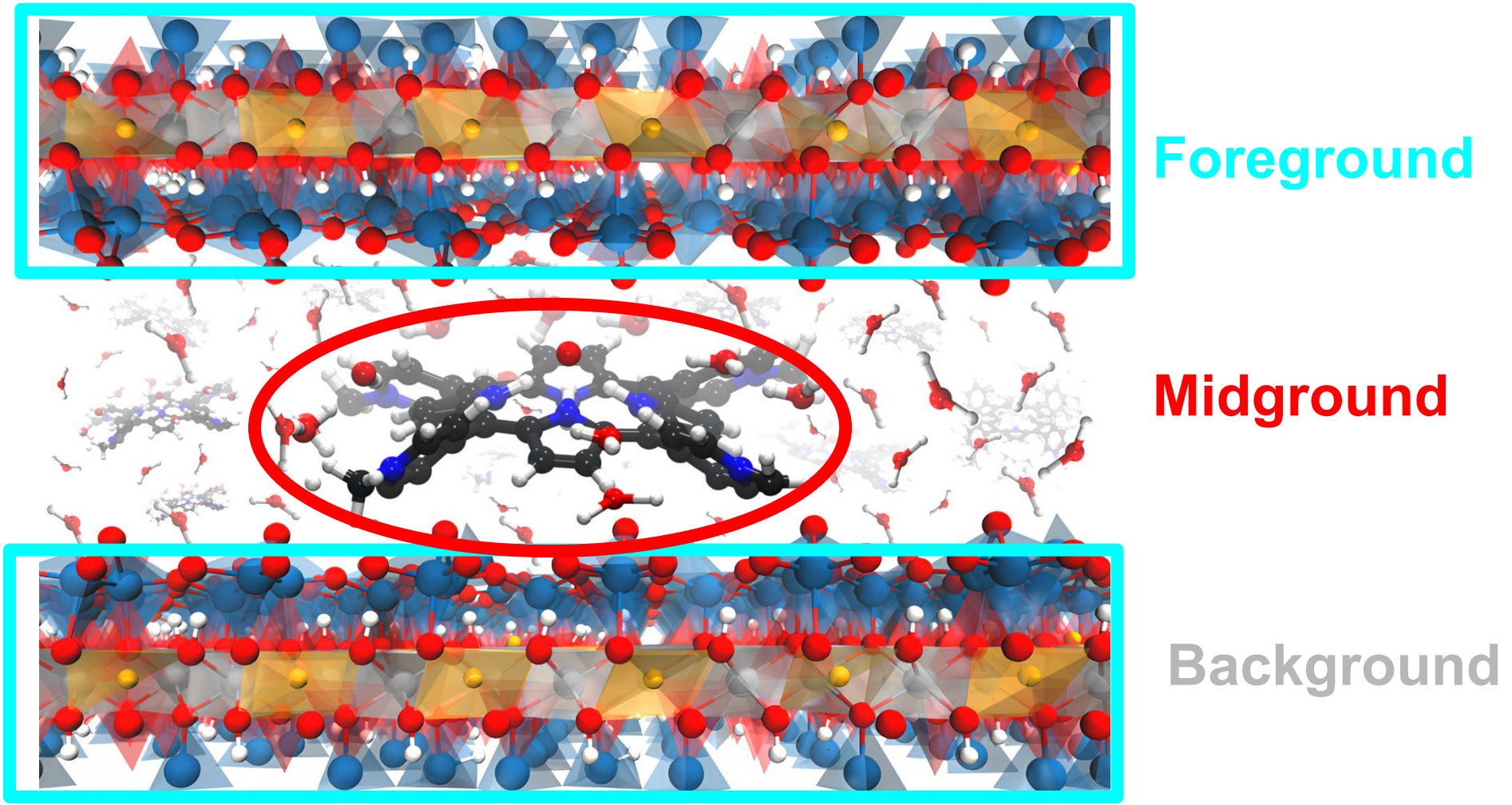
1. Composition (rule of thirds)



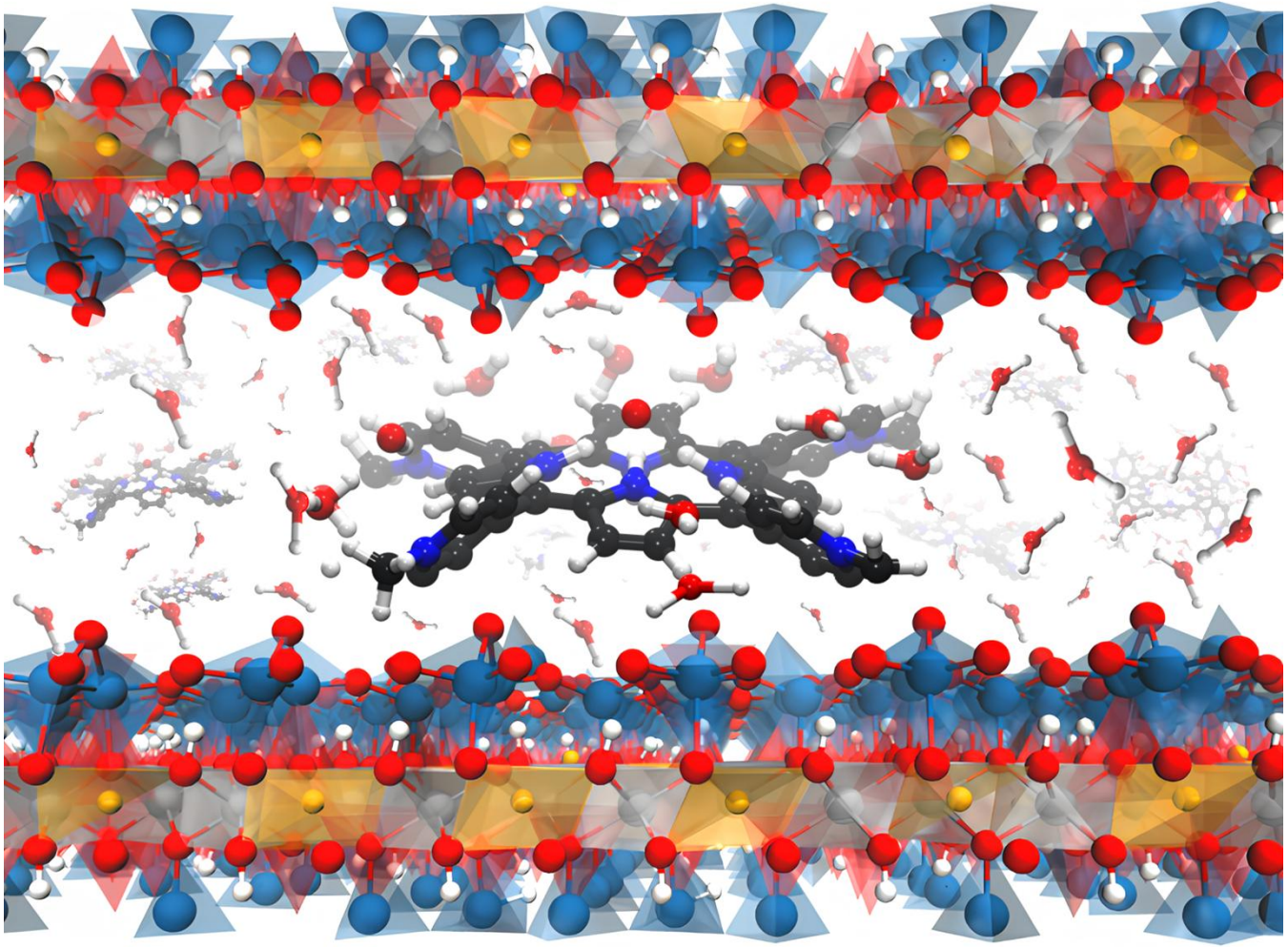
2. Focal point



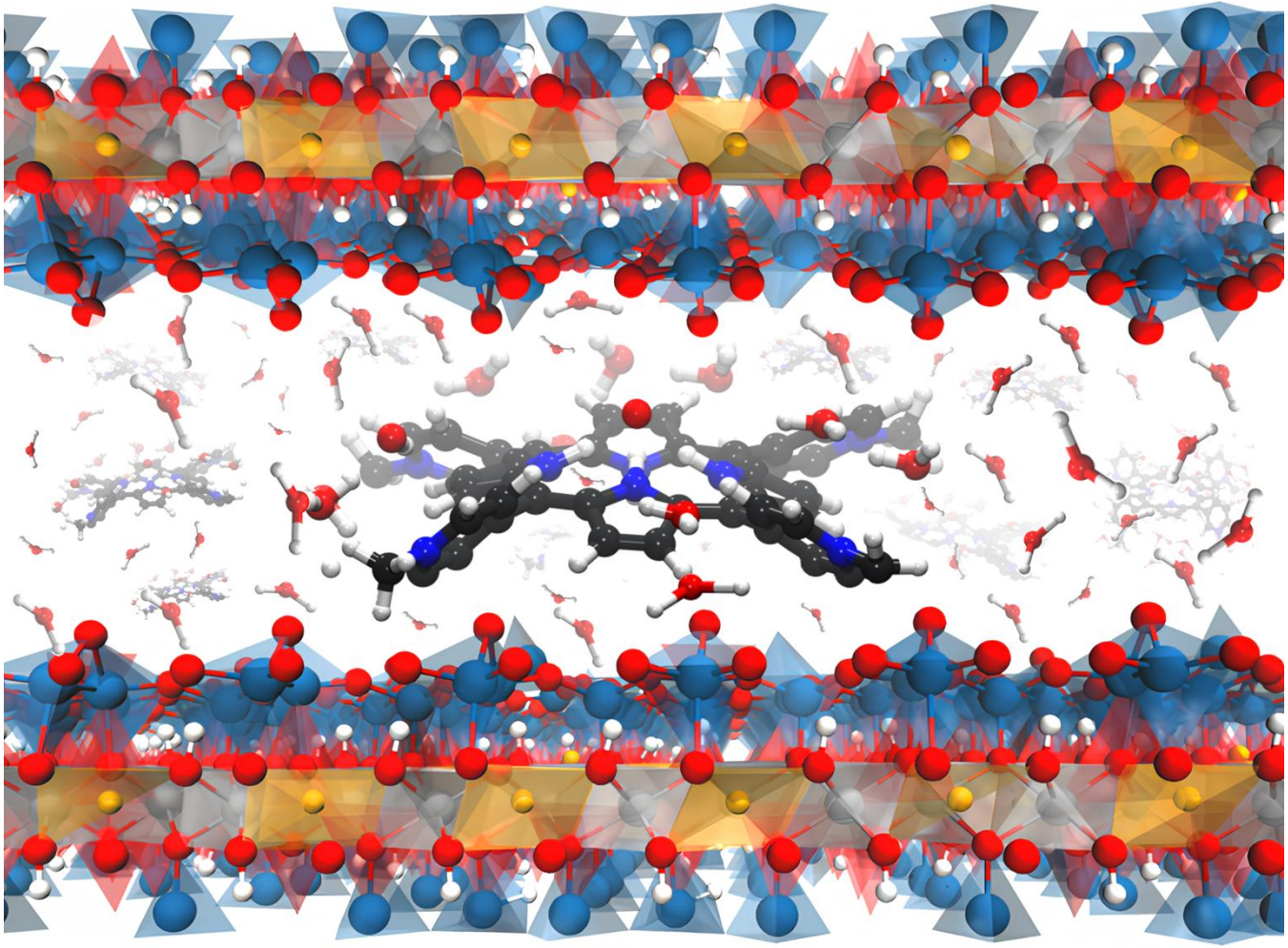
3. Depth (foreground / midground / background)


Foreground
Midground
Background

4. Light / Shadows

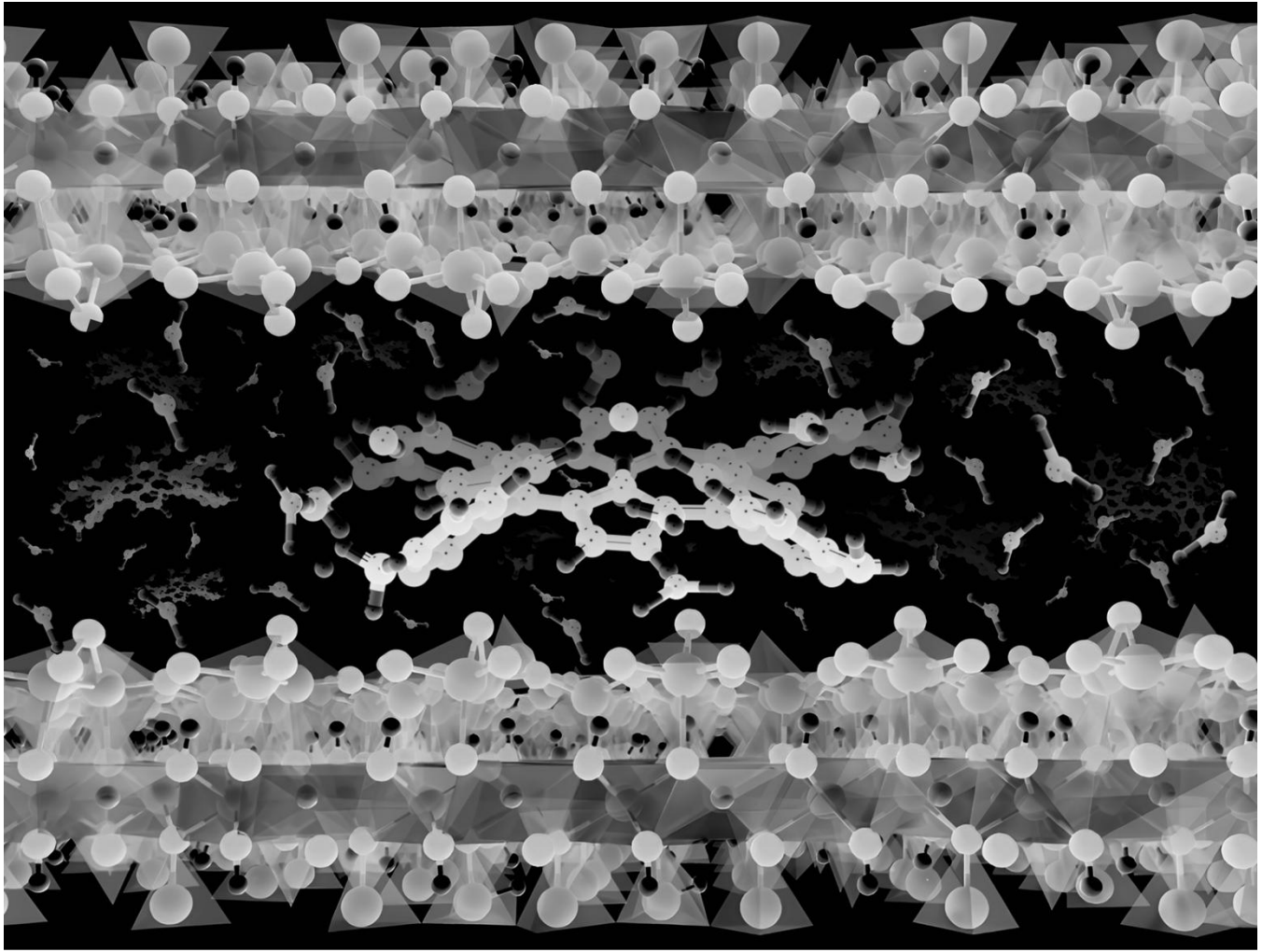


5. Contrast / Color

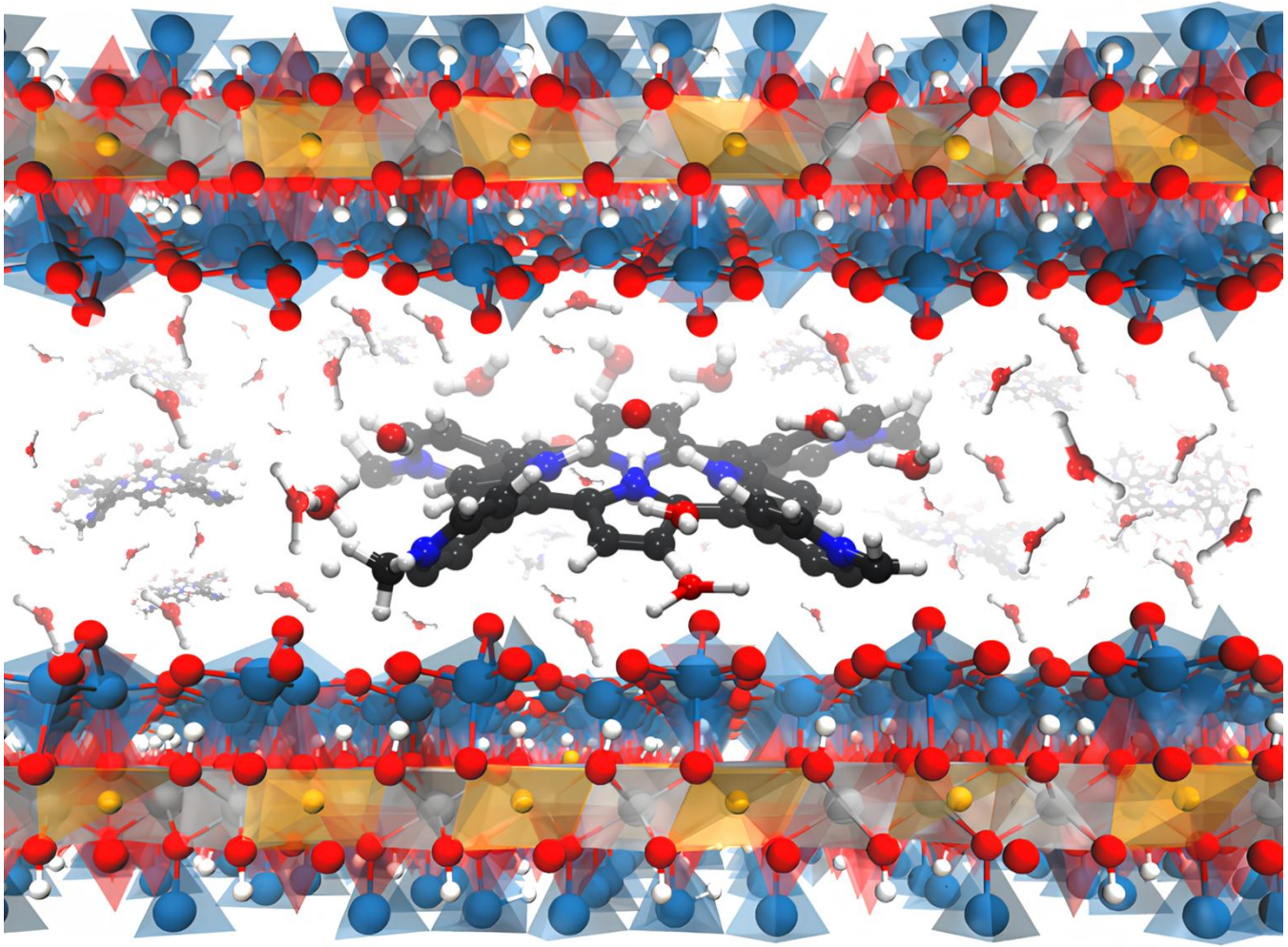



Reds
Oranges
Yellows
Yellows Greens
Greens
Blue Greens
Blues
Blue Violets
Violets
Mauves
Mauve Pinks
Pinks

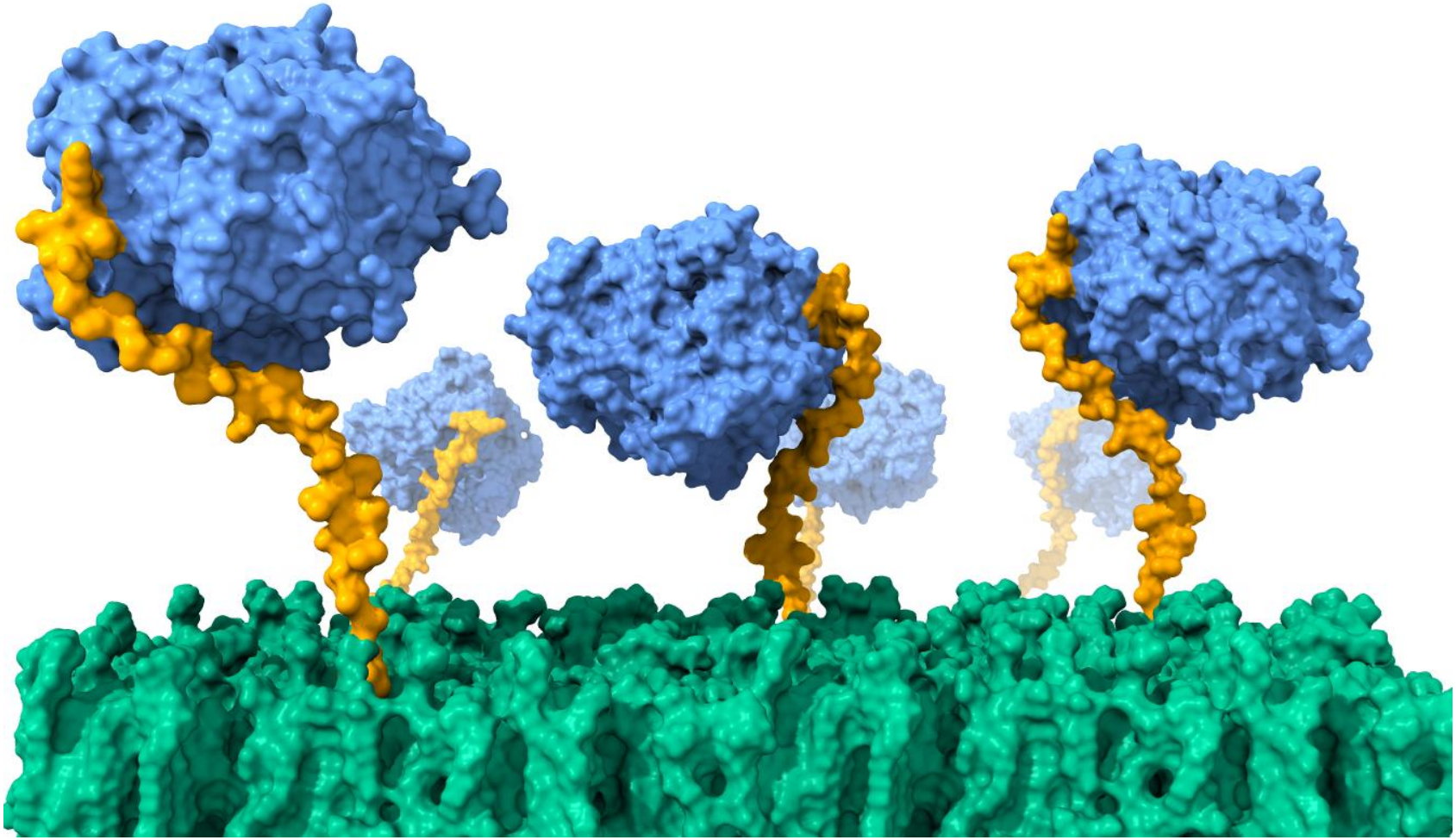
6. Negative space

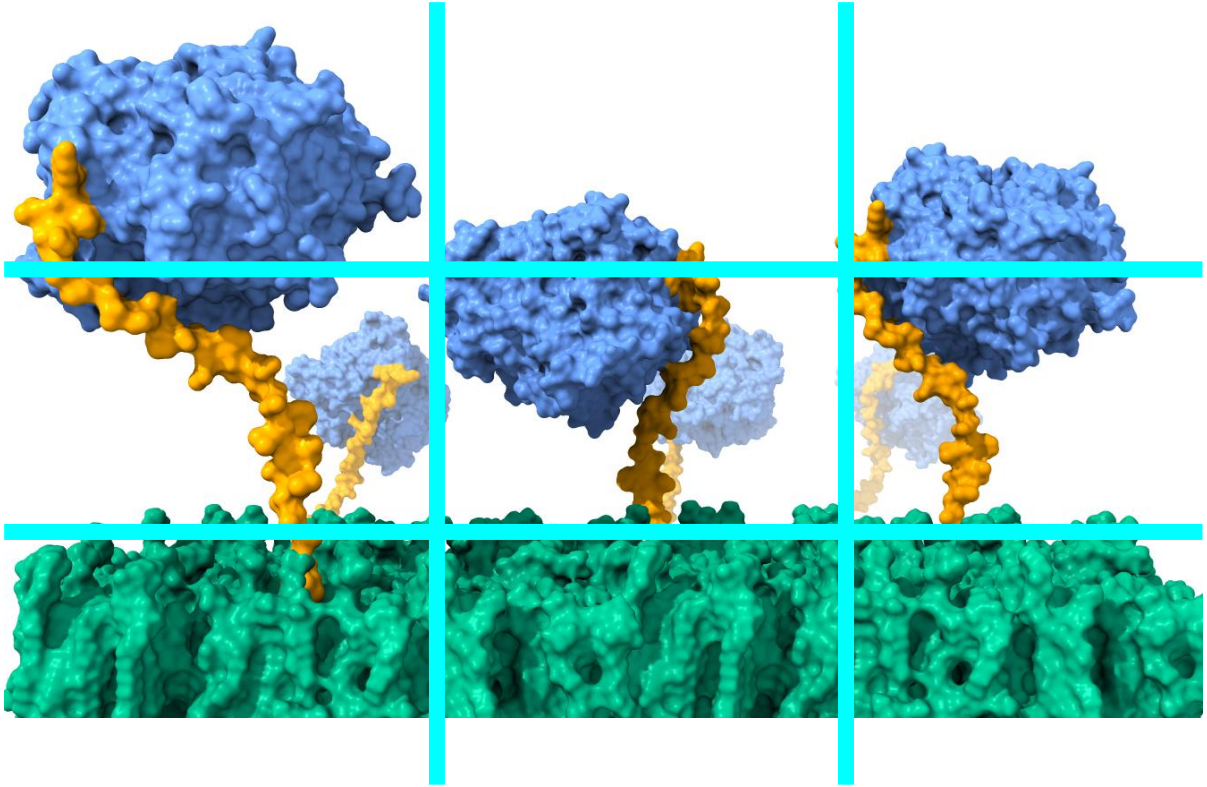


7. Storytelling

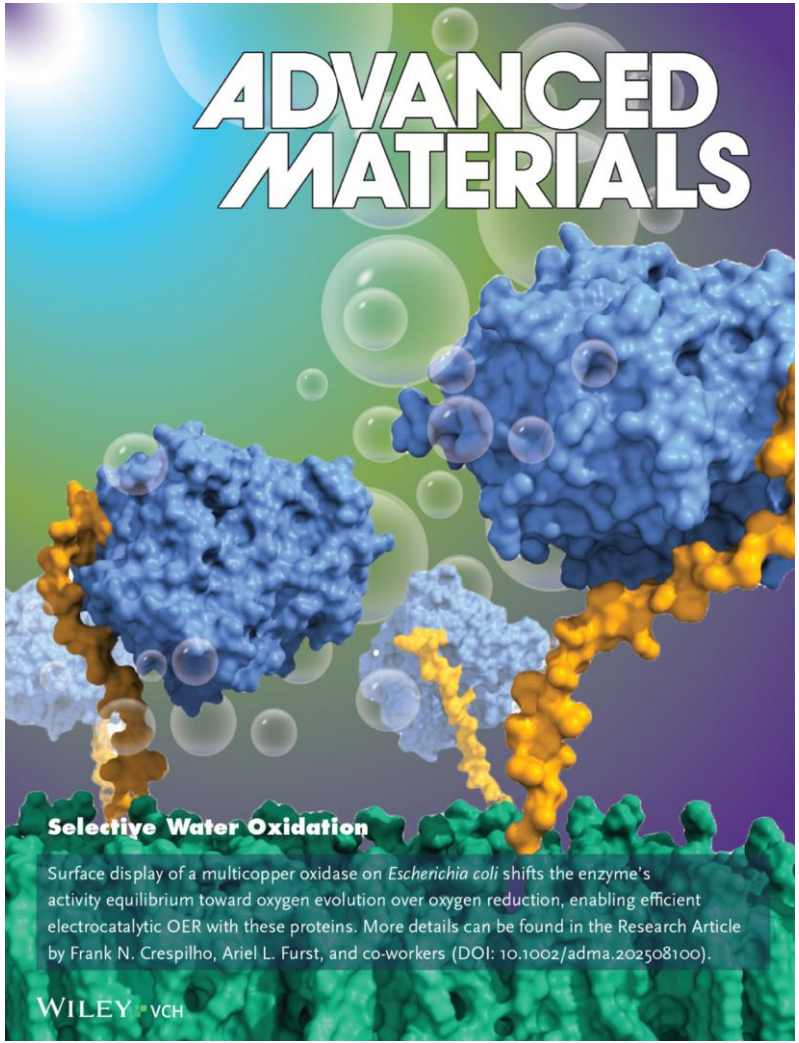


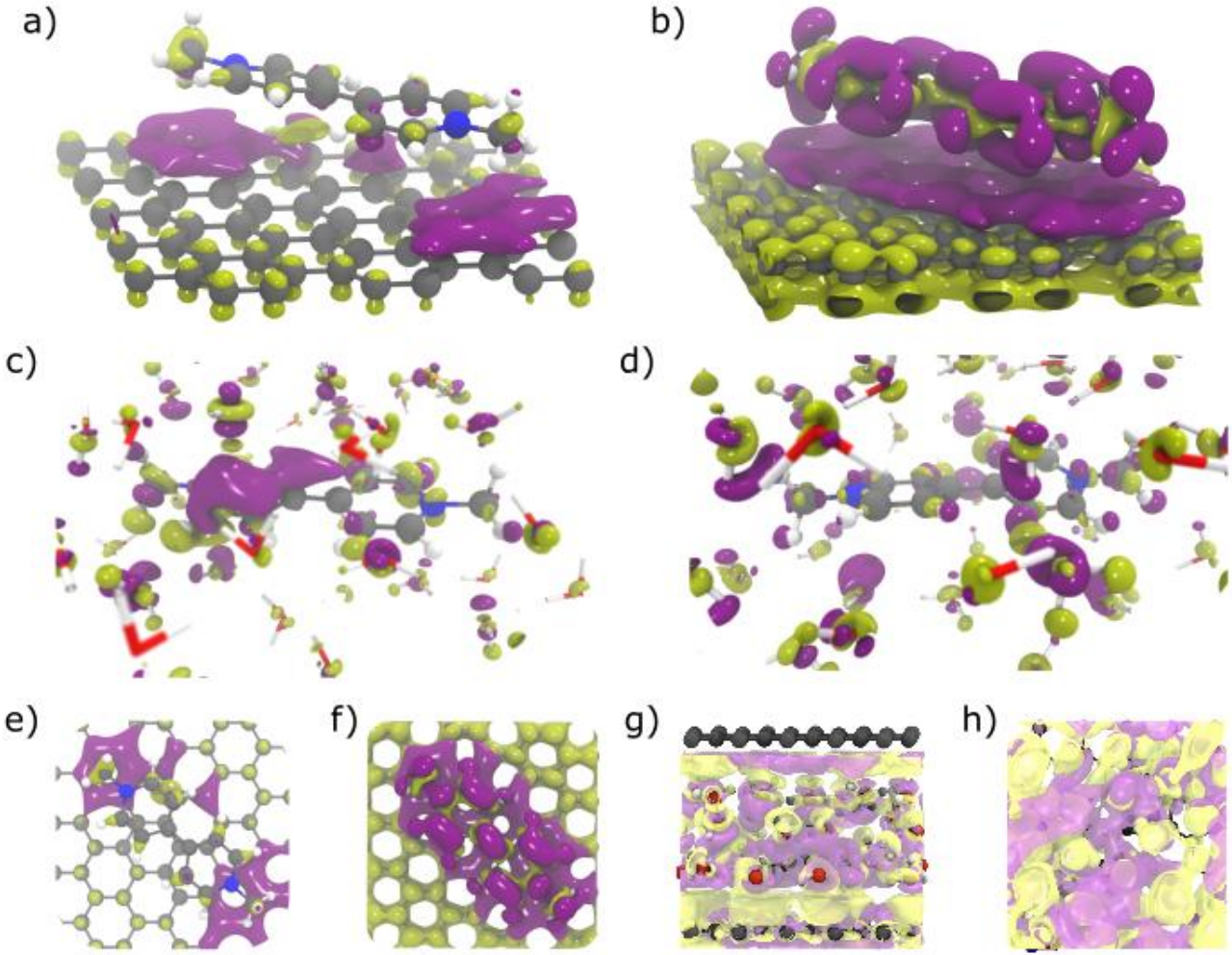
Another examples

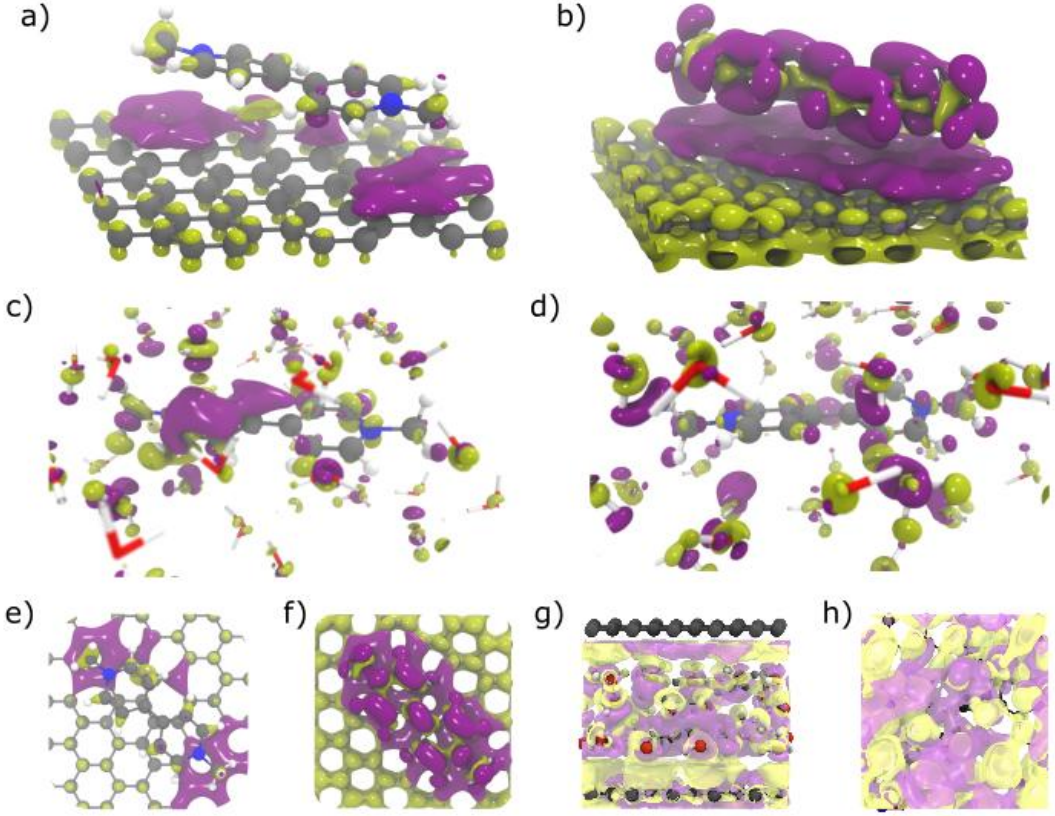


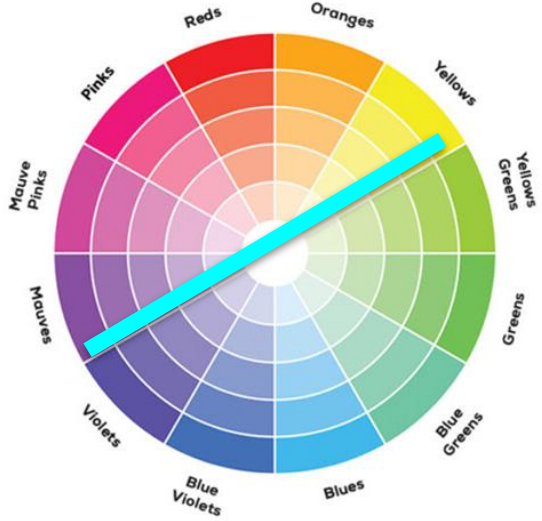


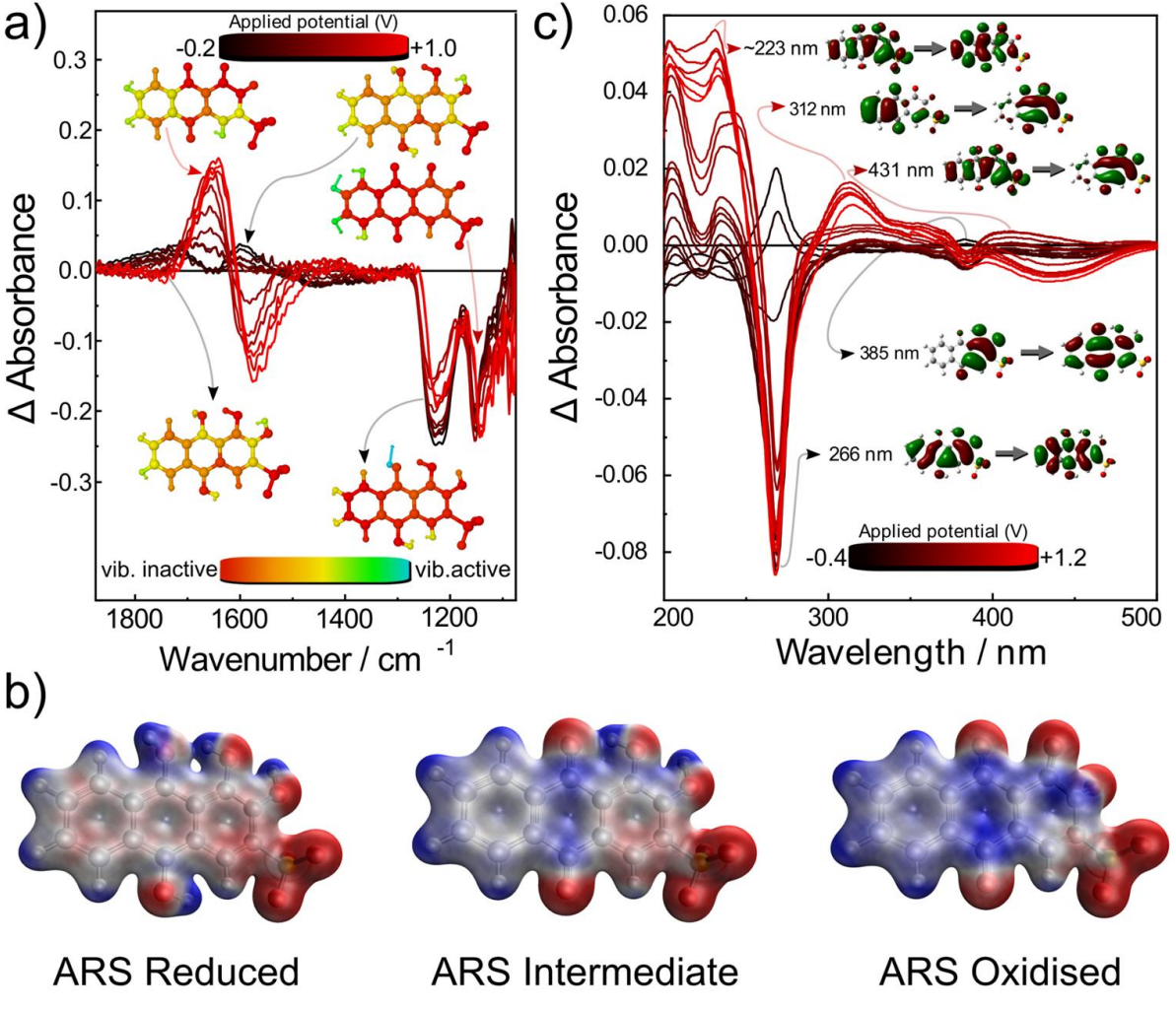

Reds
Oranges
Yellows
Yellows Greens
Greens
Blue Greens
Blues
Blue Violets
Violets
Mauves
Mauve Pinks
Pinks


ADVANCED MATERIALS
Selective Water Oxidation
Surface display of a multicopper oxidase on *Escherichia coli* shifts the enzyme's activity equilibrium toward oxygen evolution over oxygen reduction, enabling efficient electrocatalytic OER with these proteins. More details can be found in the Research Article by Frank N. Crespilho, Ariel L. Furst, and co-workers (DOI: 10.1002/adma.202508100).
WILEY VCH

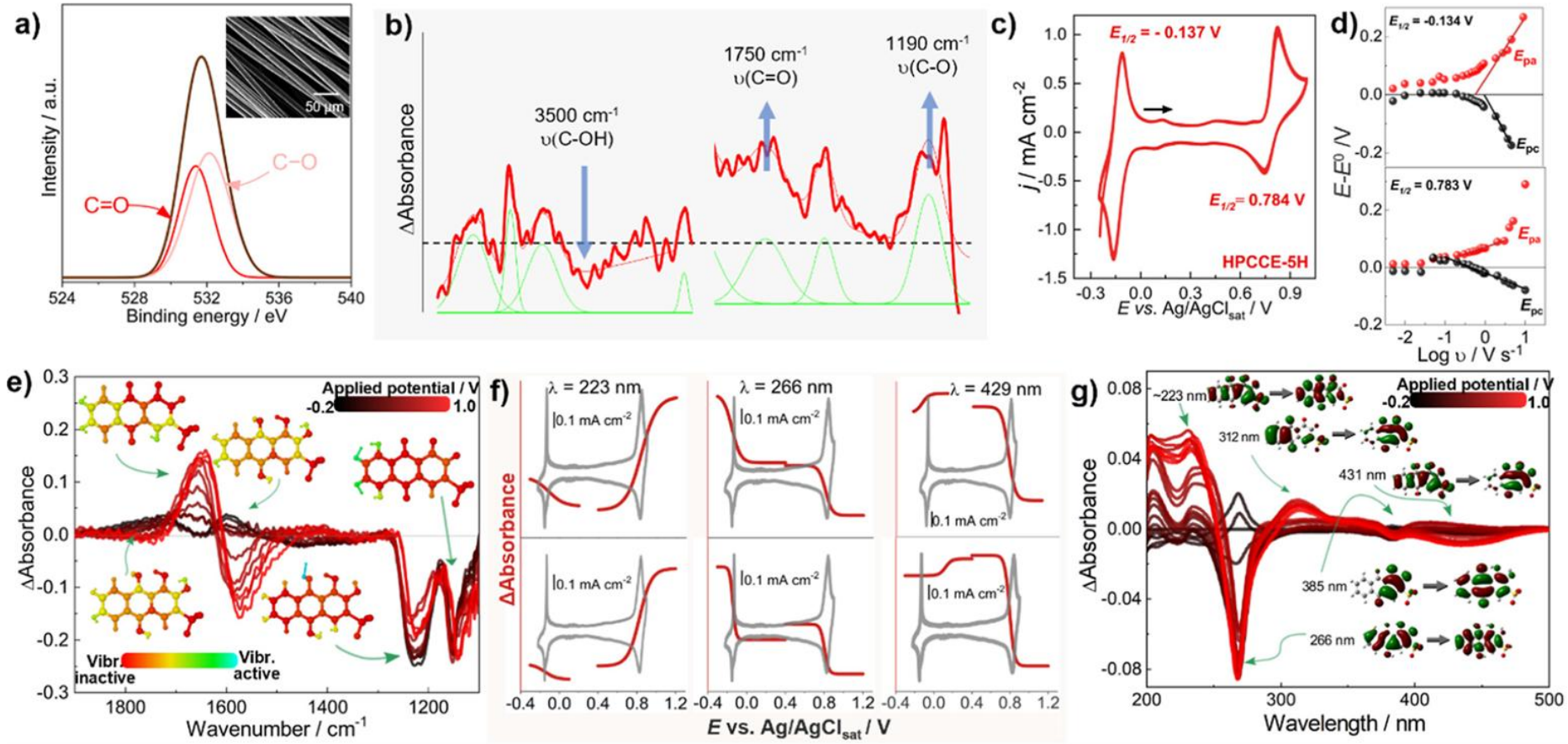

a)
b)
c)
d)
e)
f)
g)
h)


a)
b)
c)
d)
e)
f)
g)
h)

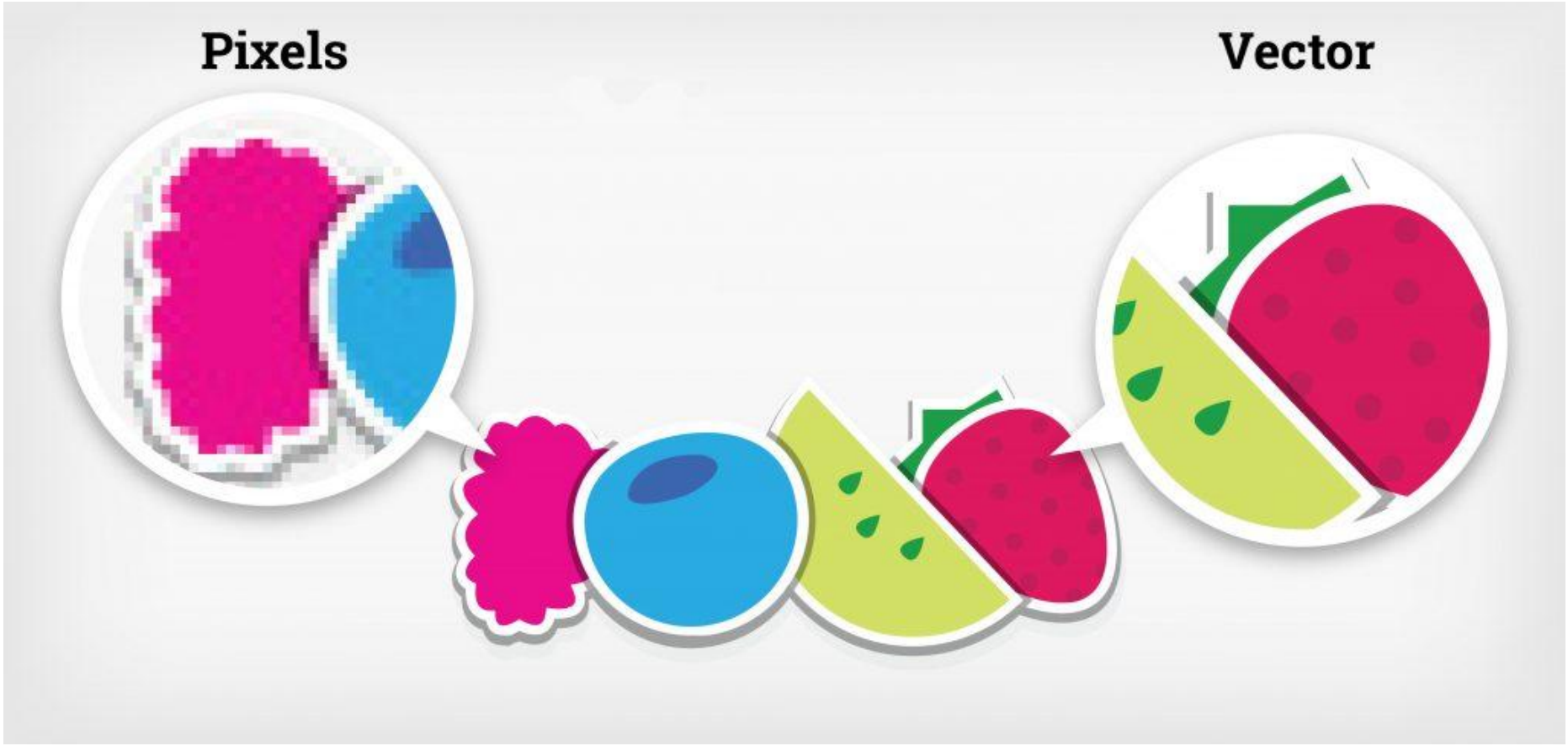

Reds
Oranges
Yellows
Yellows Greens
Greens
Blue Greens
Blues
Blue Violets
Violets
Mauves
Mauve Pinks
Pinks


a)
Applied potential (V)
-0.2
+1.0
vib. inactive
vib.active
Δ Absorbance
Wavenumber / cm -1
1800
1600
1400
1200
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
c)
~223 nm
312 nm
431 nm
385 nm
266 nm
Applied potential (V)
-0.4
+1.2
Δ Absorbance
Wavelength / nm
200
300
400
500
0.06
0.04
0.02
0.00
-0.02
-0.04
-0.06
-0.08
b)
ARS Reduced
ARS Intermediate
ARS Oxidised


Reds
Oranges
Yellows
Yellows Greens
Greens
Blue Greens
Blues
Blue Violets
Violets
Mauves
Mauve Pinks
Pinks


a)
Intensity / a.u.
C=O
C–O
50 µm
524
528
532
536
540
Binding energy / eV
b)
ΔAbsorbance
3500 cm-1
υ(C-OH)
1750 cm-1
υ(C=O)
1190 cm-1
υ(C-O)
c)
E1/2 = - 0.137 V
E1/2= 0.784 V
HPCCE-5H
j / mA cm-2
E vs. Ag/AgClsat / V
d)
E1/2 = -0.134 V
Epa
Epc
E1/2 = 0.783 V
E-E0 /V
Log υ / V s-1
e)
Applied potential / V
-0.2
1.0
ΔAbsorbance
Vibr. inactive
Vibr. active
Wavenumber / cm-1
f)
λ = 223 nm
λ = 266 nm
λ = 429 nm
0.1 mA cm-2
ΔAbsorbance
E vs. Ag/AgClsat / V
g)
Applied potential / V
-0.2
1.0
~223 nm
312 nm
431 nm
385 nm
266 nm
ΔAbsorbance
Wavelength / nm

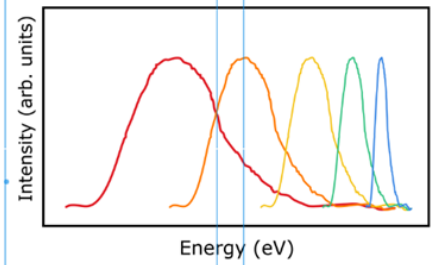
Pixels vs Vectors

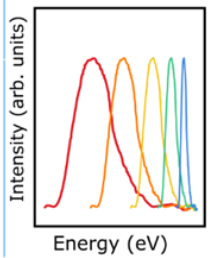

Pixels
Vector

*Novo documento 1 - Inkscape

Arquivo Editar Visualizar Camada Objeto Caminho Texto Filtros Extensões Ajuda

X: 178,743 Y: 65,169 L: 159,968 A: 97,912 mm





Preenchimento: N/D
Contorno: N/D
O: 100
Camada 1
Nenhum objeto selecionado. **Clique**, **Shift+Clique**, **Alt+Rolar** o mouse sobre os objetos ou **arraste** em volta dos objetos para selecioná-los.
X: -125,10
Y: 107,87
Z: 54%
R: 0,00°

How about GIMP?

How about canva or any other software?

Warning!

Molecules / slabs / crystals are only **pixels images**

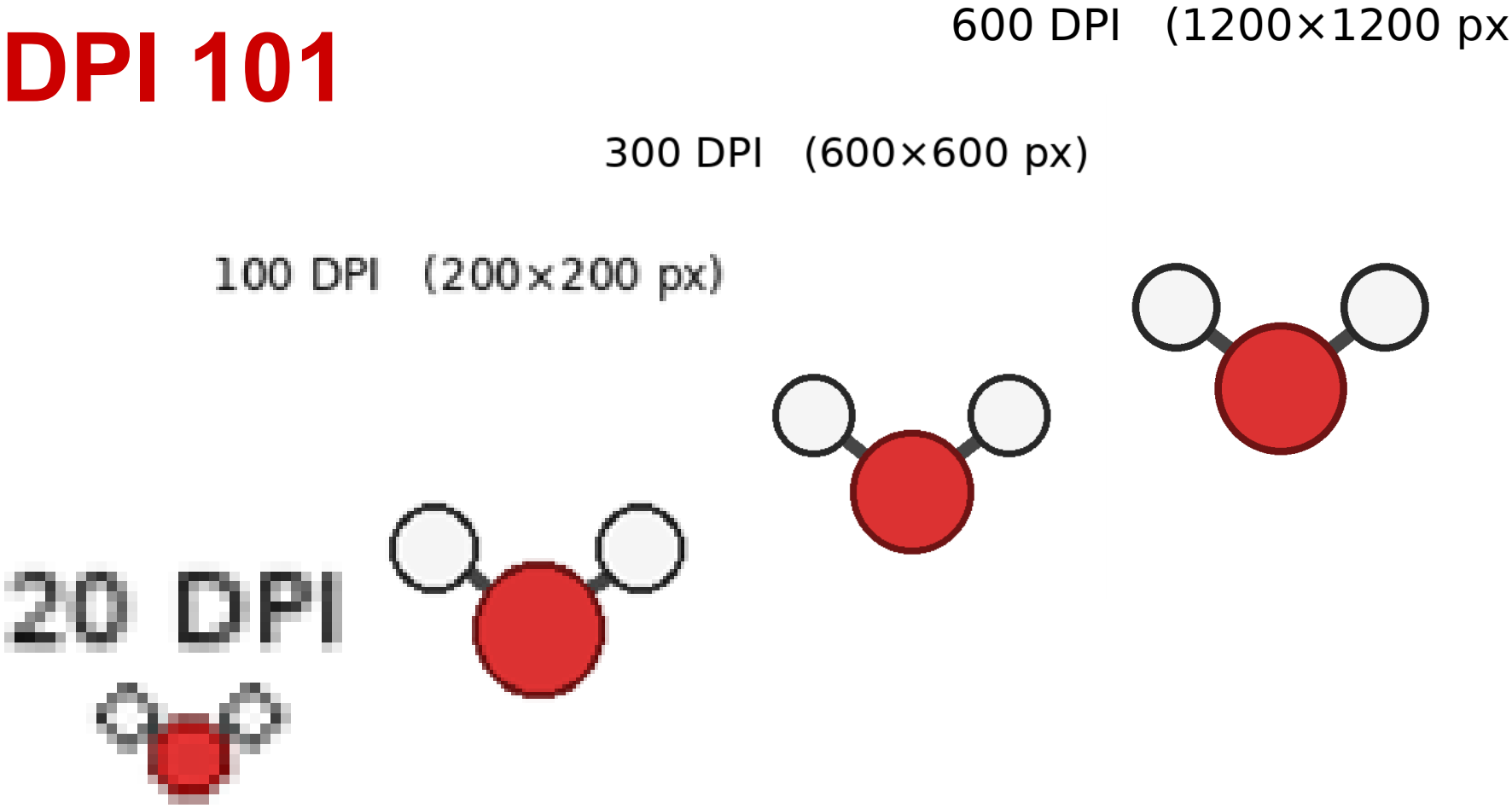
Export with:

high resolution (bigger than ~ 1000 x 1000 px)

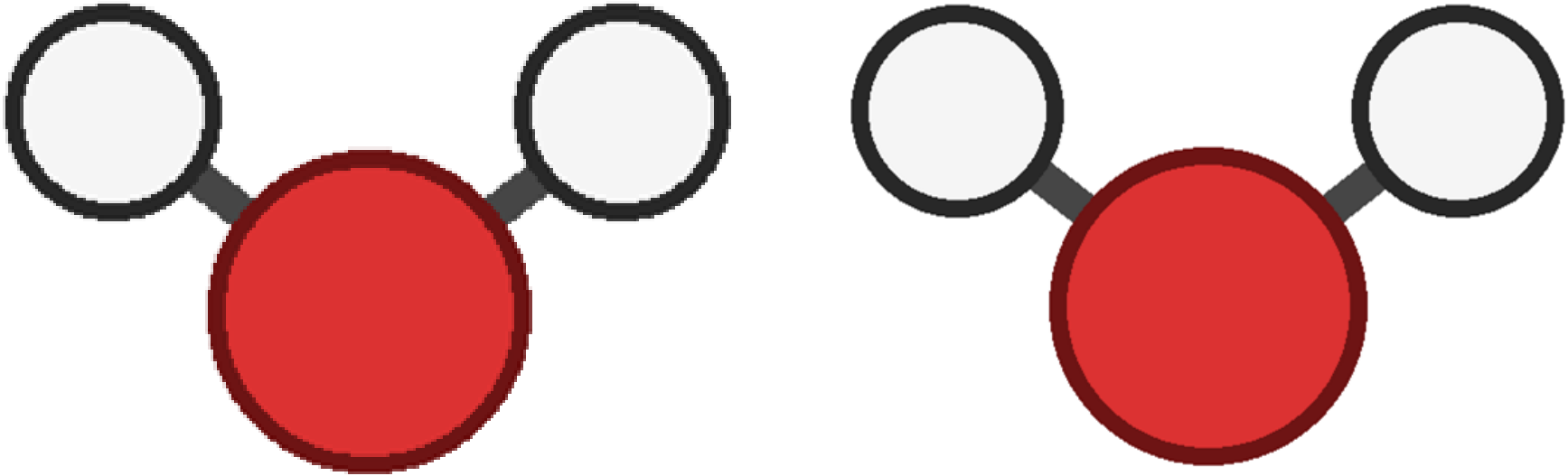
high DPI (pixel density per inch)

Transparent background if available.

DPI 101



DPI 101



My workflow

Which software should I use to draw my systems?

Softwares that I use for molecules/systems:

~~xcrysden, ASE-GUI, Avogadro, Biovia Discovery Visualizer~~

Jmol + povray

VMD + optix/geforce

ChimeraX

Pymol + povray

iboview (only windows)

Doesn’t matter the software I use for graphs

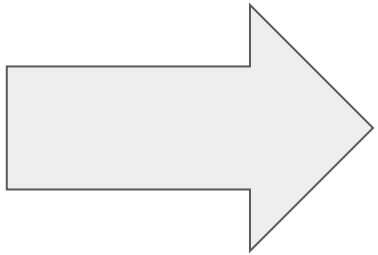
Python (matplotlib)

Xmgrace

Origin

Qtiplot

Gnuplot



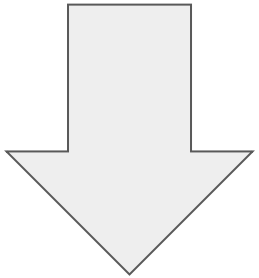
Export as:

.svg

.pdf

.eps

.ps



Fine tune your figure using **inkscape**.

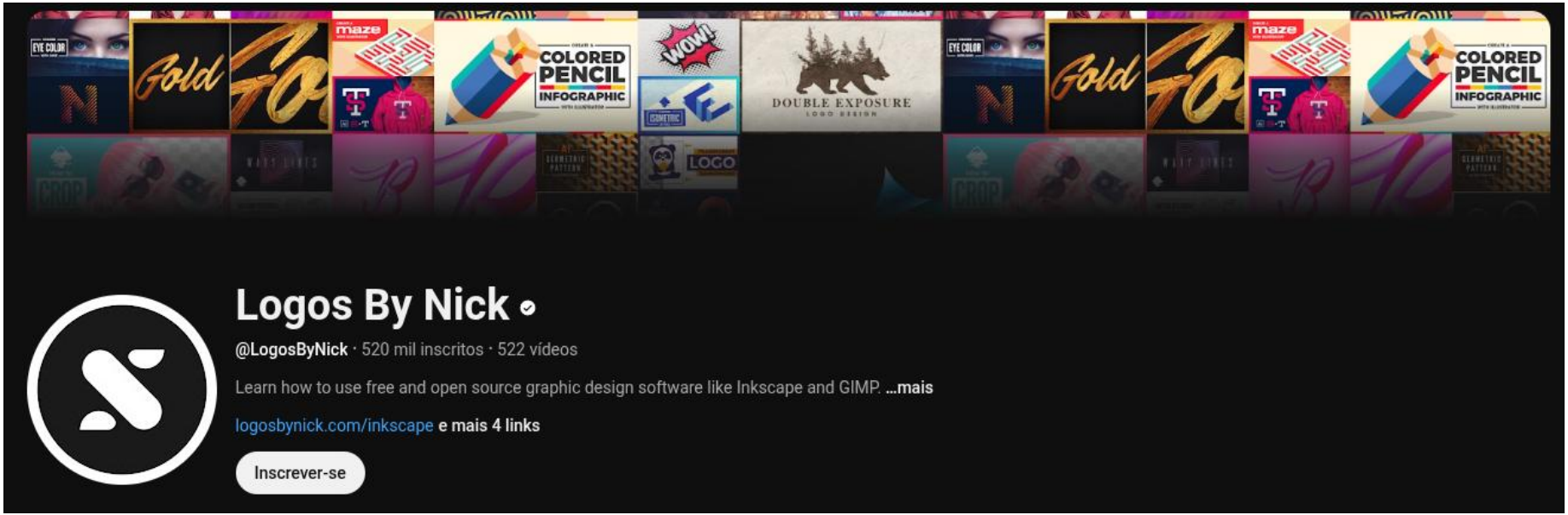
Softwares/services that I use

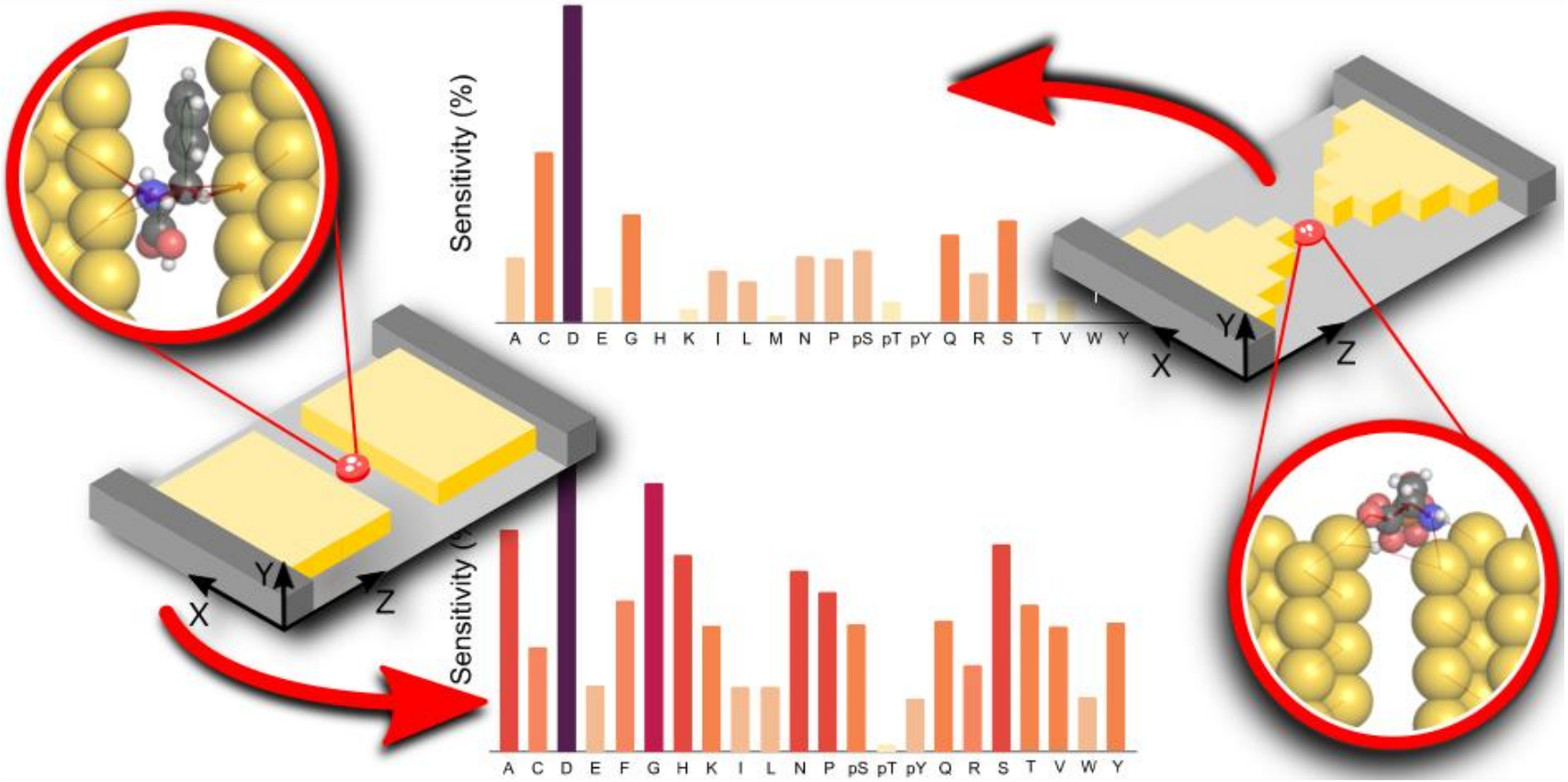
One last thing…

How can I improve?

Studying inkscape

https://www.youtube.com/c/logosbynick




Sensitivity (%)
A C D E G H K I L M N P pS pT pY Q R S T V W Y
Y
X
Z
Sensitivity (%)
A C D E F G H K I L N P pS pT pY Q R S T V W Y
Y
X
Z

Studying photos


RESTAURANT
BEER WINE
P
100円
150円

Asking AI


ENJOY

Thank you!

fdlima@ifsp.edu.br