

August 2025

#### STARTING TIPS: MAKING FIGURES AND IMAGES

Wang Materials Group Meeting Tutorials

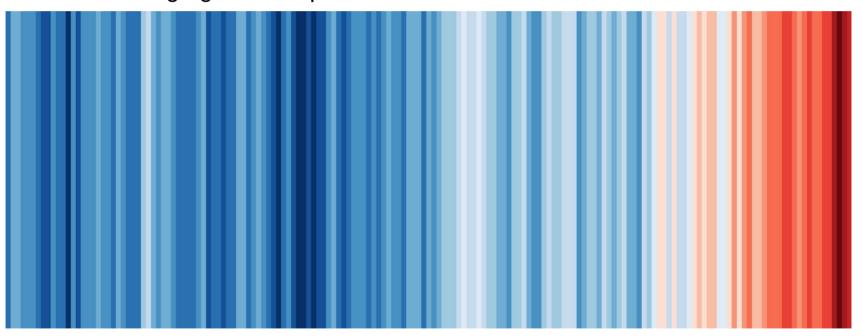
Wennie Wang
Wang Materials Group (https://wangmaterialsgroup.com)
The University of Texas at Austin, McKetta Department of Chemical Engineering

### Why bother making a nice figure?

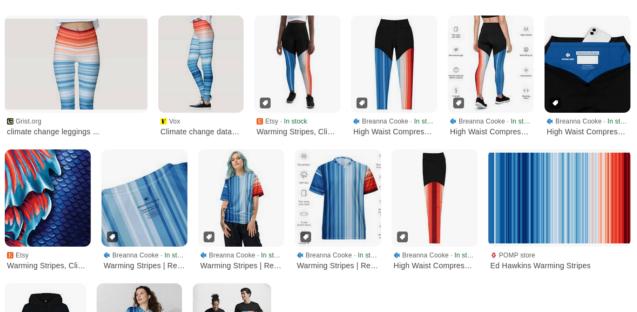
- •A figure is worth a thousand words
- •It is often the first impression you make to the reader
- •It is sometimes the only thing a reader looks at
- •Visual communication is just as powerful a form of communication as written!

#### Good design is memorable

Example: Warming stripes, Ed Hawkins Annual average global temperature 1850-2010



# Good design is memorable





POMP store
Ed Hawkins Warmi...



◆ Breanna Cooke · In st...

Warming Stripes | R...



Redbubble
 Australia climate a...

#### Figures are a form of visual design

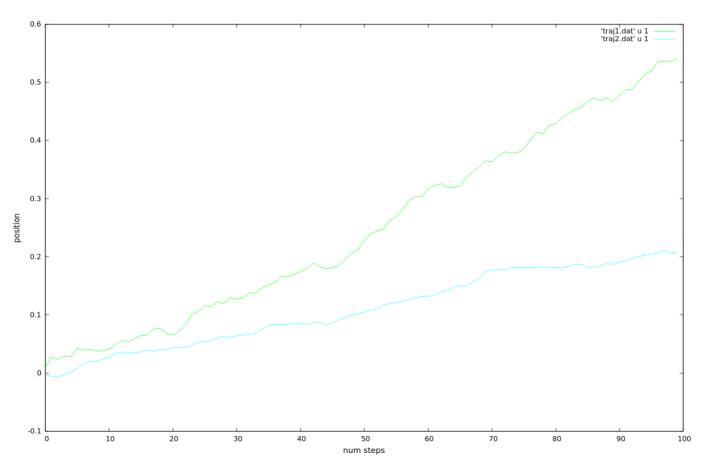
- Design with intent
- Do not just directly copy a figure in a paper into a presentation
- The visual design will not always translate
  - adjust the relative scale of axes labels, tick marks, etc.
  - break down a complex figure

#### Always take the time to typeset

- LaTeX is your friend (klatex for generating image equations)
- The hyphen (-), the minus (-), the en dash (-, denote range), the em dash (-, separate parts of sentence)
- Times (x, not 'x')
- Subscript, Superscript (cm-1 v cm-1)
- Element names are not italicized (CuO<sub>2</sub>, not CuO<sub>2</sub>)
- Variables are italicized (or in math mode)
- Approximately (≈, not ~)
- Space between value and units (2.0 eV, not 2.0eV);
   if there is a newline, keep the value and units together
- Much greater than ( $\gg$ , not >>)
- Bra-ket notation ( $\langle \rangle$ , not  $\langle \rangle$ )

Generated with gnuplot, a command-line graphic utility

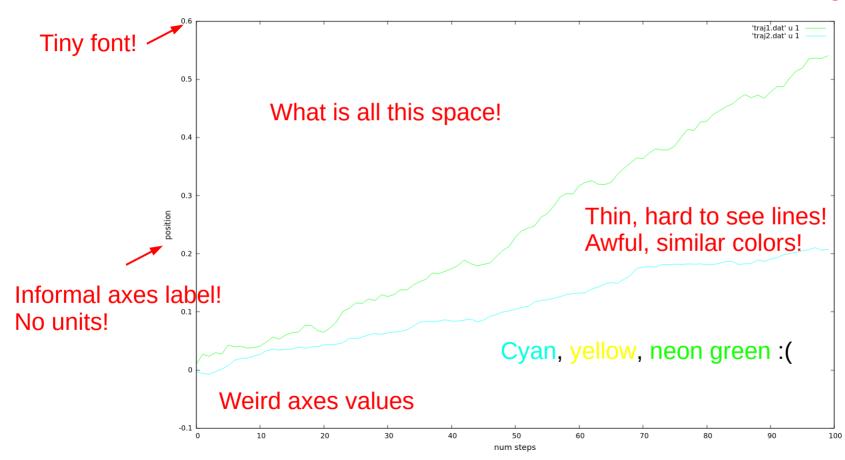
## A bad figure



Ok for quick visualization Not ok for paper figure

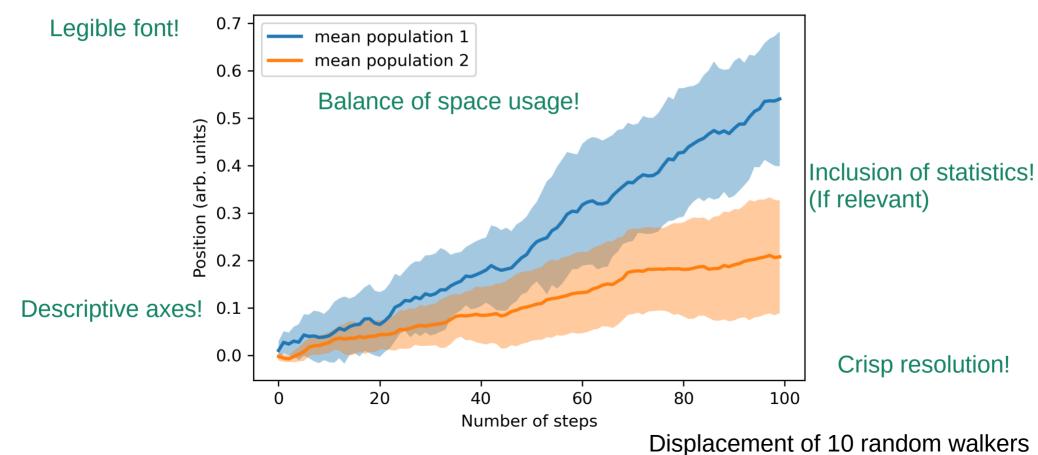
#### A bad figure

Meaningless key!



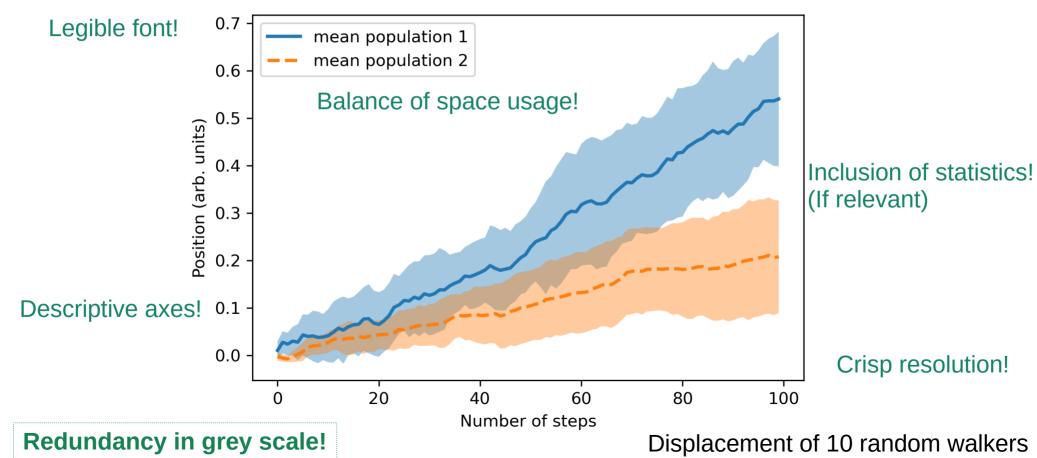
#### A better figure

Clear lines with contrasting, complementary colors!



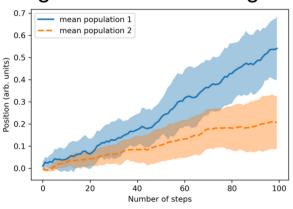
#### A better figure

Clear lines with contrasting, complementary colors!



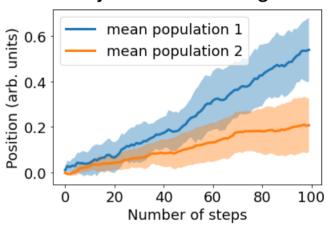
#### Make it scalable

#### Original scaled down figure



versus

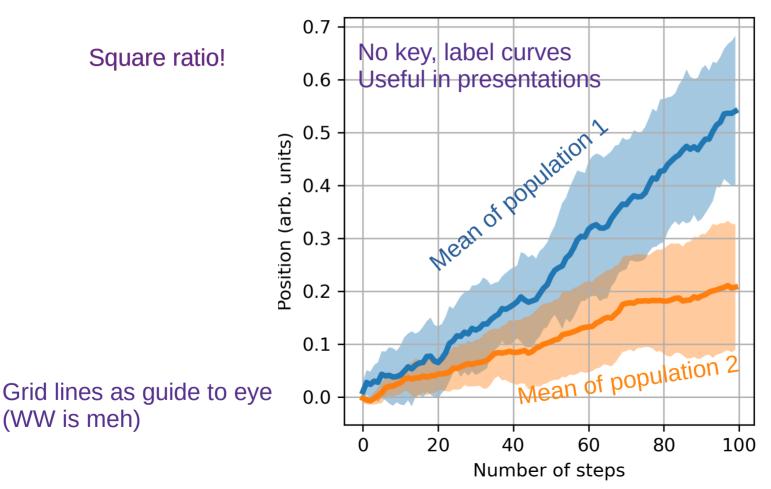
#### Re-adjusted scaled figure



The font size is scaled to match the scaling of the figure

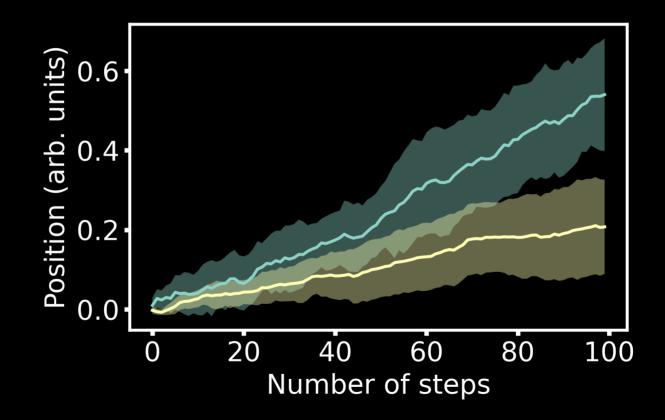
You can save space without compromising on the readability of the figure!

### Some things of personal choice



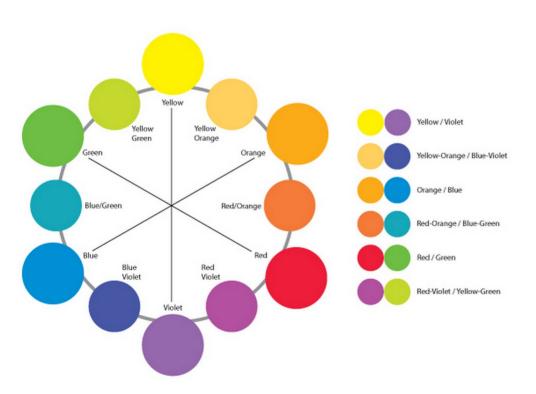
### Dark Background?

It can work, but you need to be careful of visibility

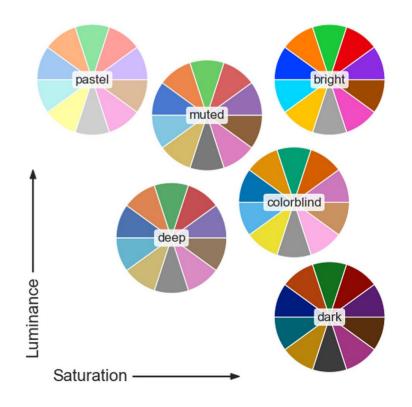


### Color is important

#### Complementary colors



#### seaborn color palettes



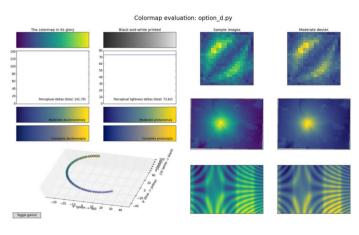
#### Color Maps

Avoid default jet (rainbow) setting... not great



https://youtu.be/xAoljeRJ3IU

Viridis, Parula are better!



https://bids.github.io/colormap/

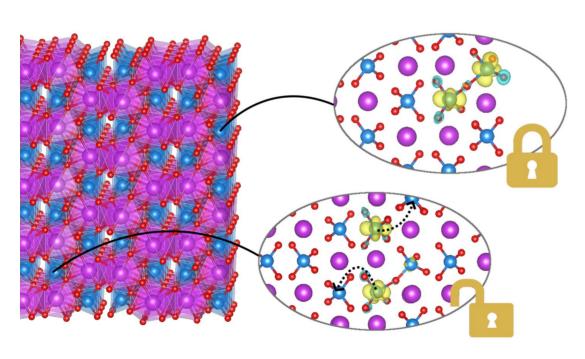
Perceptually uniform, Translates well to greyscale, Better for the colorblind,...

### Example Tools (open source!)

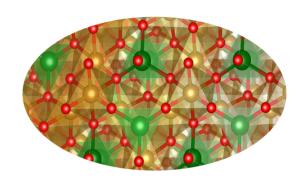
- GIMP (bitmap images)
- Inkscape (vector image)
- Xmgrace, gnuplot (plotting from terminal or script)
- Python, matplotlib, seaborn
- VESTA, Xcrysden, ASE (visualize structure); Ovito (animations)
- Blender (3D rendering and animation)
- TikZ, Asymptote (vector graphics for textbook-like schematics, scriptable)
- · ...many, many more

R. Schmied. Using Mathematica for Quantum Mechanics: A Student's Manual. https://arxiv.org/pdf/1403.7050.pdf

### Crystal structures



**VESTA + GIMP** 



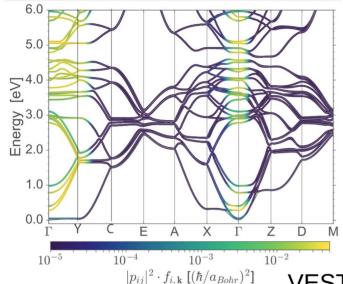


w/ VESTA (plus some tuning)

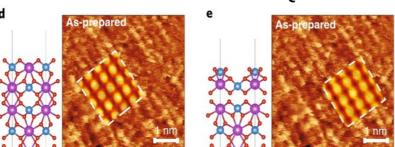
#### Python matplotlib

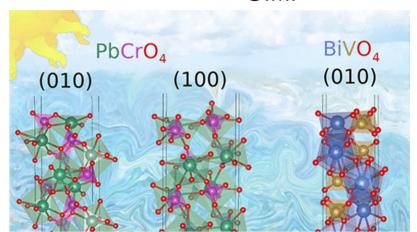
#### Example Figures

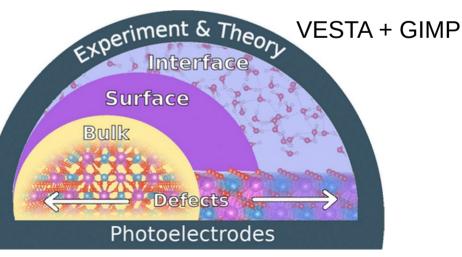
VESTA + Pixabay + GIMP



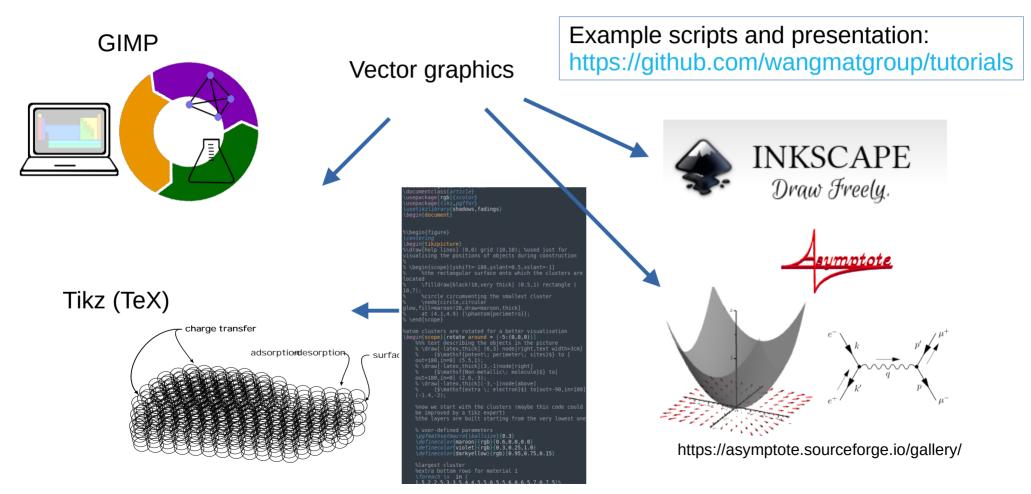
VESTA + GIMP + Quantum Espresso



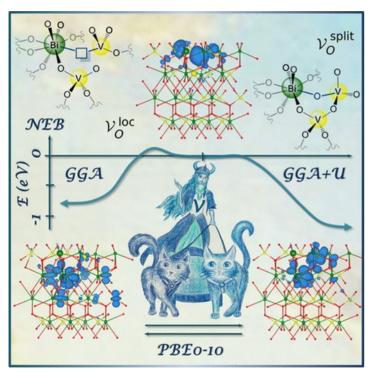




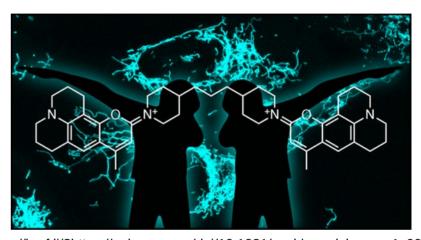
### **Example Figures**



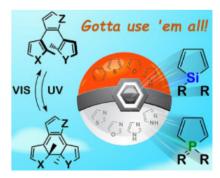
#### TOC graphics



https://pubs.acs.org/doi/10.1021/acs.jpclett.9b02552



https://href.li/?https://pubs.acs.org/doi/10.1021/acsbiomedchemau.1c00068

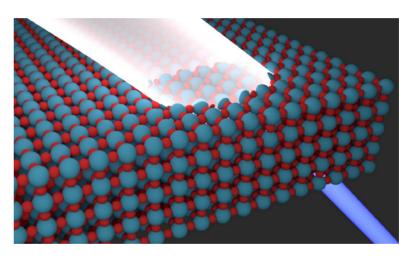


https://href.li/?https://www.sciencedirect.com/science/article/pii/S0022328X21004721?dgcid=rss\_sd\_all

## Fancier figures

3<sup>rd</sup> party+ GIMP





VESTA structure file + Blender

#### Random tips

- Save in the native file format of the editing program
- Use layers to your advantage
- Save intermediate files- there will be many times you need to slightly modify a figure
- Save a final high-resolution version that can be converted to other file formats
- Ask for feedback on your plots

#### Other resources on visual design

- Jean-Luc Doumont, Felice Frankel
- MRS Science as art
- Ram Seshadri's Preparing Figures

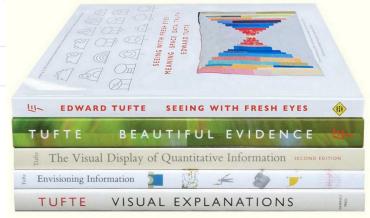
Fundamentals of graphic design—essential tools for effective visual science communication

Authors: Karen J. Murchie 

and Dylan Diomede | AUTHORS INFO & AFFILIATIONS

Publication:FACETS · 11 June 2020 · https://doi.org/10.1139/facets-2018-0049

**OPEN ACCESS** | Science Applications Forum



#### This presentation & related scripts are @

https://github.com/wangmatgroup/tutorials/tree/main/Figure-making