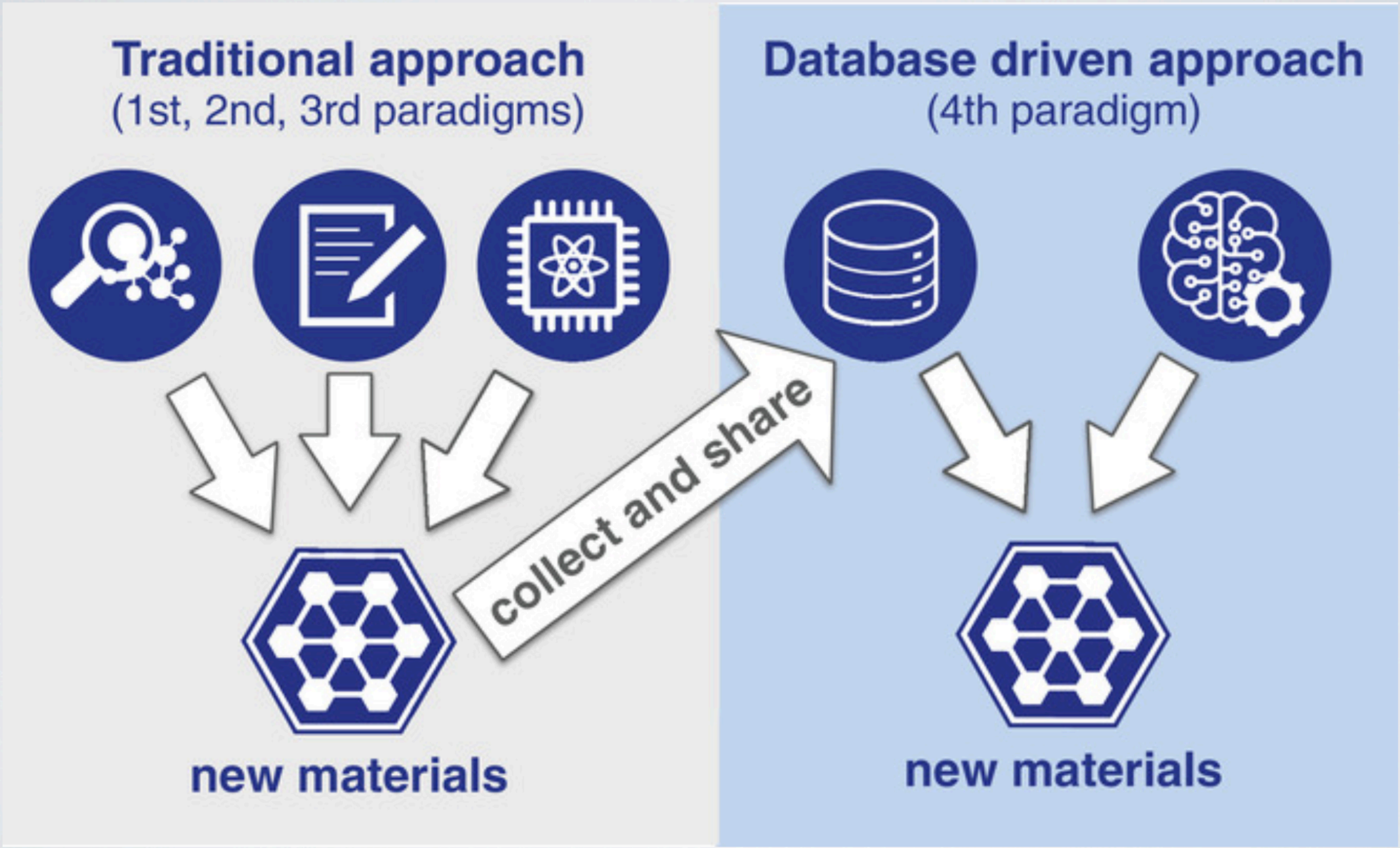
Data-driven design as 4th paradigm



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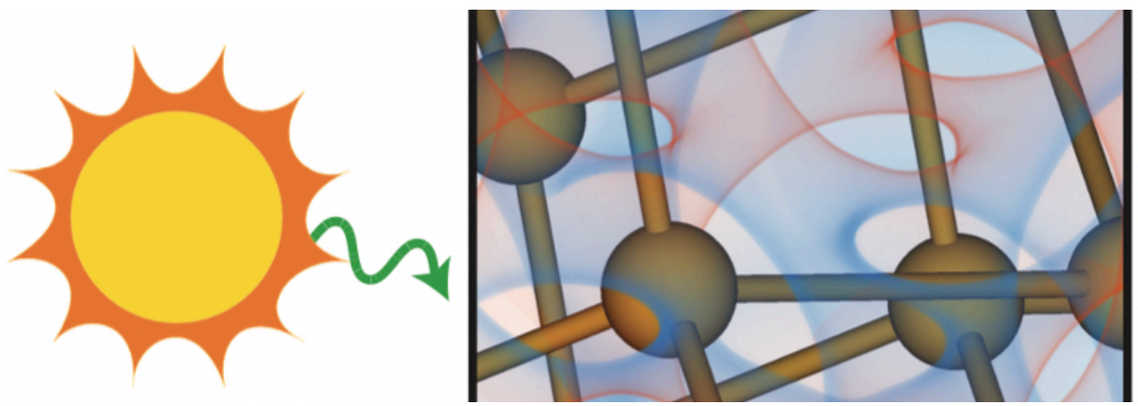
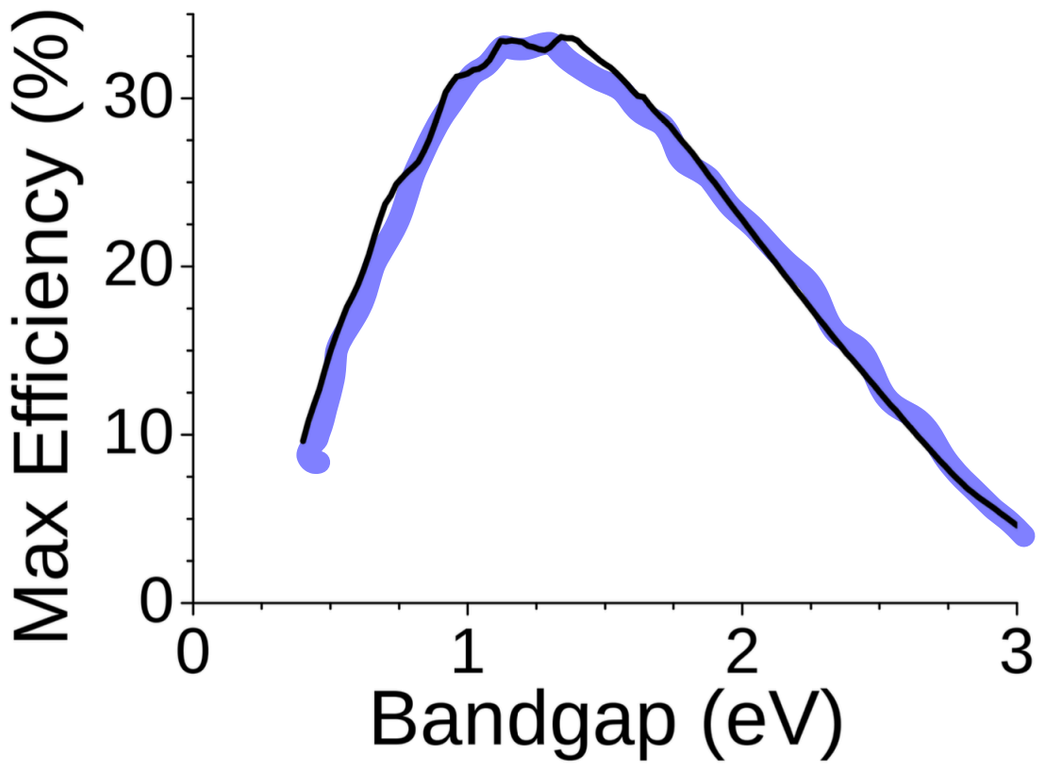
Solar Cells



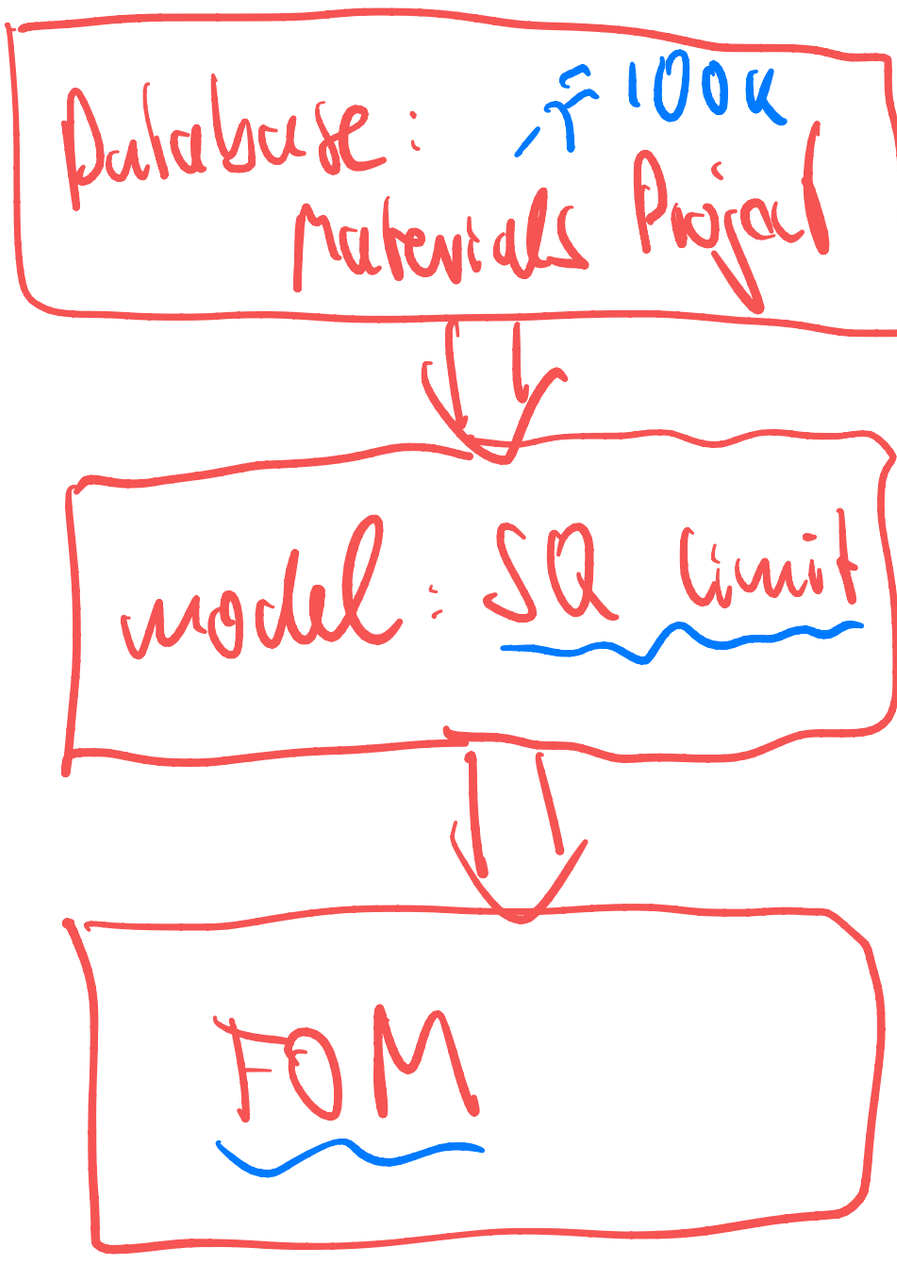
- Light is absorbed by a material, creating energetic charge carriers
- These move through a circuit, which corresponds to electricity

Solar Cells

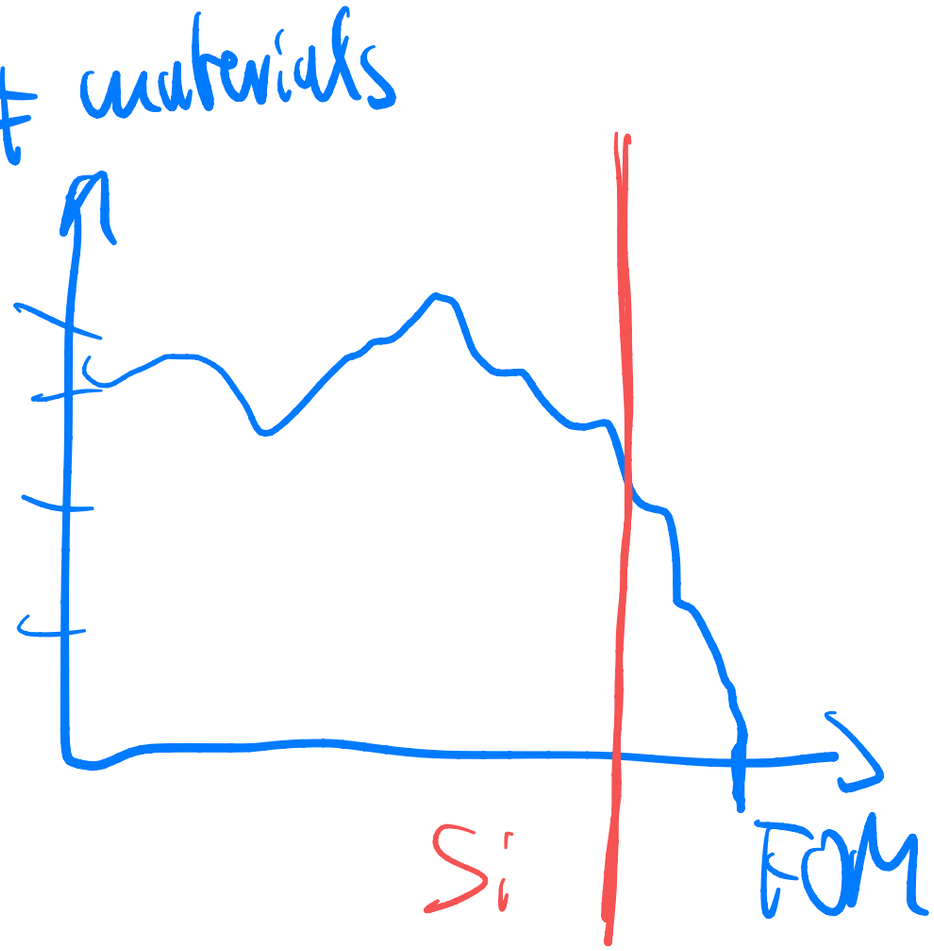


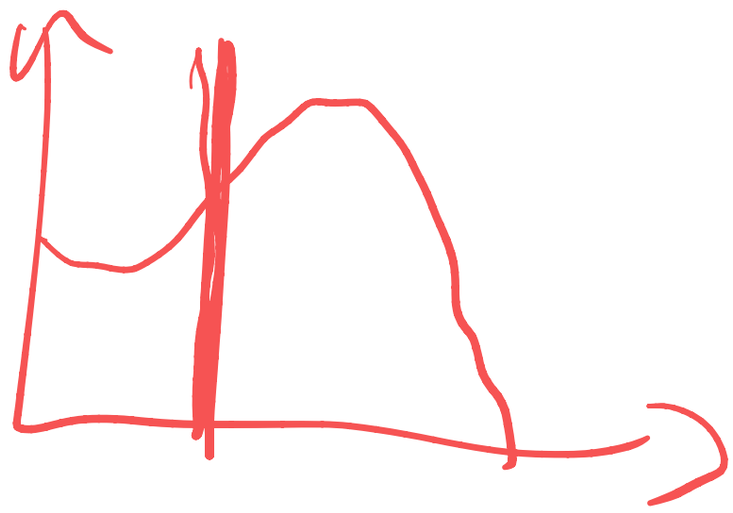
- Shockley-Queisser limit
- Theoretical maximum from detailed balance

Materials and Data

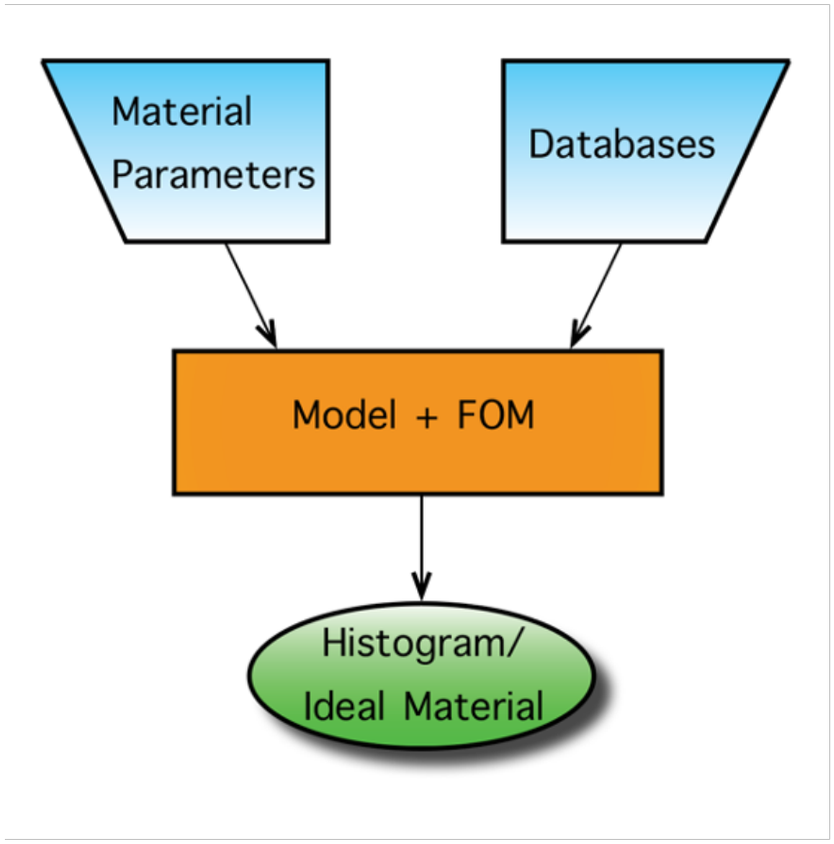


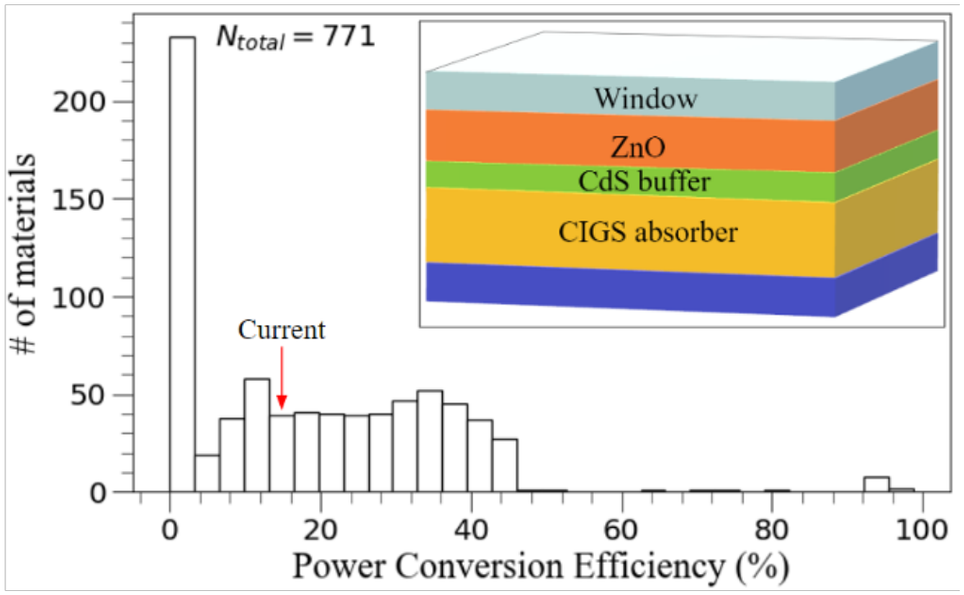
Histogram





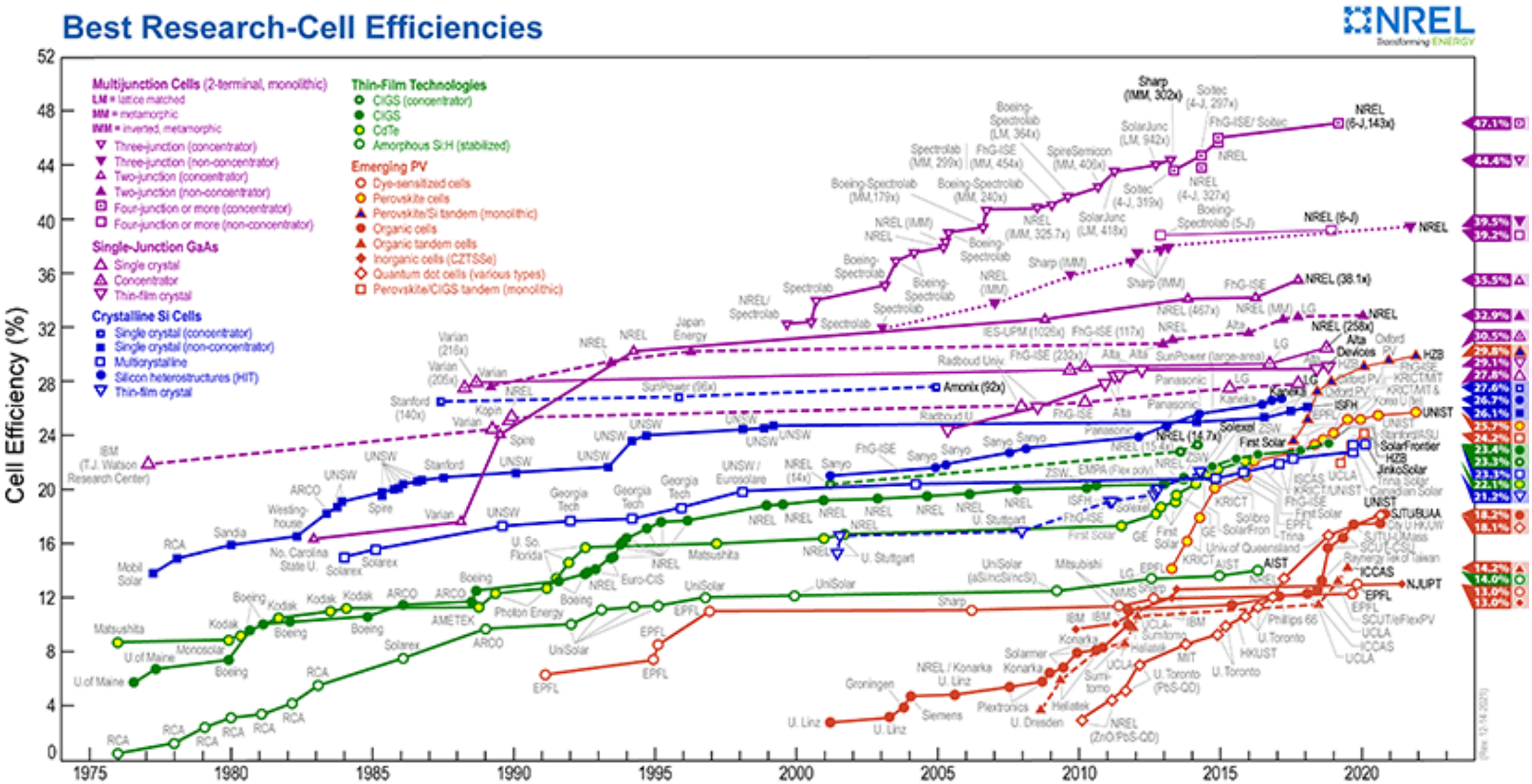
Materials and Data





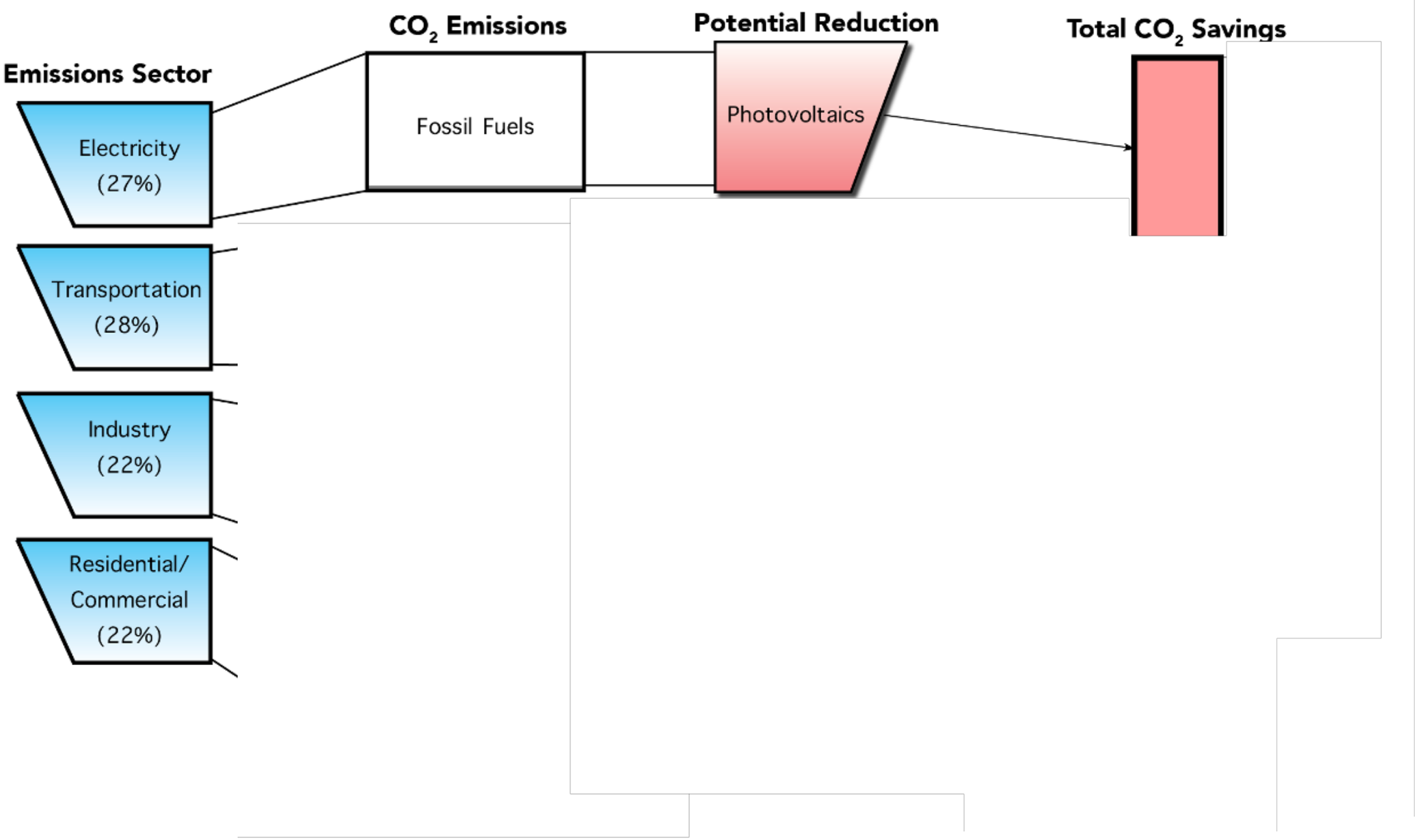
- This gives a range of what can be achieved within a specific model/paradigm
- Different paradigm needed to go beyond (Interesting for Materials Science!)

Materials and Data

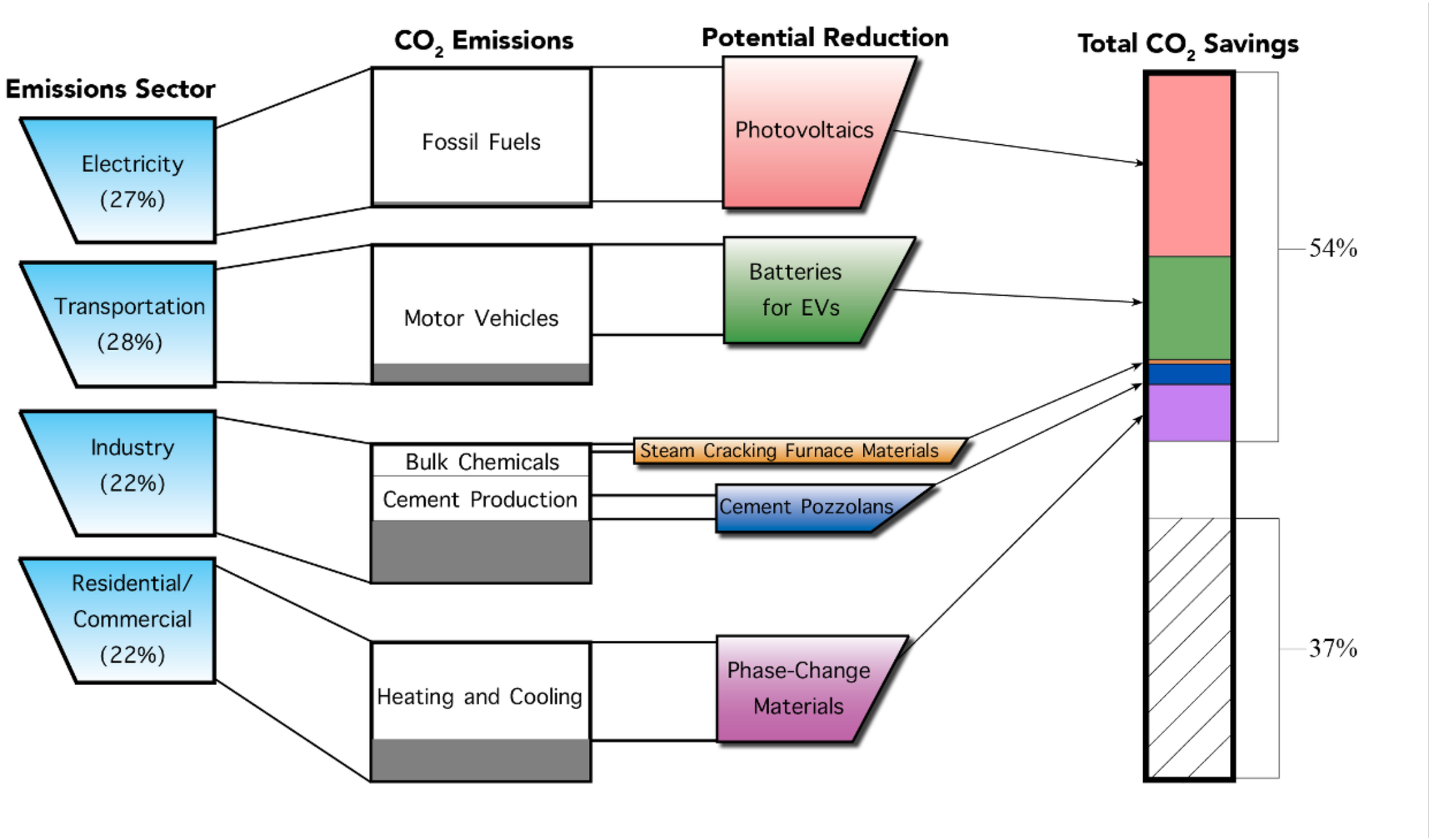


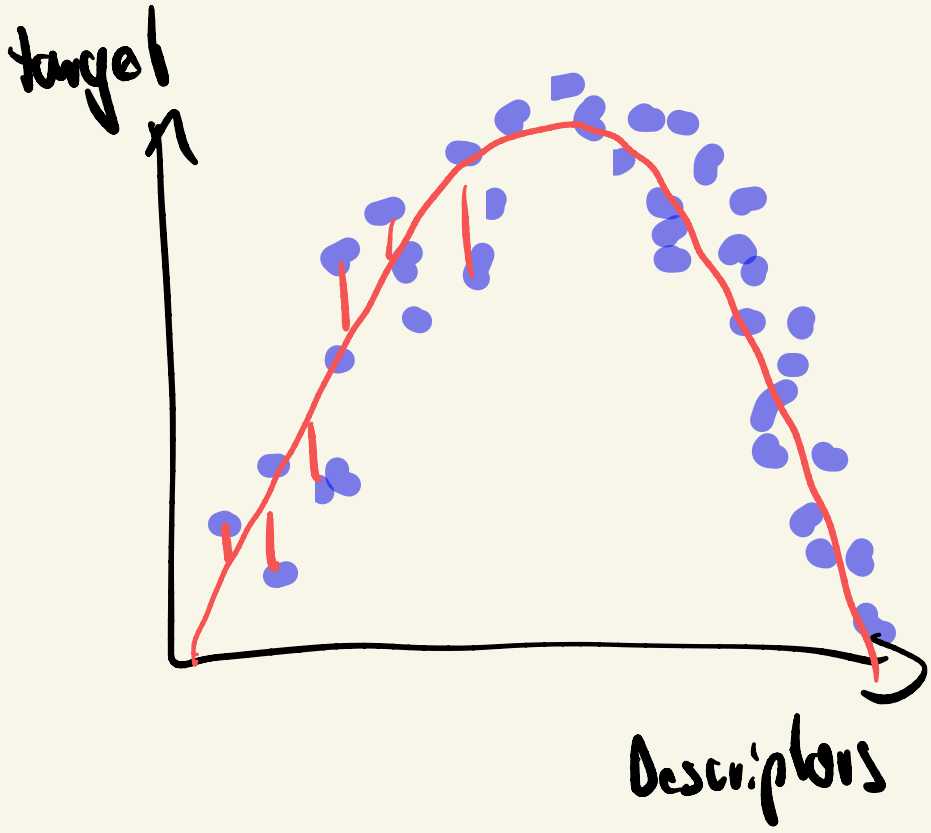
- Takes all practicalities into account;
- Challenging experimentation

Materials and Data



Materials and Data




target
Descriptors

Python demo

Go to https://colab.research.google.com/

Walkthrough

Python demo

In this exercise, we will plot the total positive test results as function of time:

- Get data from https://covidtracking.com/api/v1/states/daily.csv
- Convert the dates in the data to Pandas datetime objects.
- Plot the number of positive tests as a function of time and the positivity as a function of time.
- Document how you retrieved the above from the data.
- Make a comment about the positivity and number of positive tests. Are they correlated?
- Choose an implementation in your group for the presenter to explain to the rest of the class.
- Make any fixes, export to a PDF

Python demo

F	Xie, Dajie	Nolan, Gillian Margaret	Ni, Hsu-Chih	Bean, Chris	Lee, Yi-Ting
M	Aboutaleb, Sohaila Mostafa Gamaleldin	Zhang, Zhixin	Paranjape, Salil	Yin, Kaijun	Yardas, Olek
P	Desilva, Charith Ravana	Furlanetto Ferrari, Paolo	Pak, Angela Areum	Han, Joon Su	Palmer, Dan
S	Krishnan, Siddharth	Hwang, Kelly	Lo, Tzu-Hsiang	Foiles, Dreycen	Lin, Tsai-Wei
D	Chee, Gwendolyn Jin Yi	Nahid, Shahriar Muhammad	Ellis-Mohr, Austin Russell	Li, Shuchen	Bipasha, Ferdaushi Alam
F	Sin, Phillip Hyun	Celebi, Orcun Koray	Wonner, Sara Katlyn	Xu, Rui Hua Jeff	He, Jimmy
D					Brandvold, Ally

Facilitator: Make sure that the goals are all achieved

Moderator: Make sure that everyone's ideas are heard, finds resolutions to disagreements.

Presenter: Will report experience or conclusion to the rest of class

Scribe: Screen share the response document so you can work on it collaboratively.

Devil's advocate: Quality control—does the argument make sense?

Python demo

- Plot the function sin(x) and x and choose your x and y limits appropriately.
- Generate a probability distribution and plot these random numbers.
- Draw the histogram of that distribution.
- Draw the histogram of the number of COVID test results per day
- Explain what you did to class.

- Make any fixes, include in your PDF and submit to Gradescope