

Modeling atoms to address our climate crisis

Larry Zitnick
Research Director



of interest to the whole world—
 are of the an being. It is
 e depress- y, and it a life-
 orn facts. rations to come.
 think are of the
 d in deadly peril ed
 eat. As mouths multiply, food
 will grow wheat is
 difficult and capri-
 constrained
 to show that our wheat-producing soil is to-
 the strain put upon it.

wheat-producing soil is totally
 unequal to the strain put upon it.

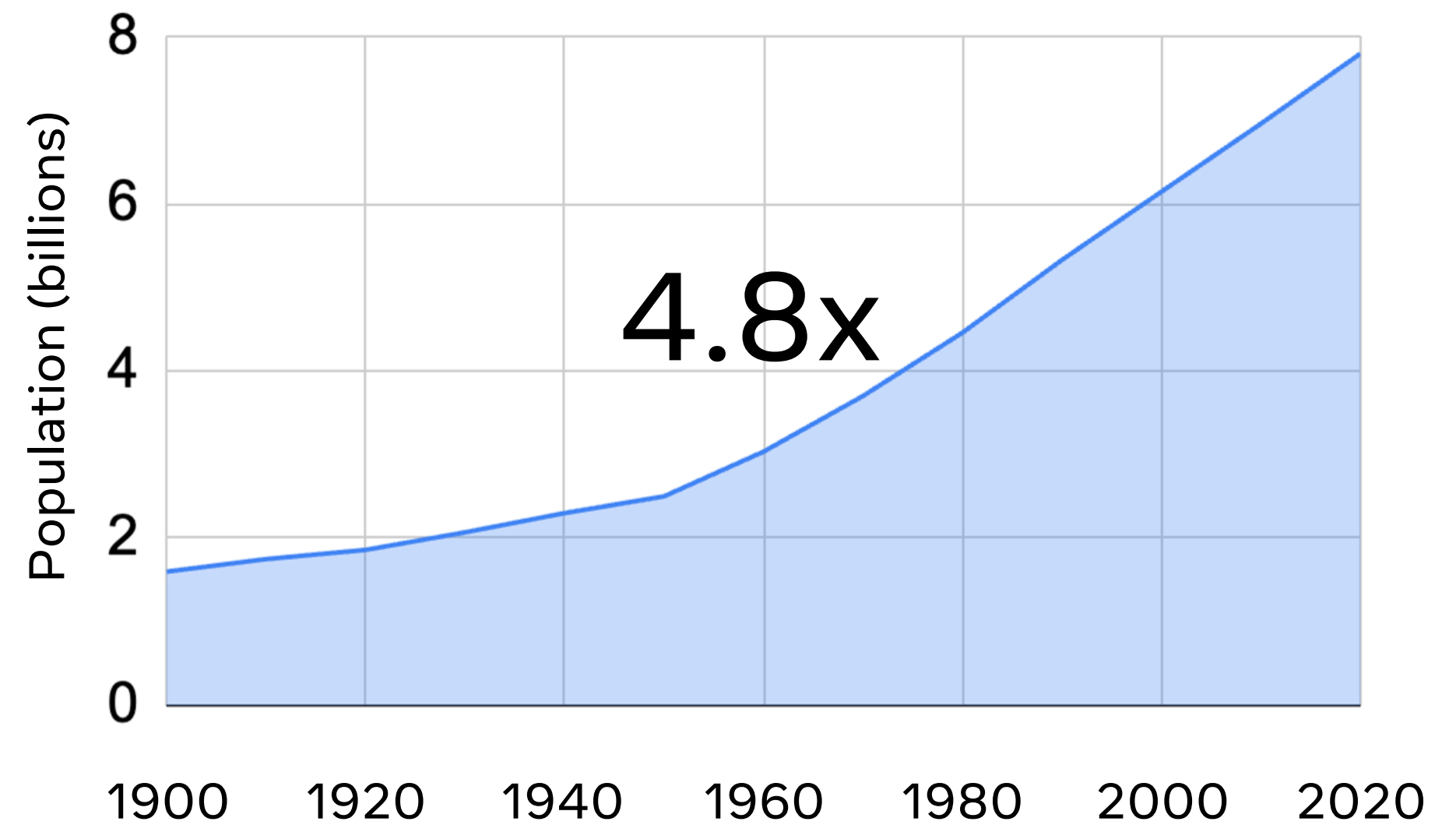
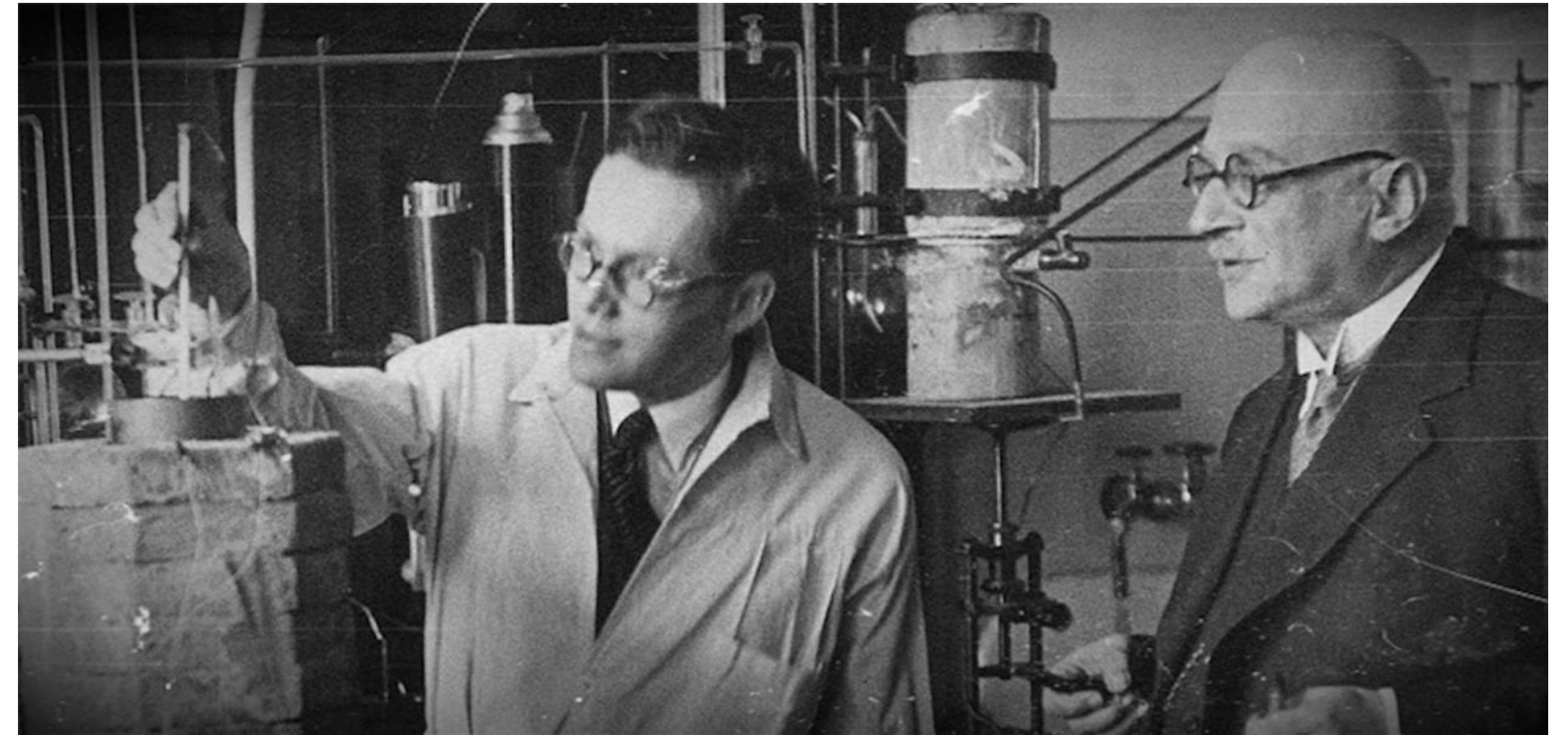
whether
 mental ely
 ings, where, by the singular laws of modern
 society, momentous announce
 sometimes first given to the world
 Playfair (then Sir Lyon Playfa
 President of the British Associa
 Aberdeen in 1885; his address on
 casion will long be remembered as
 of profound learning and luminous
 tion.

**It is the chemist who must come to the res-
 cue of the threatened communities. It is
 through the laboratory that starvation may
 ultimately be turned into plenty.**

ultimately be turned into plenty.
 The food supply of the kingdom is of pe-

Haber-Bosch Process

(ammonia fertilizer)



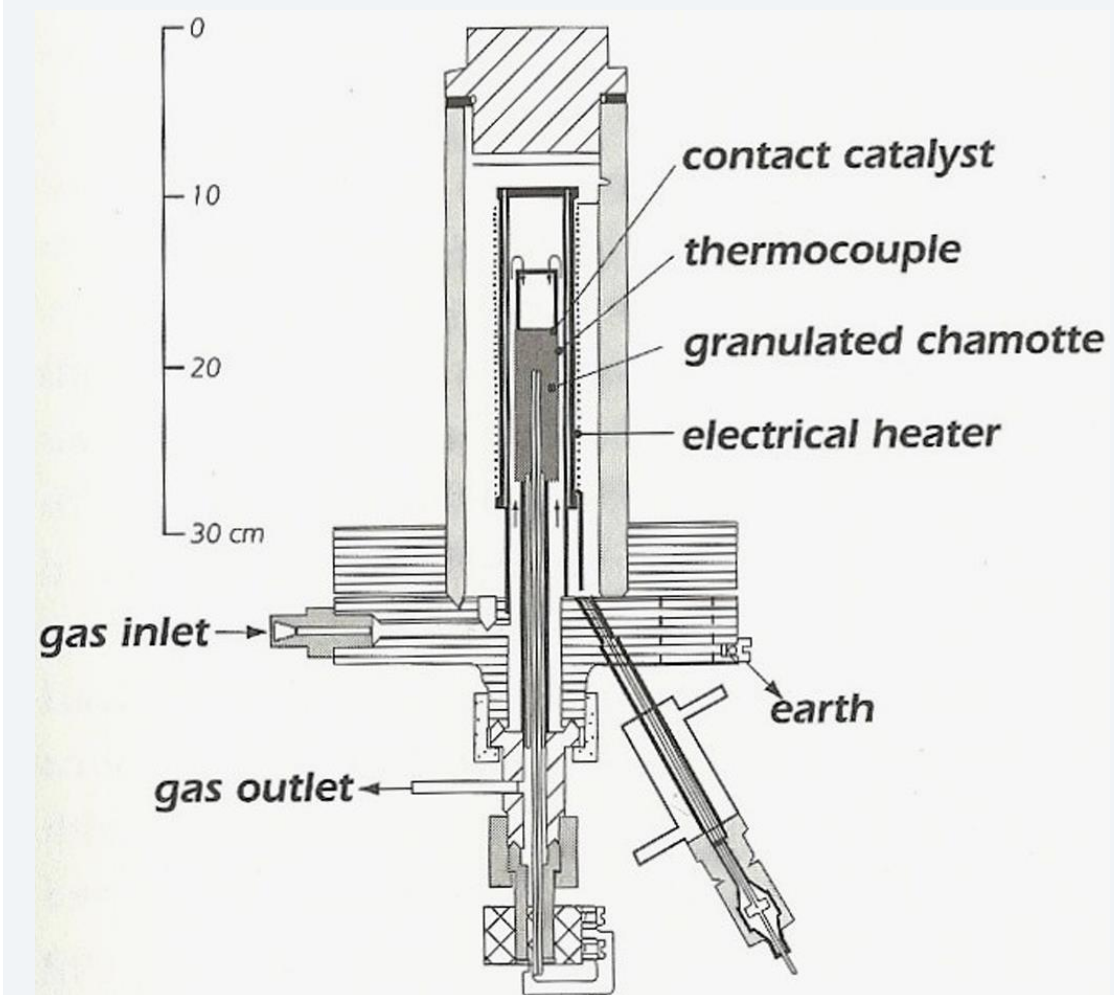
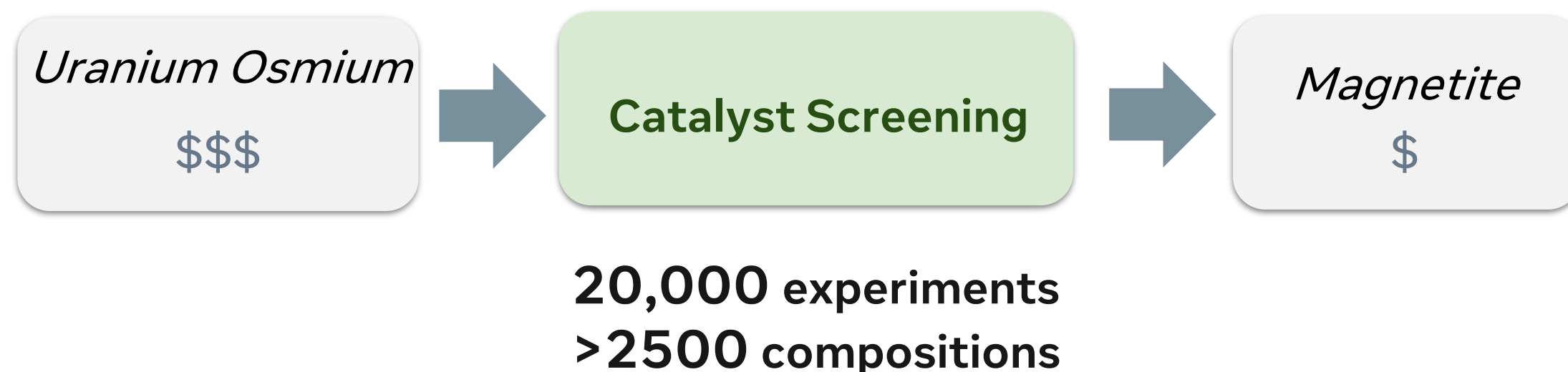
The Mittasch approach

Uranium Osmium

\$\$\$



The Mittasch approach

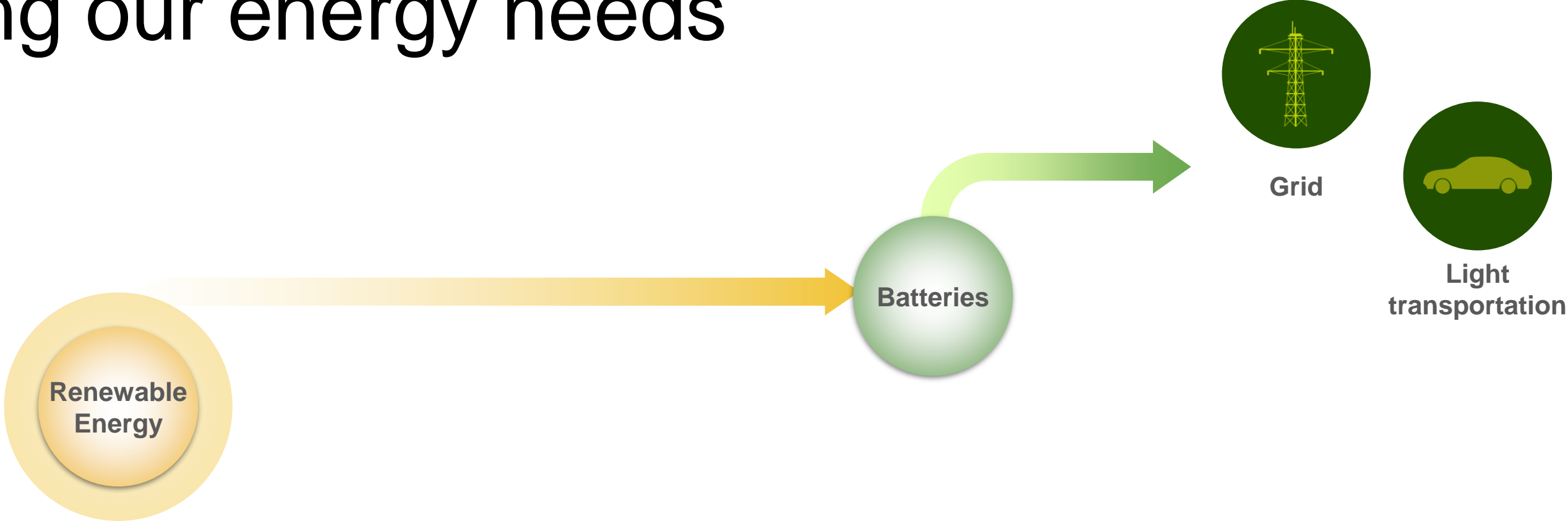


Laboratory apparatus used
by Alwin Mittasch
for testing catalyst (1910)

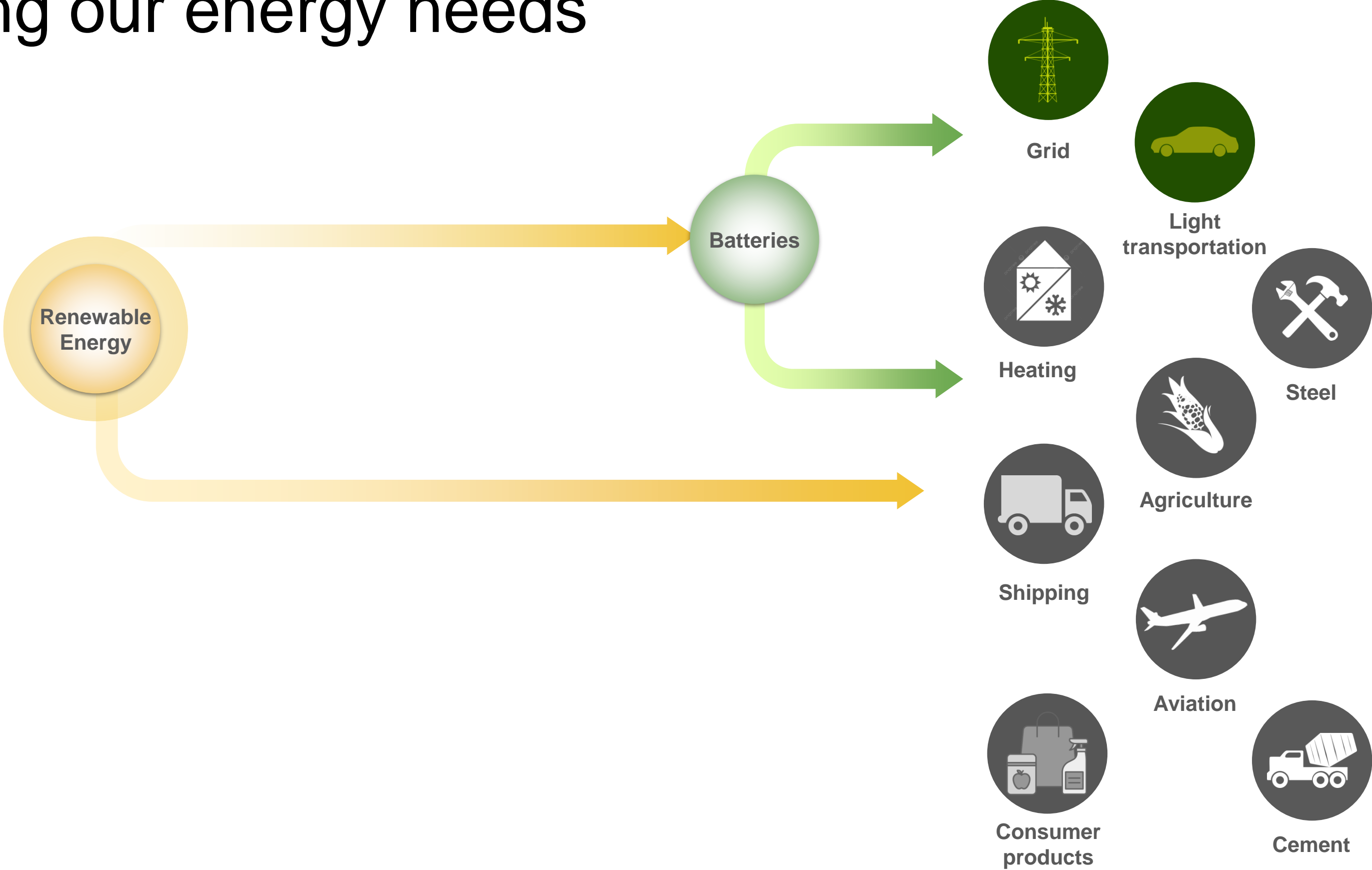
1900 ...

... 2024

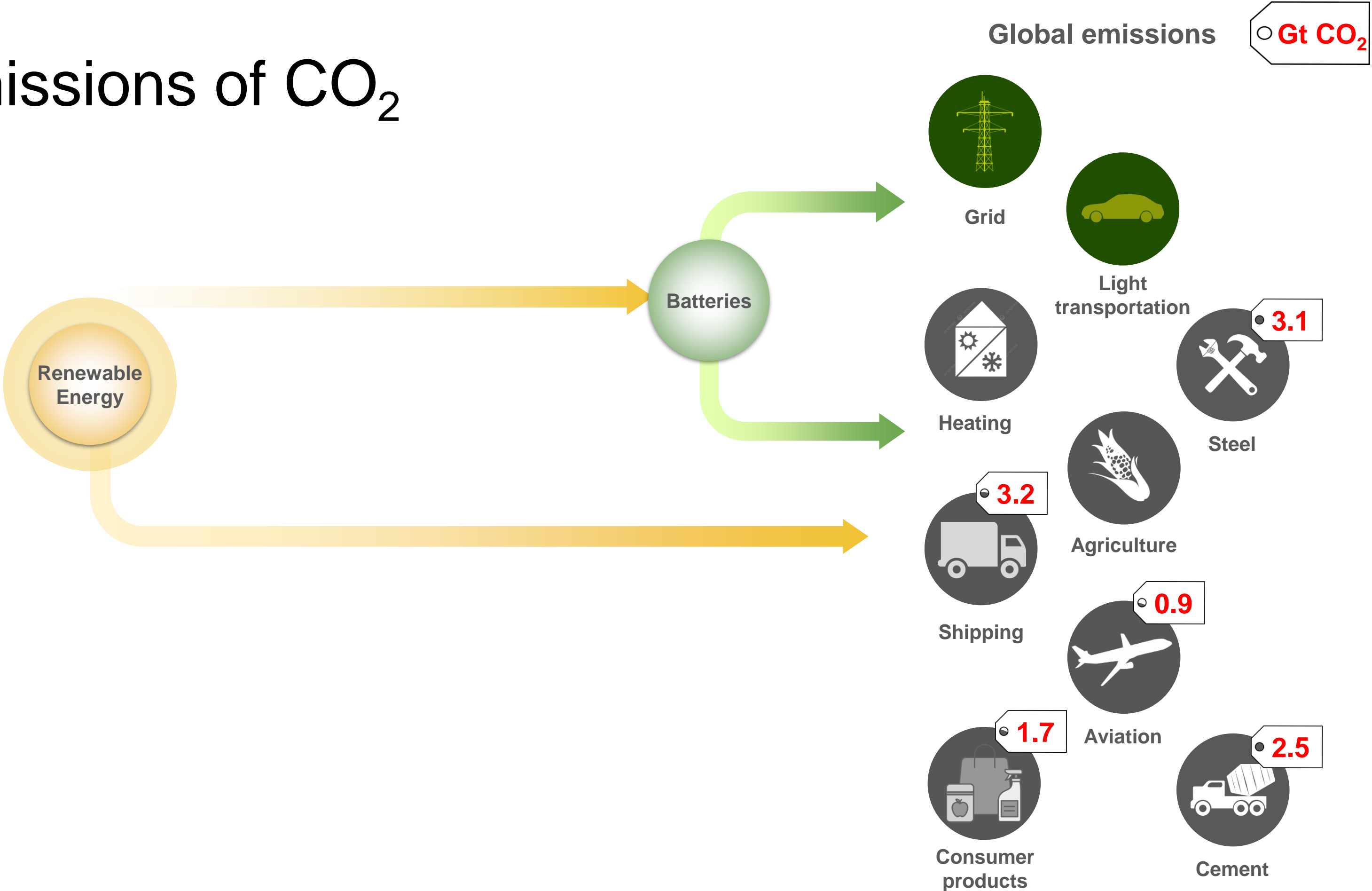
Electrifying our energy needs



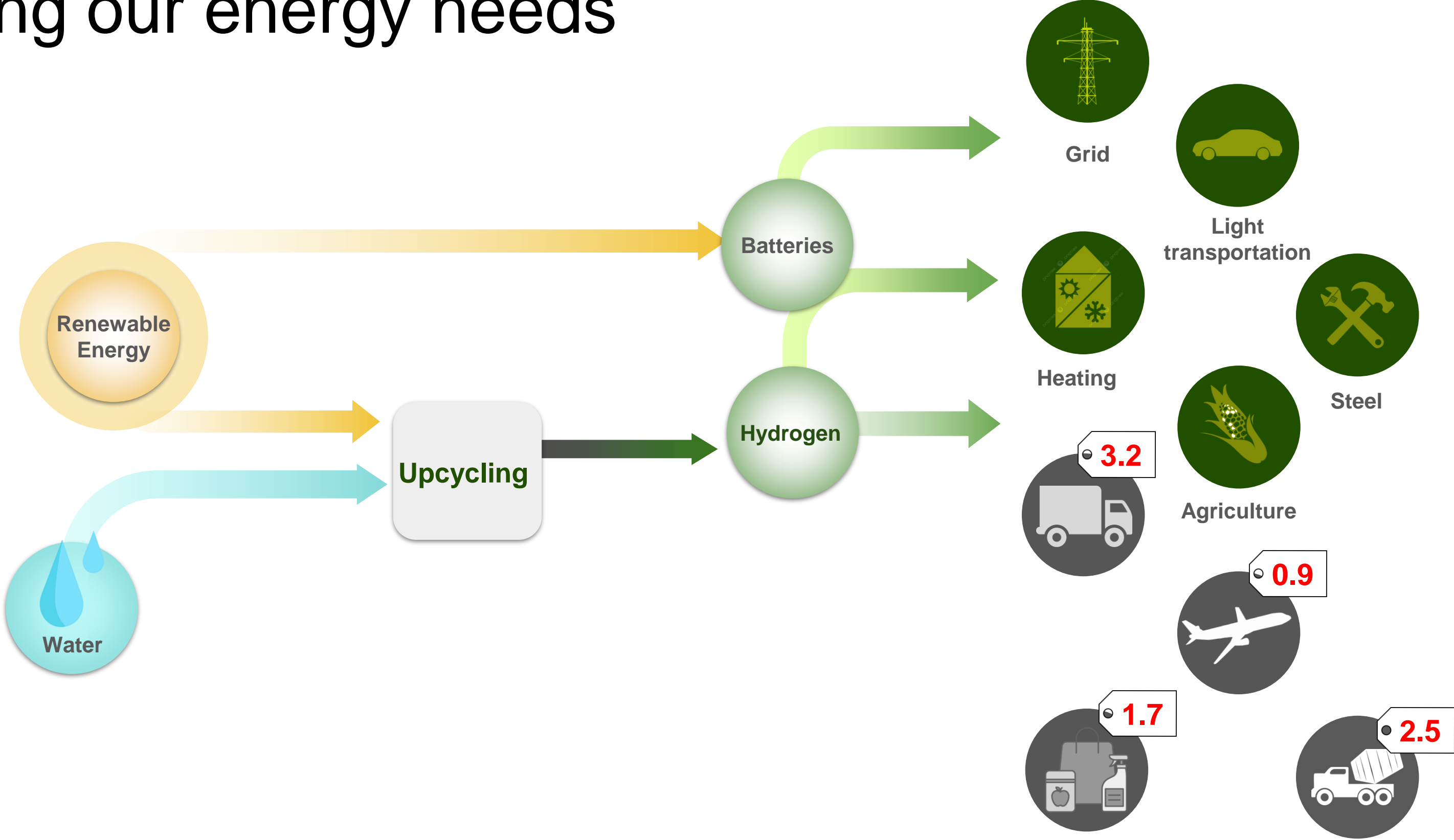
Electrifying our energy needs



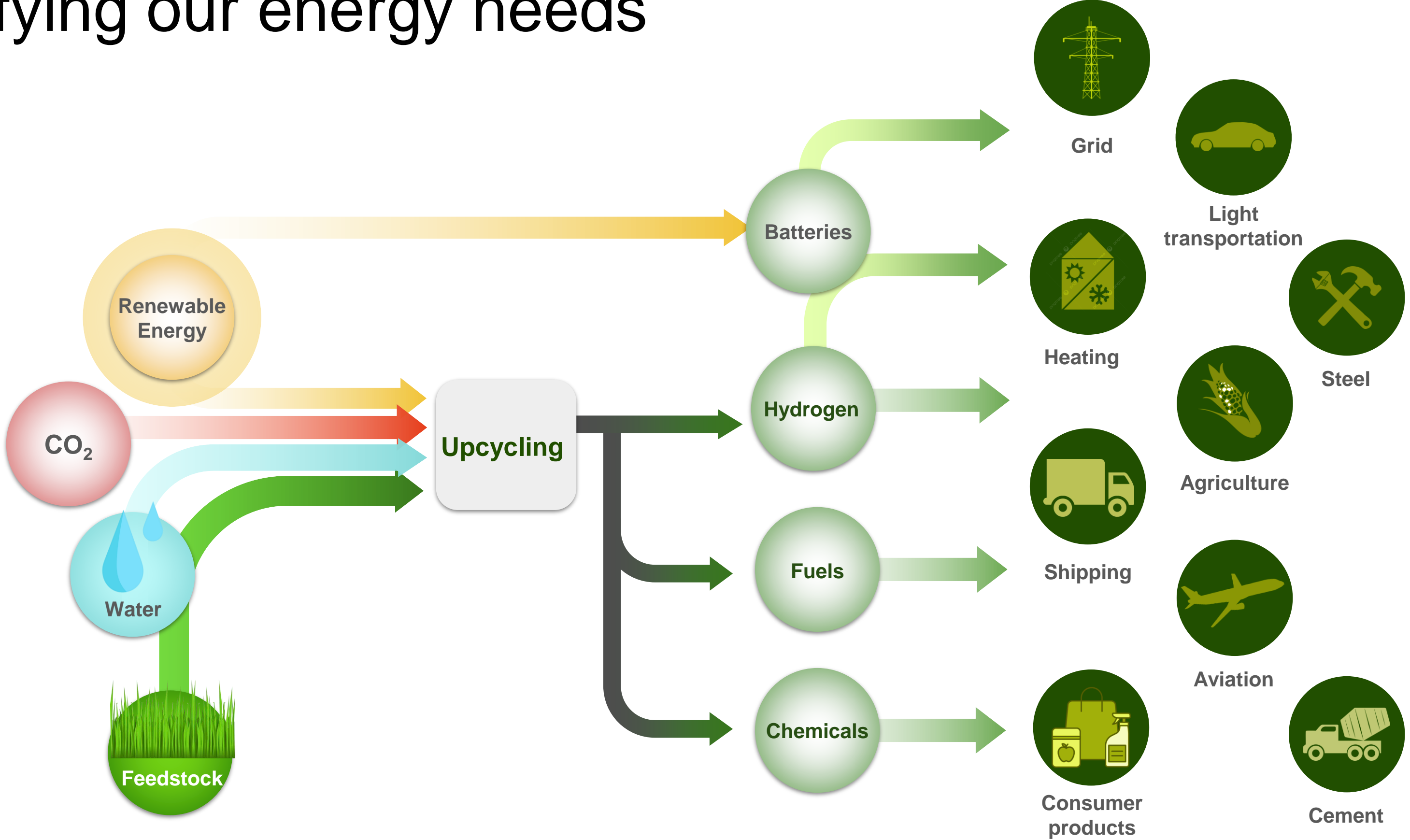
Large emissions of CO₂



Electrifying our energy needs



Electrifying our energy needs

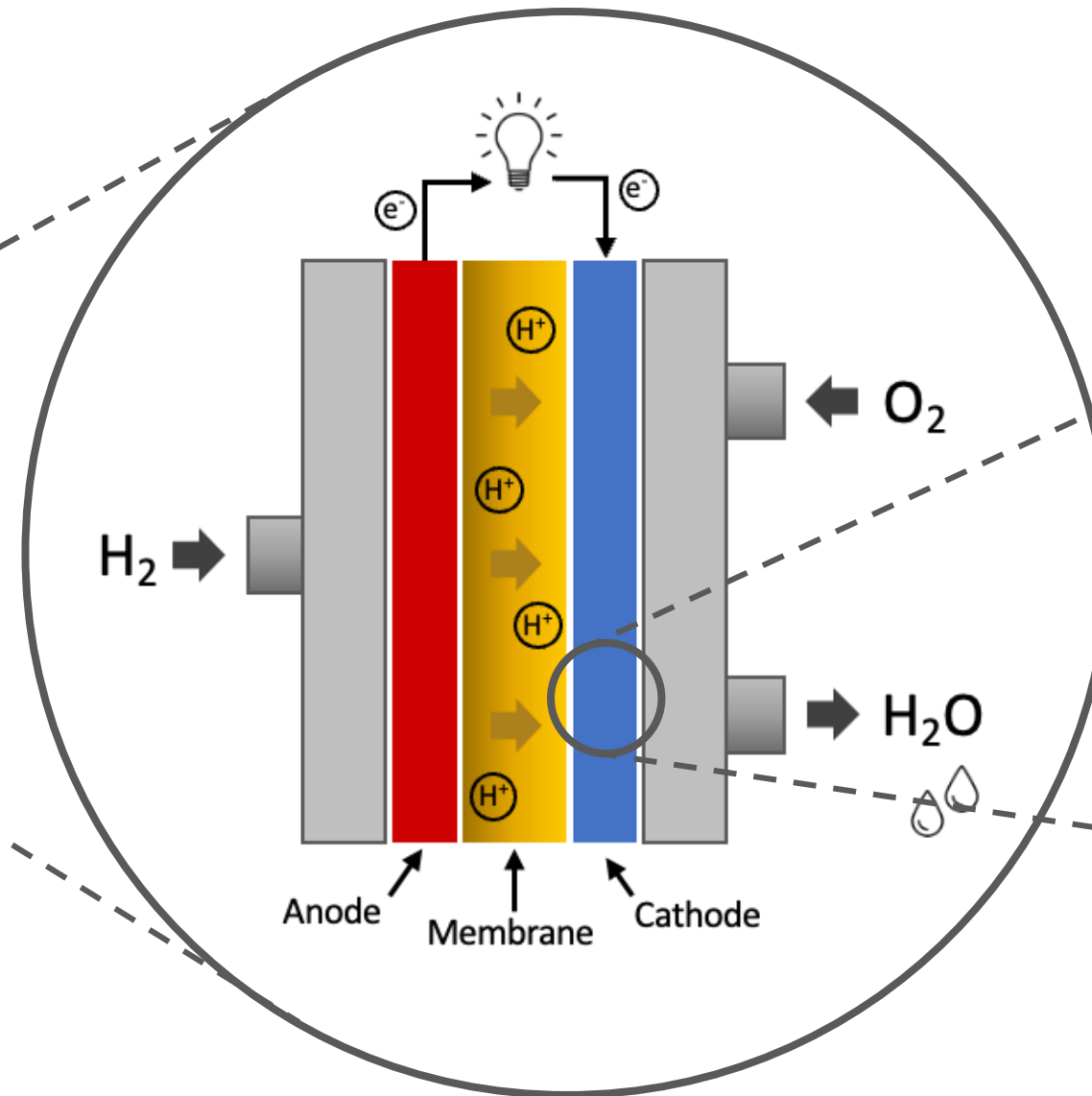


Catalyst *noun*

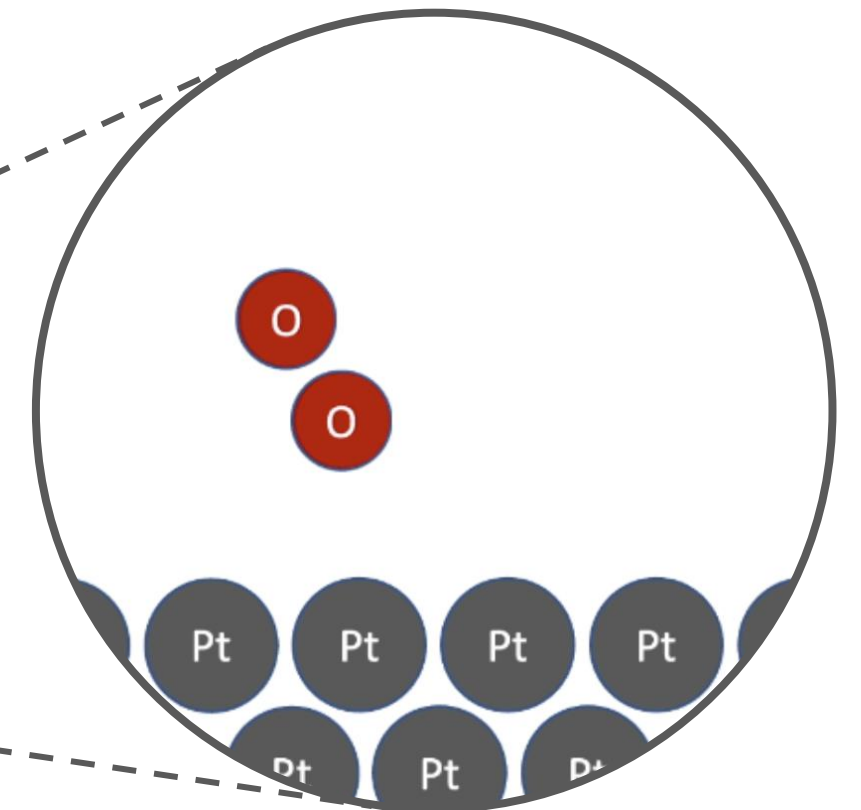
Material used to increase the rate of a chemical reaction without being consumed in the process.



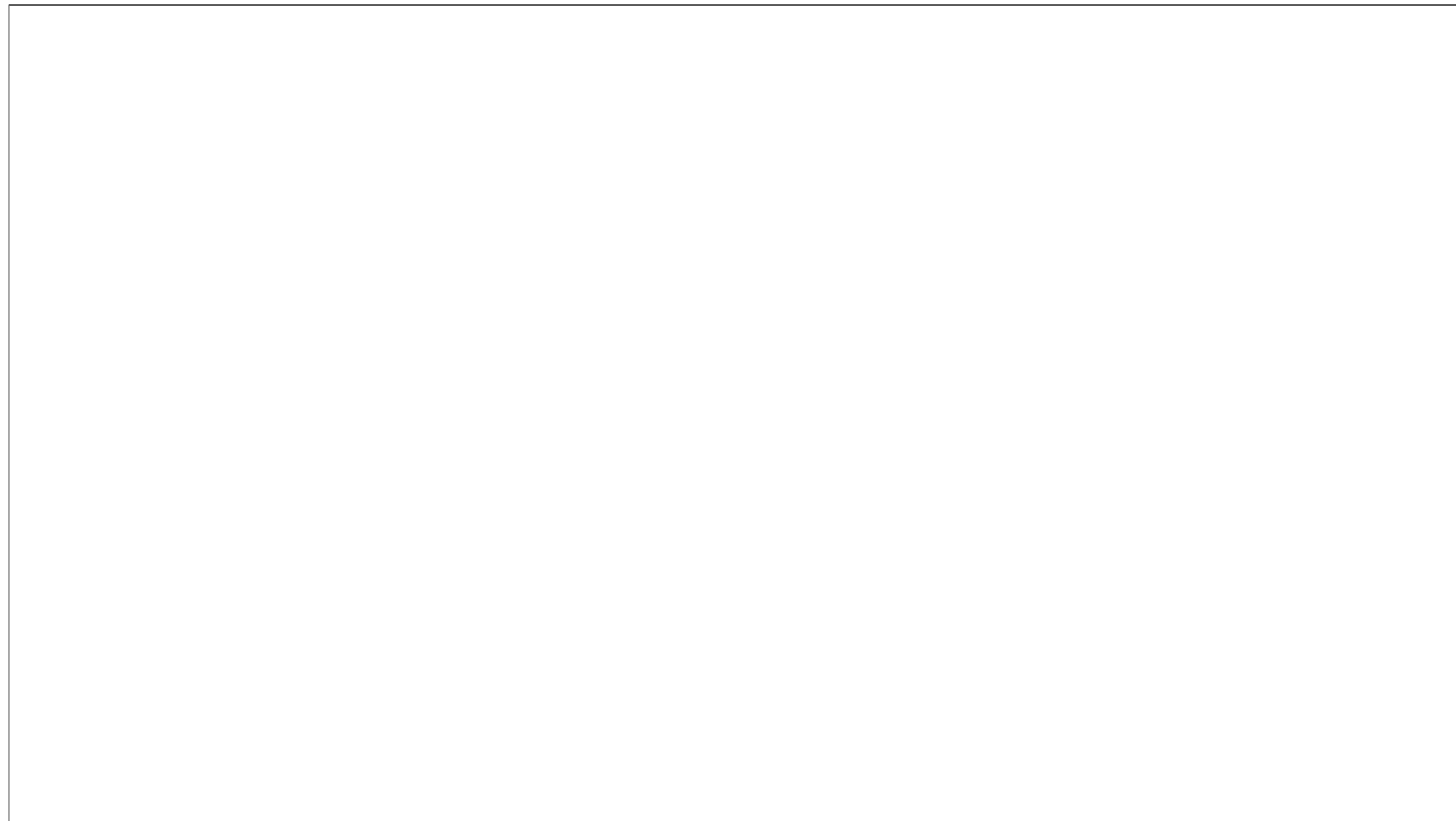
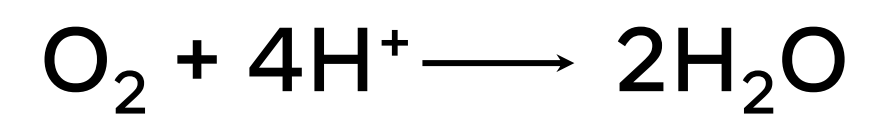
Toyota Mirai



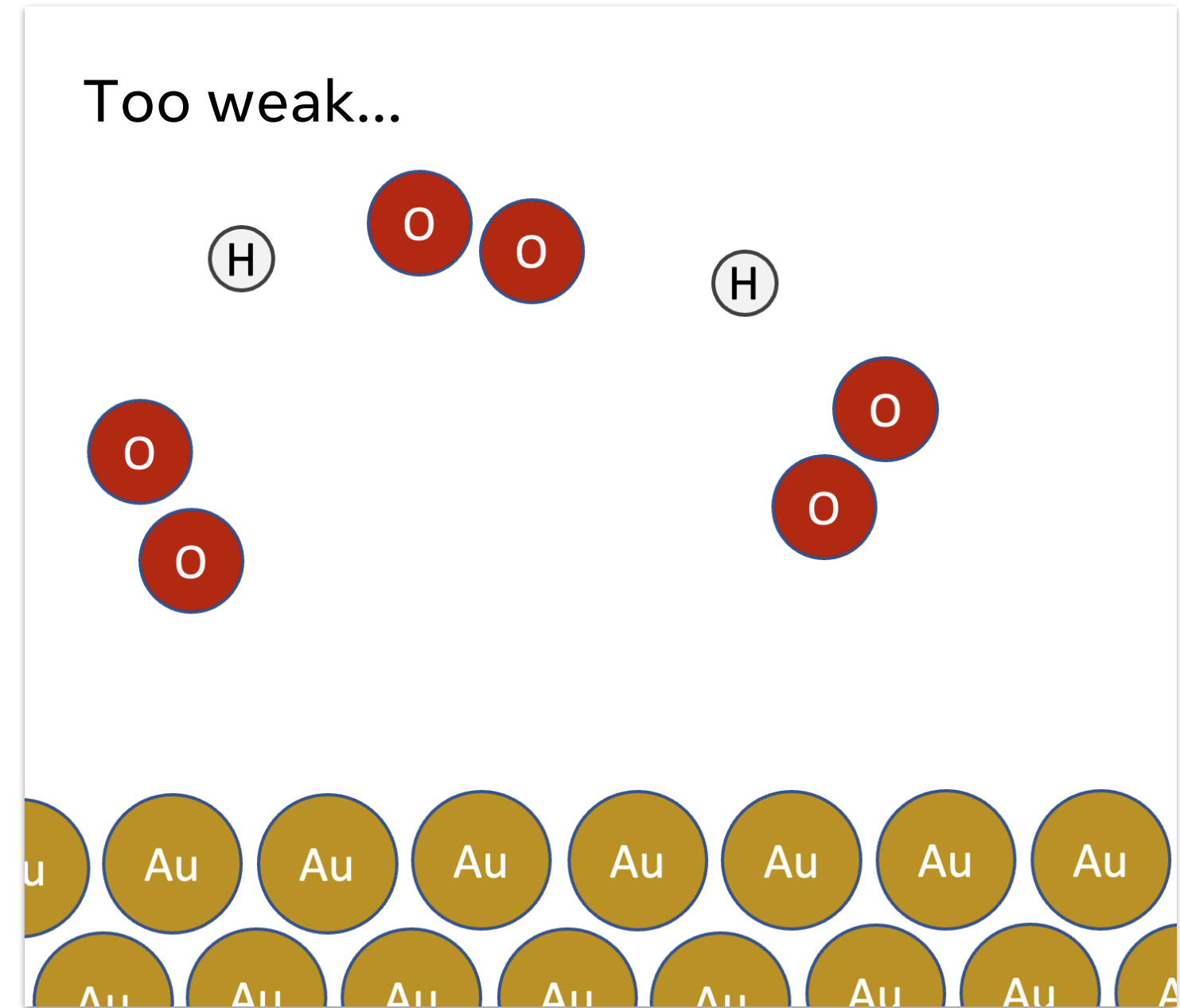
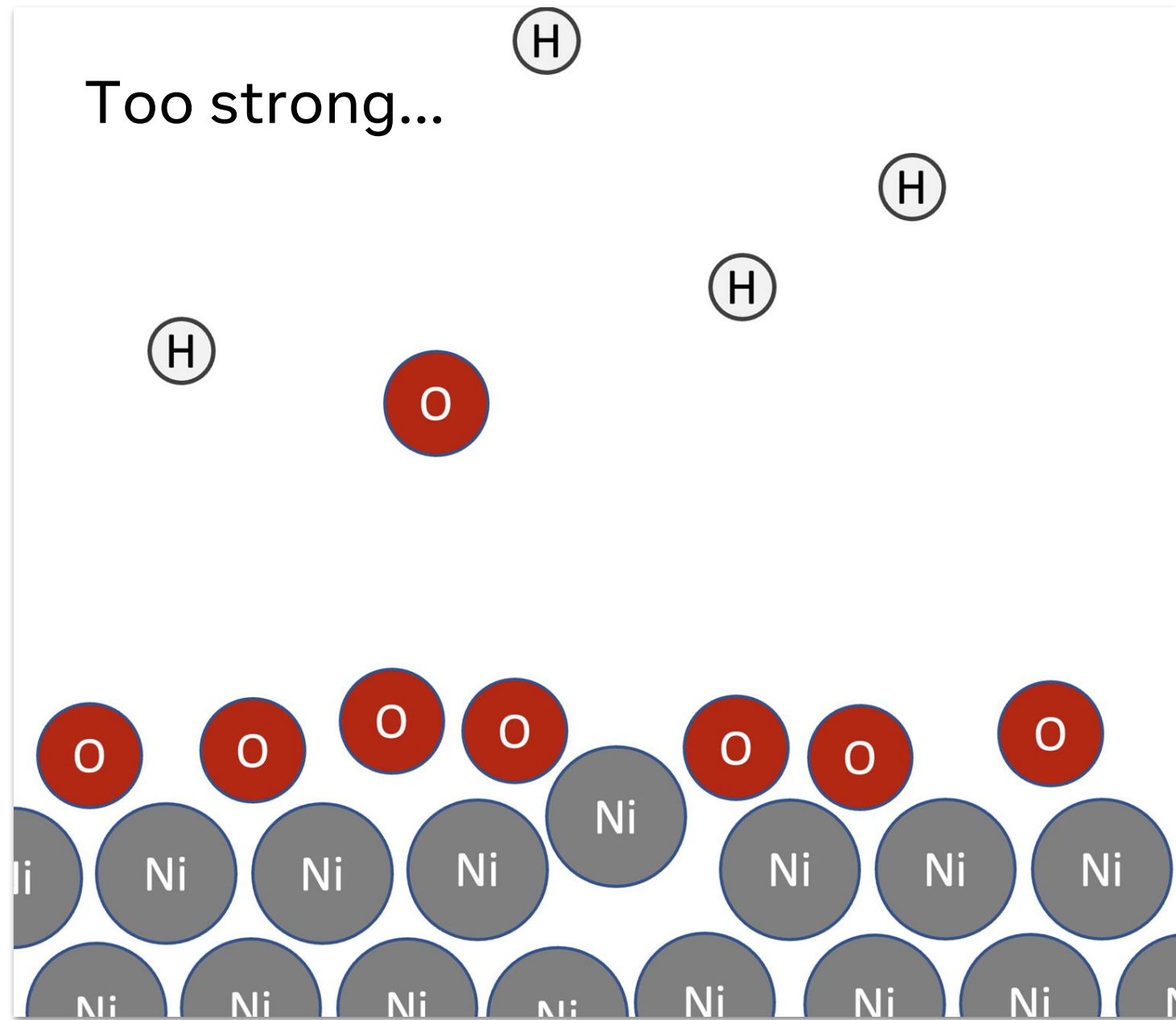
Fuel Cell



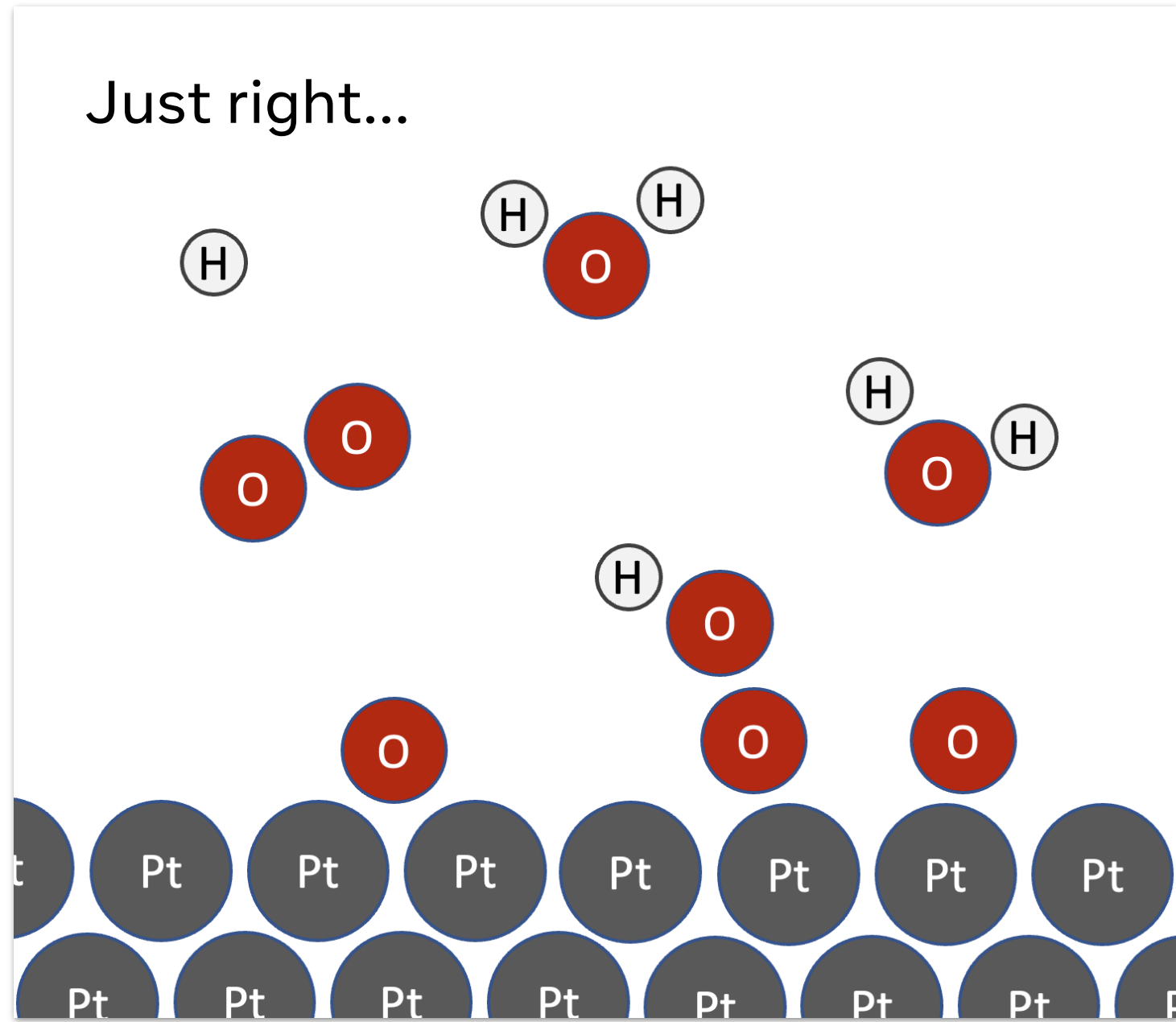
Catalyst



Goldilocks...



Goldilocks...



\$\$\$

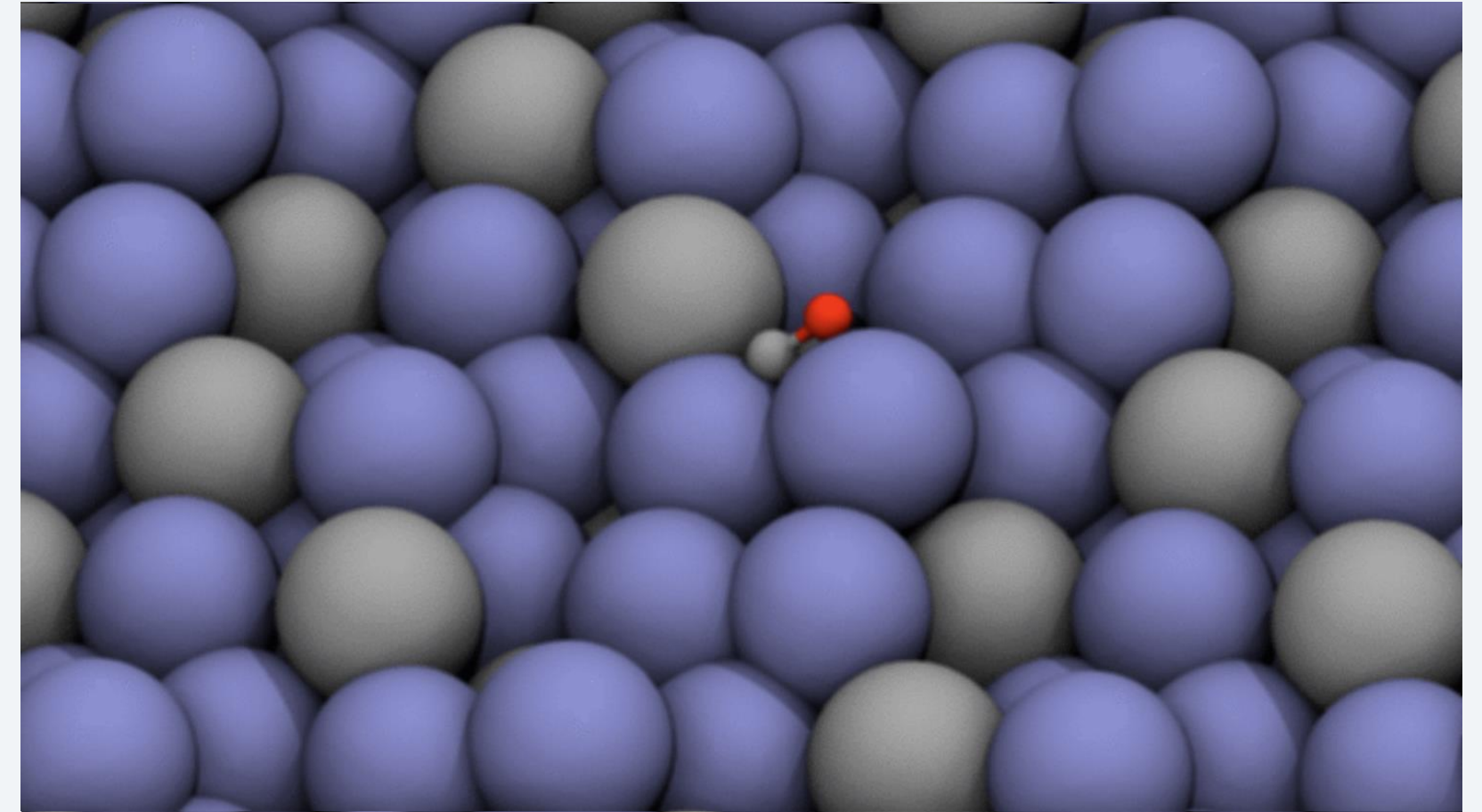
How are catalysts screened?

1. Place adsorbate near the catalyst

2. Relax atom positions

- a. Compute forces
- b. Update atom positions
- c. Repeat

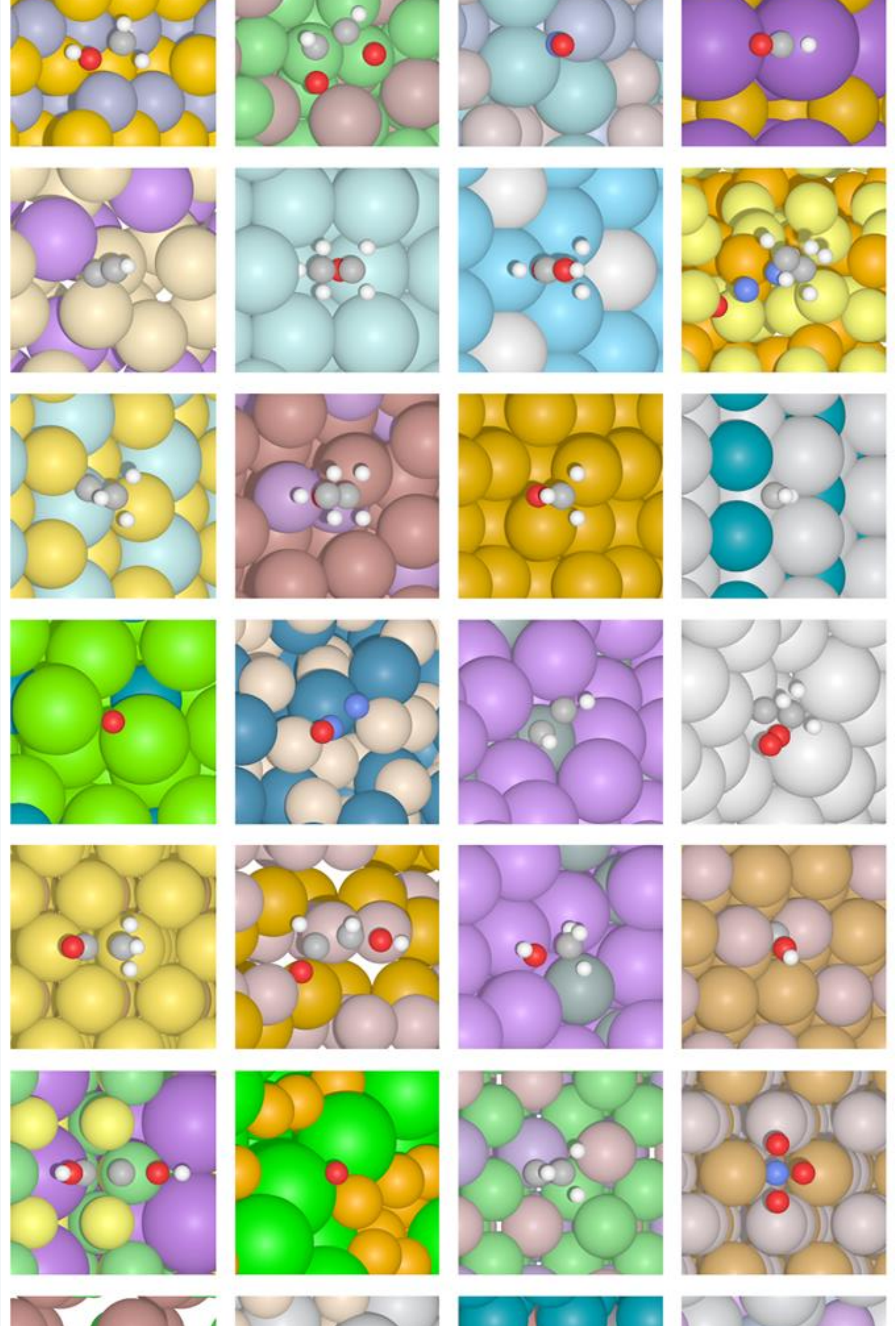
3. Use relaxed energy to estimate reaction rate trends



A single relaxation using
DFT* takes ~1 day

...billions of possibilities :(

*Density Functional Theory



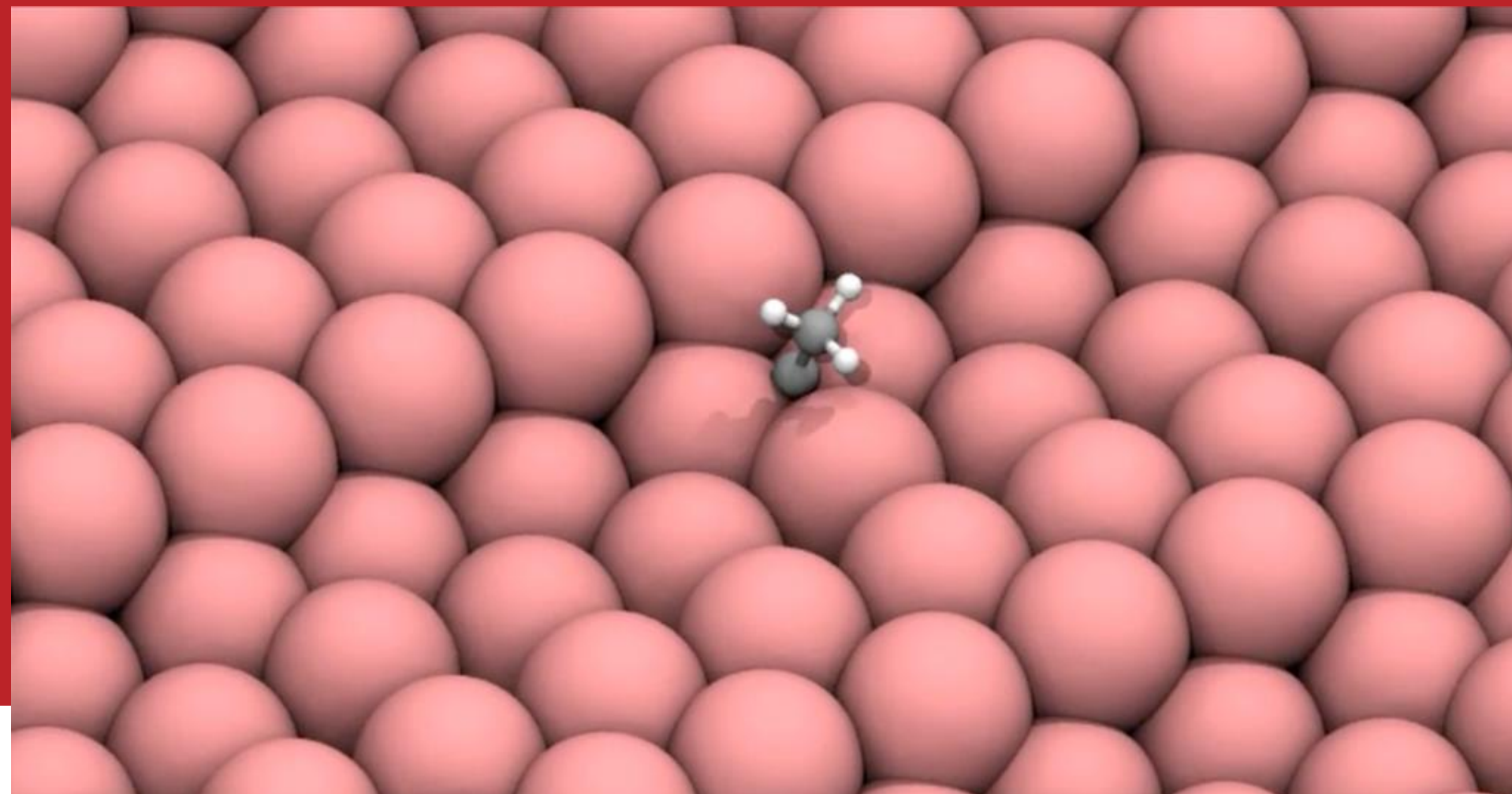
Reducing computation from 1 day to 1 second?

AI* to the rescue!

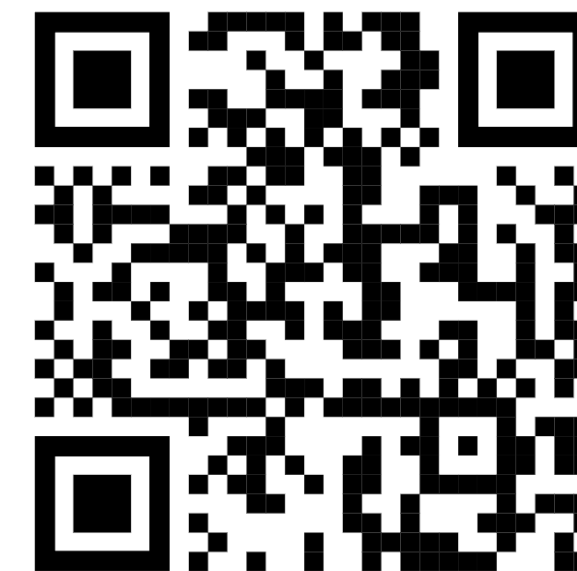
*and also chemistry :)

Open Catalyst Project

Using AI to model and discover new catalysts to address the energy challenges posed by climate change.



Carnegie Mellon University



OpenCatalystProject.org

Training data

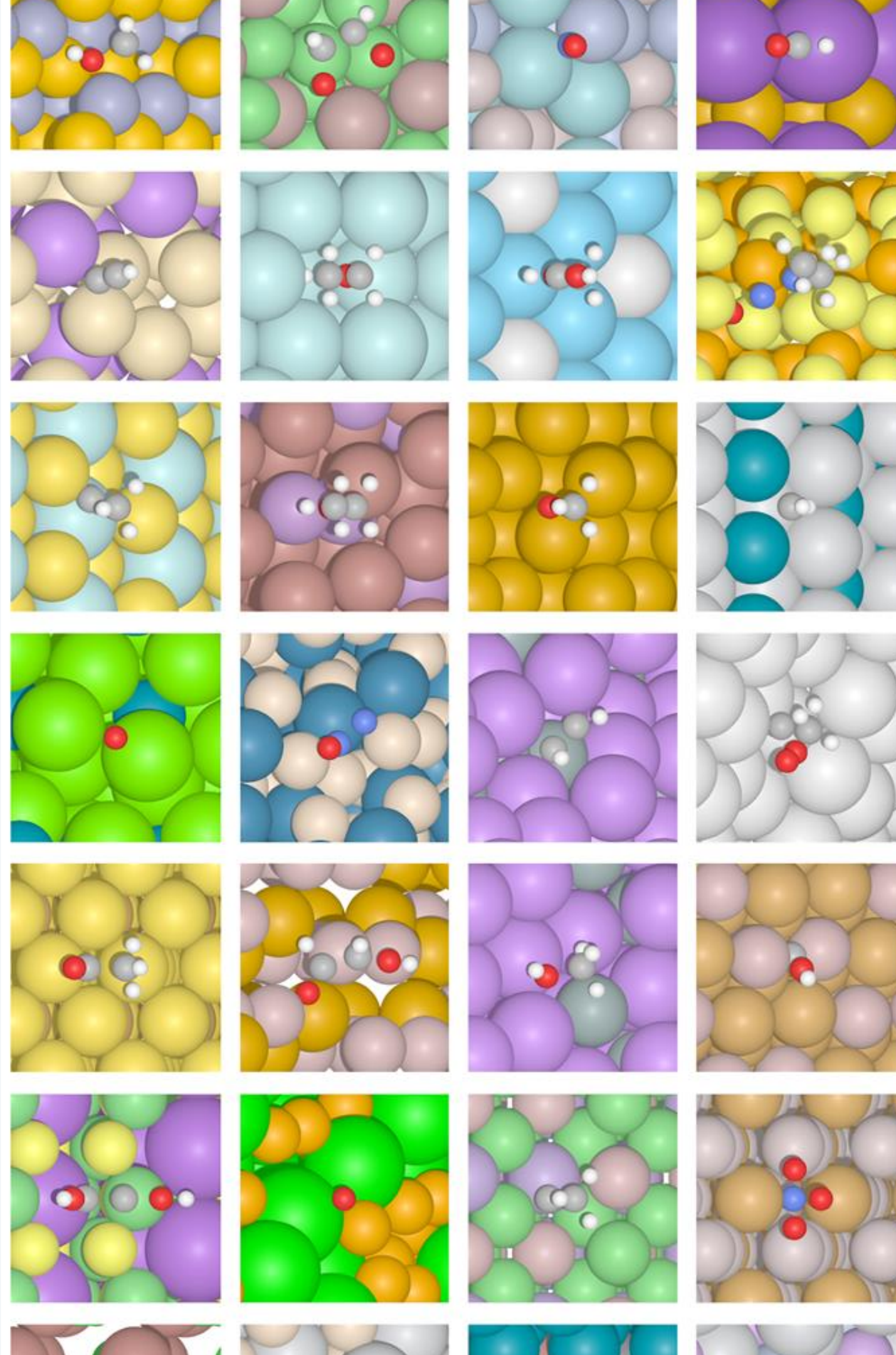
OC20 and OC22 datasets

> 140M training examples

> 500M hours of compute!

Open sourced

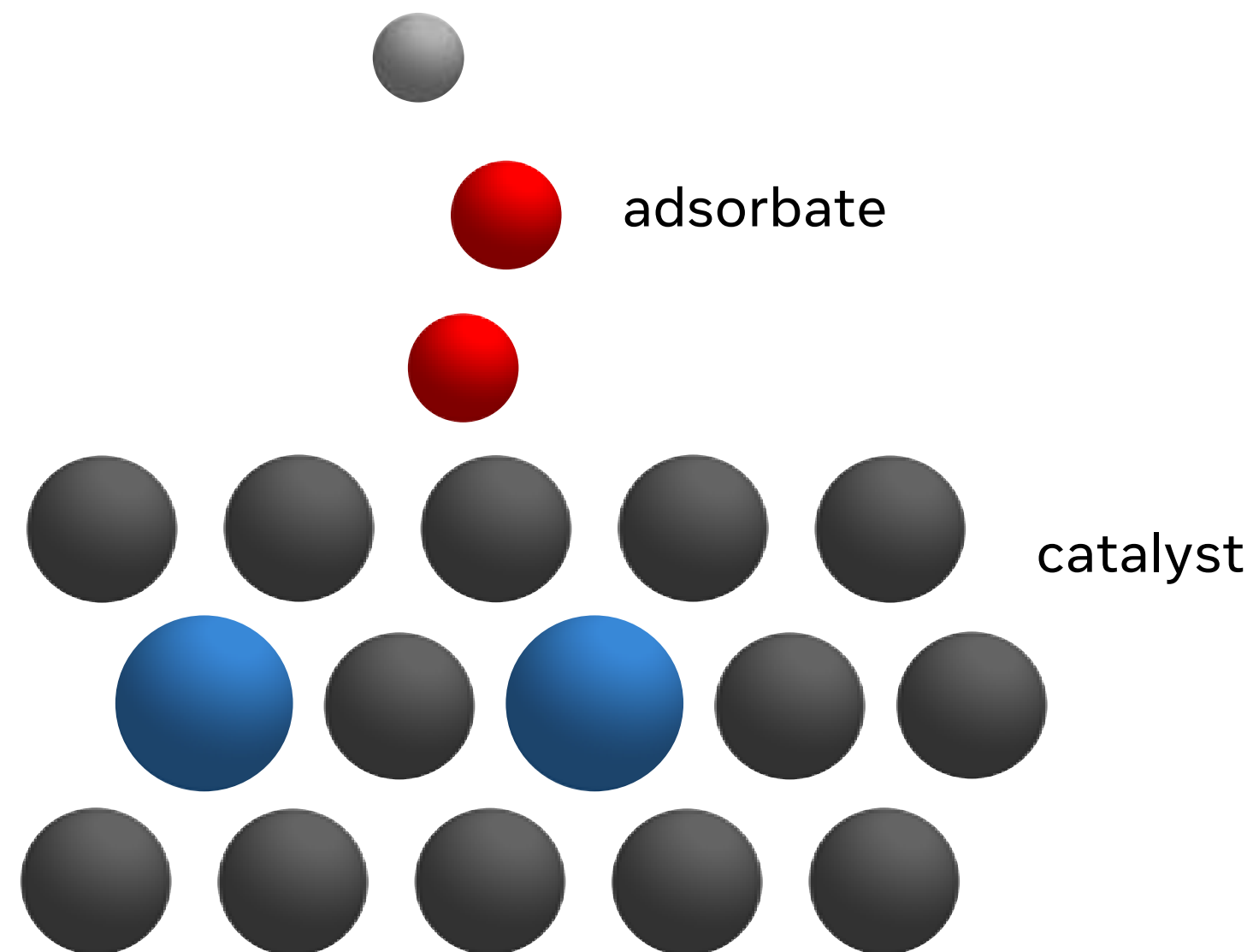
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Data

Input:

3D atom positions and atomic numbers



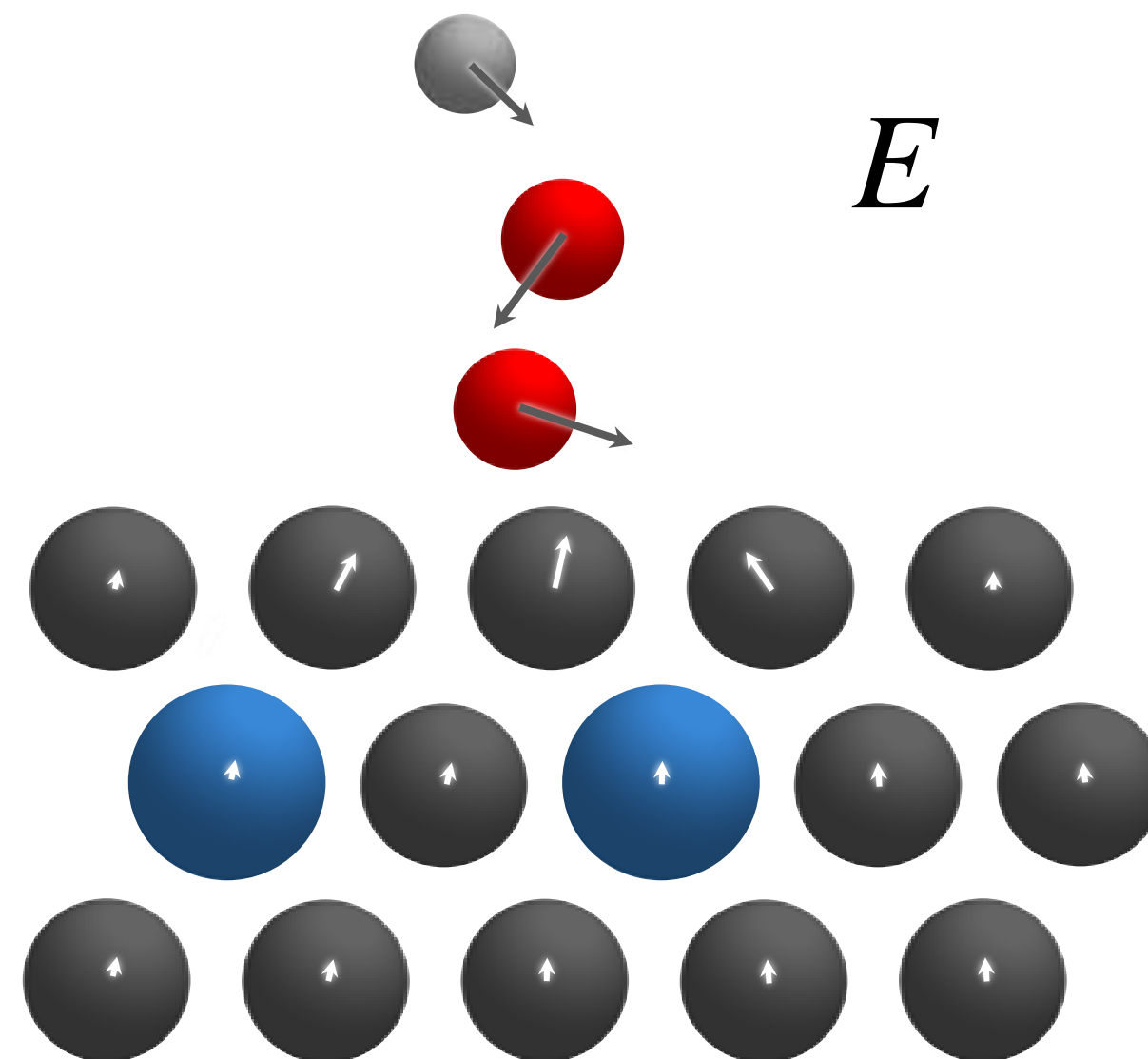
Data

Input:

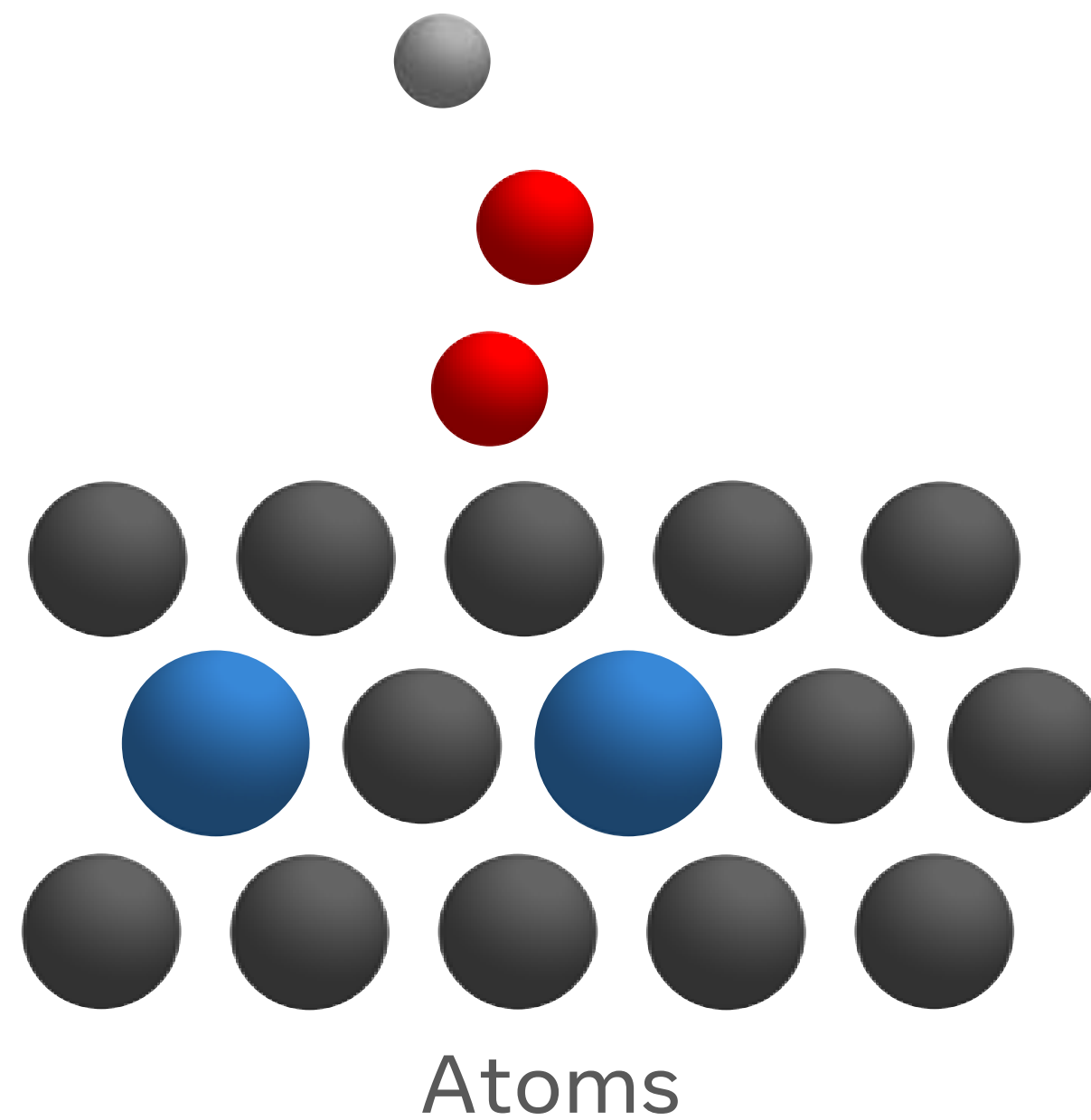
3D atom positions and atomic numbers

Output:

Energy and 3D atom forces

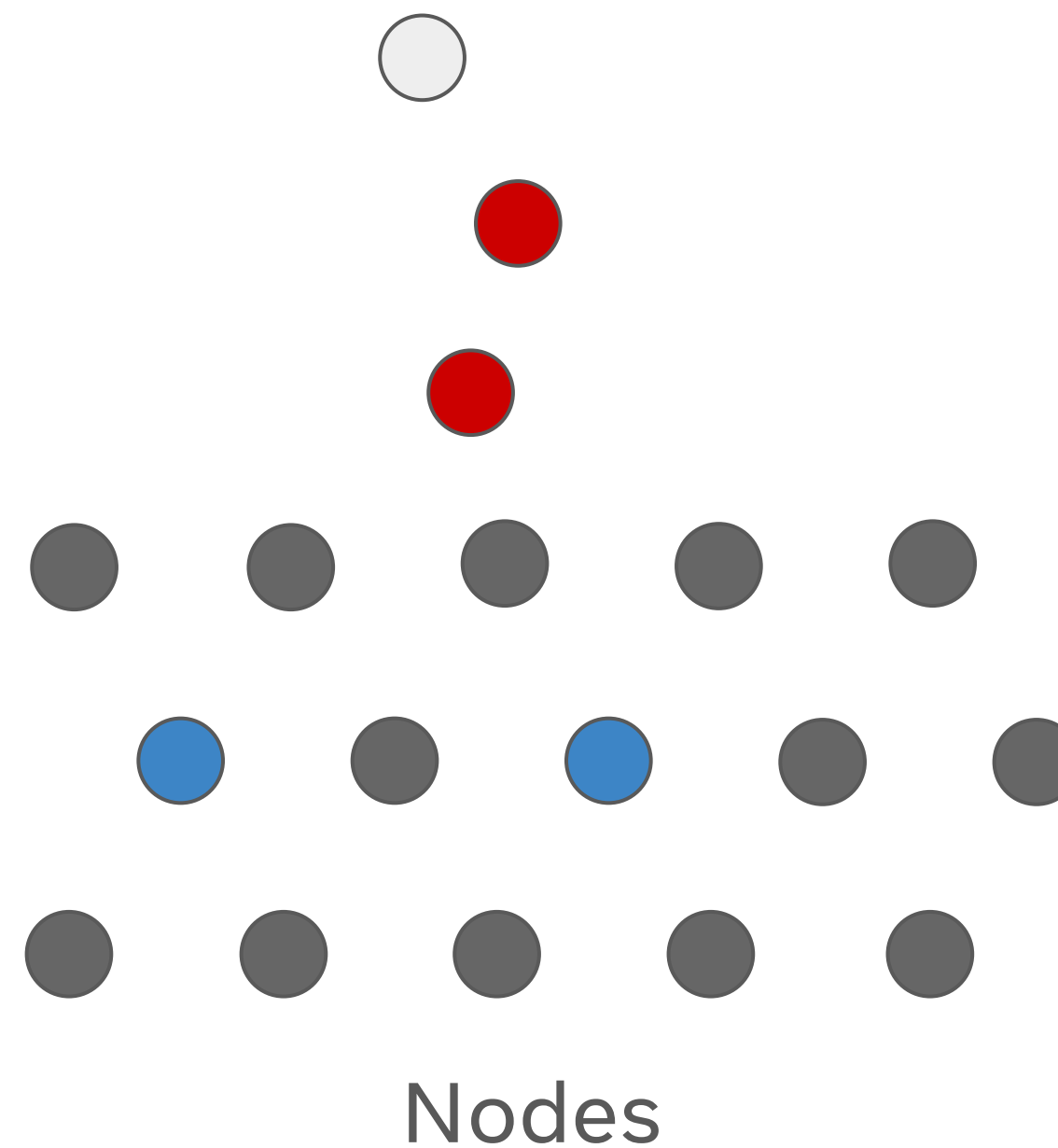


Graph Neural Network



Graph Neural Network

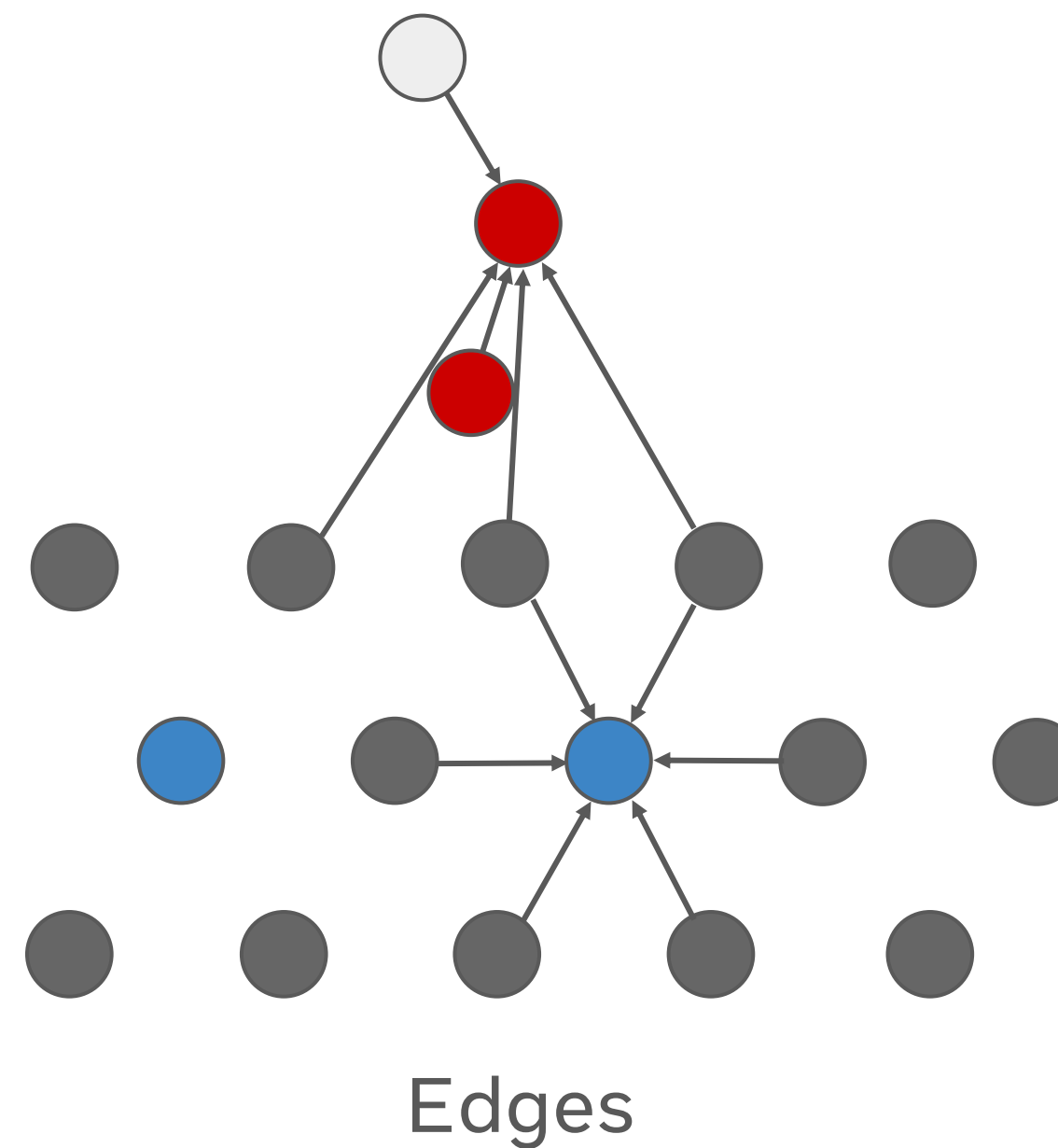
Node = Atom



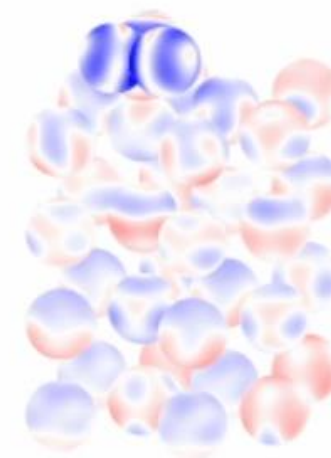
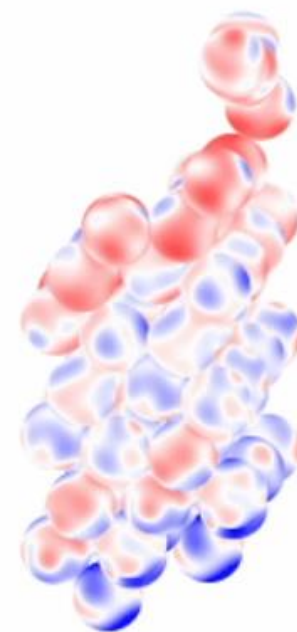
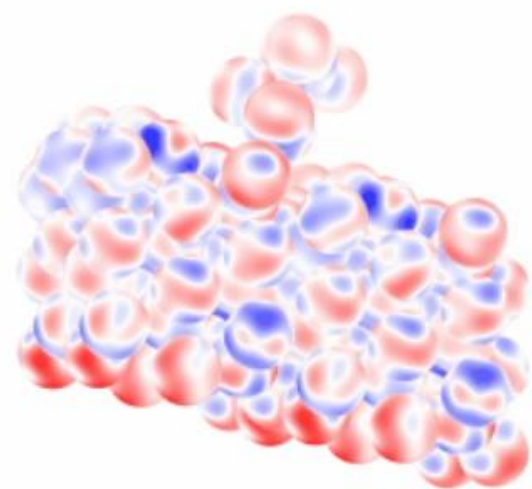
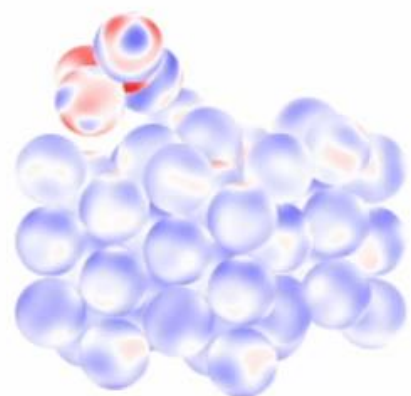
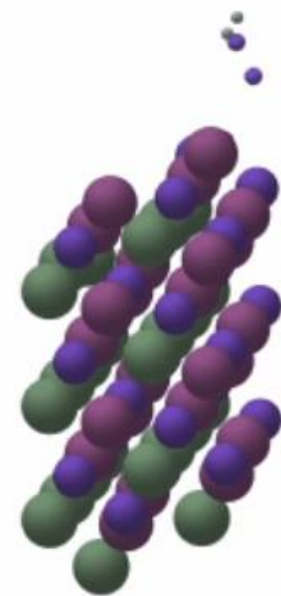
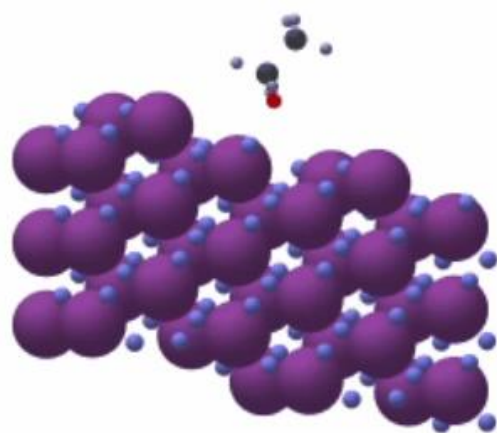
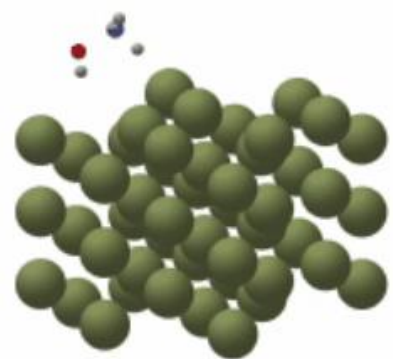
Graph Neural Network

Node = Atom

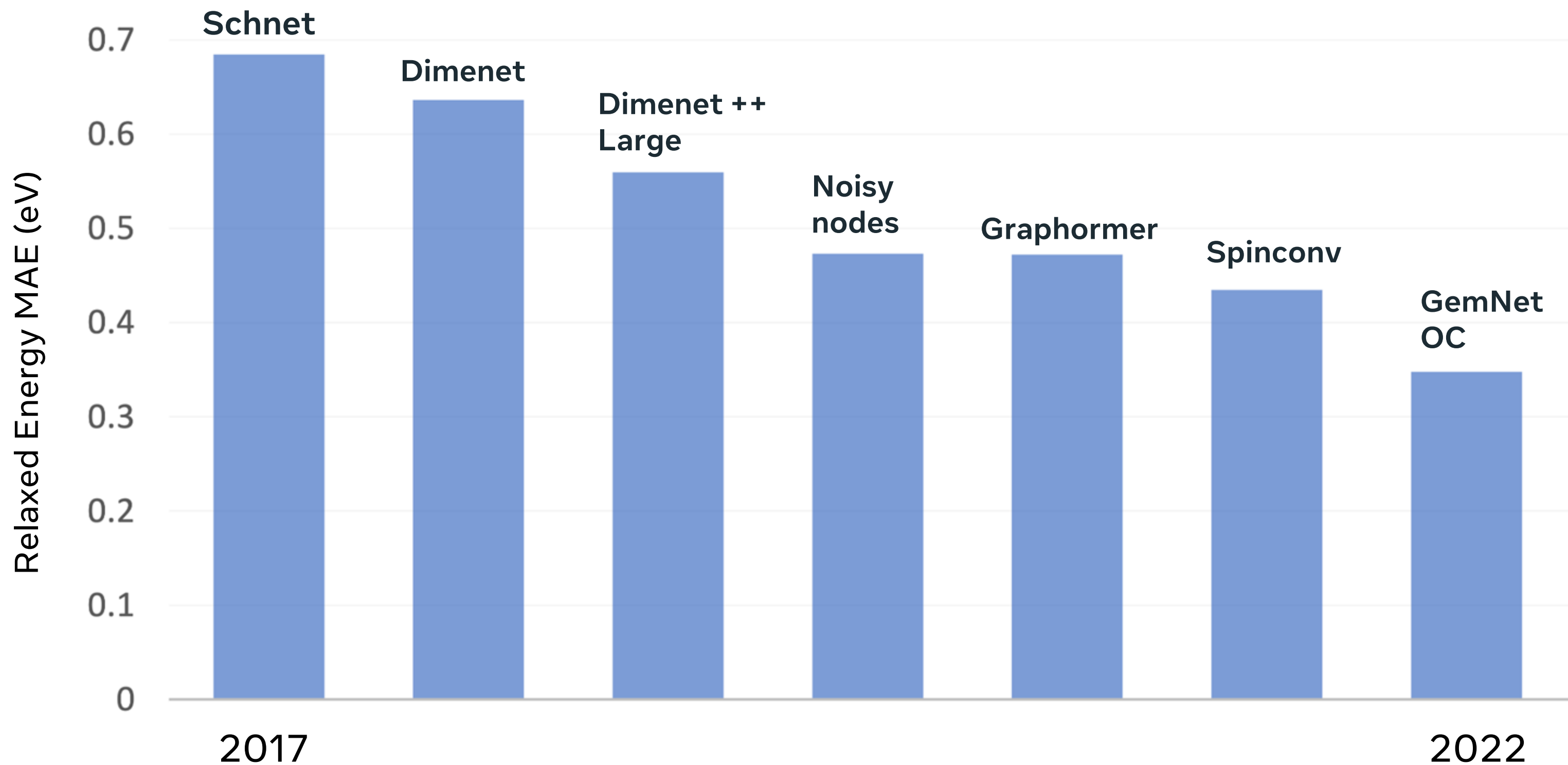
Edge = Neighbor



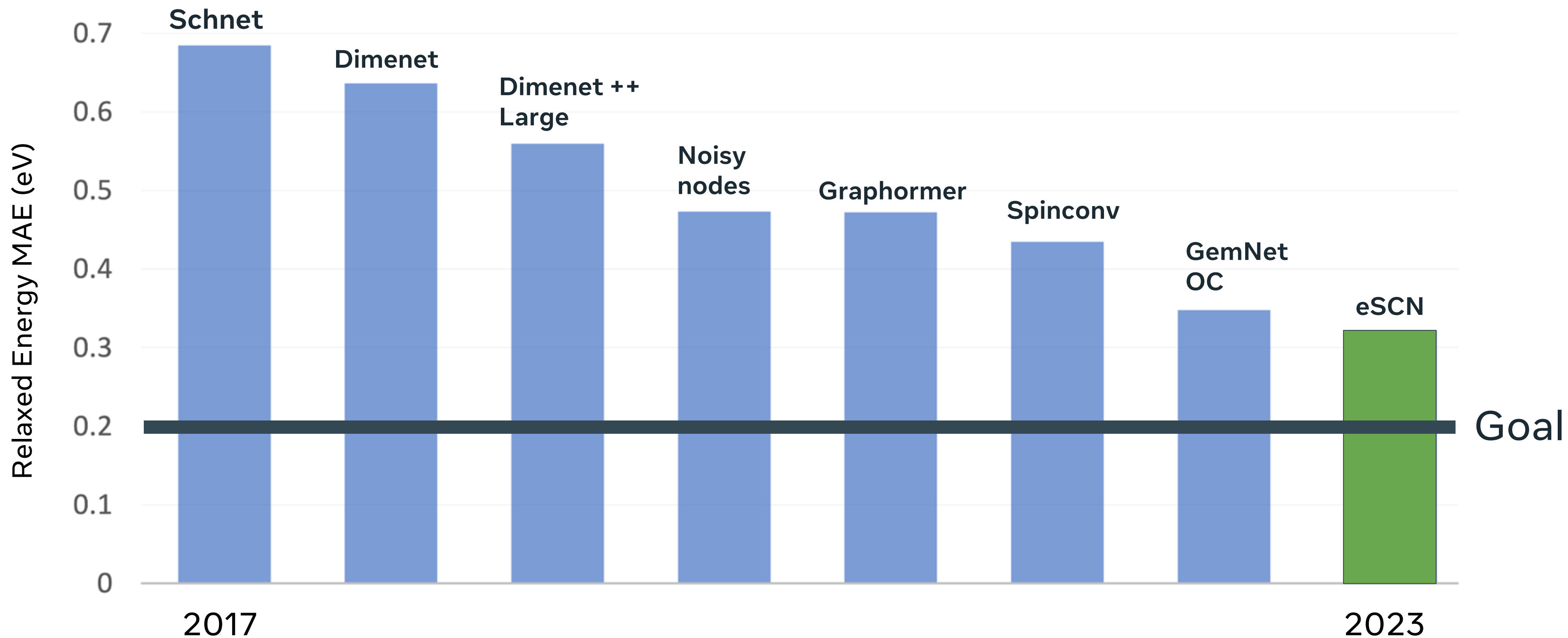
Spherical channels



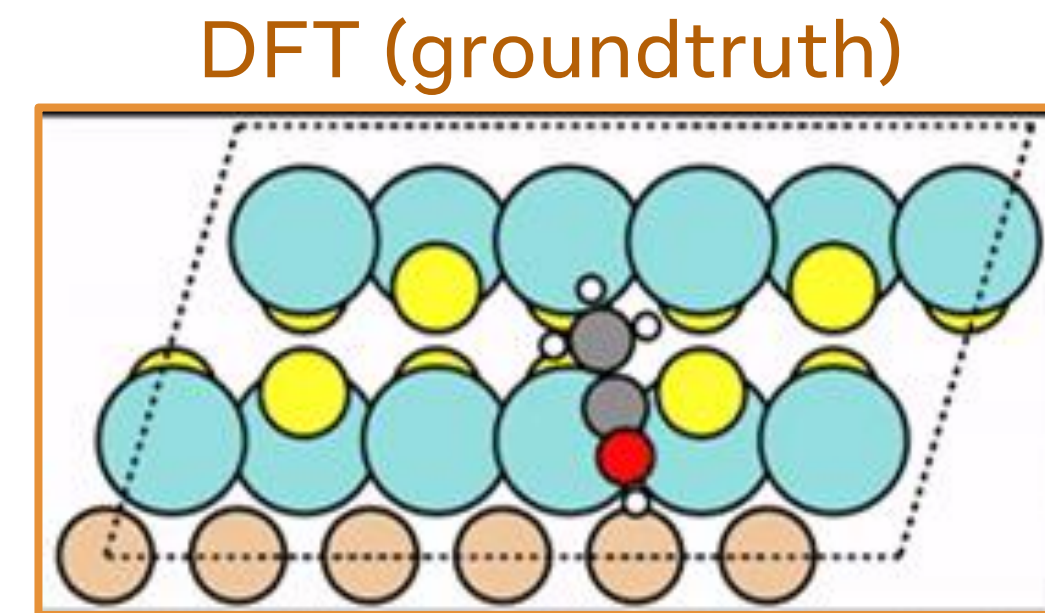
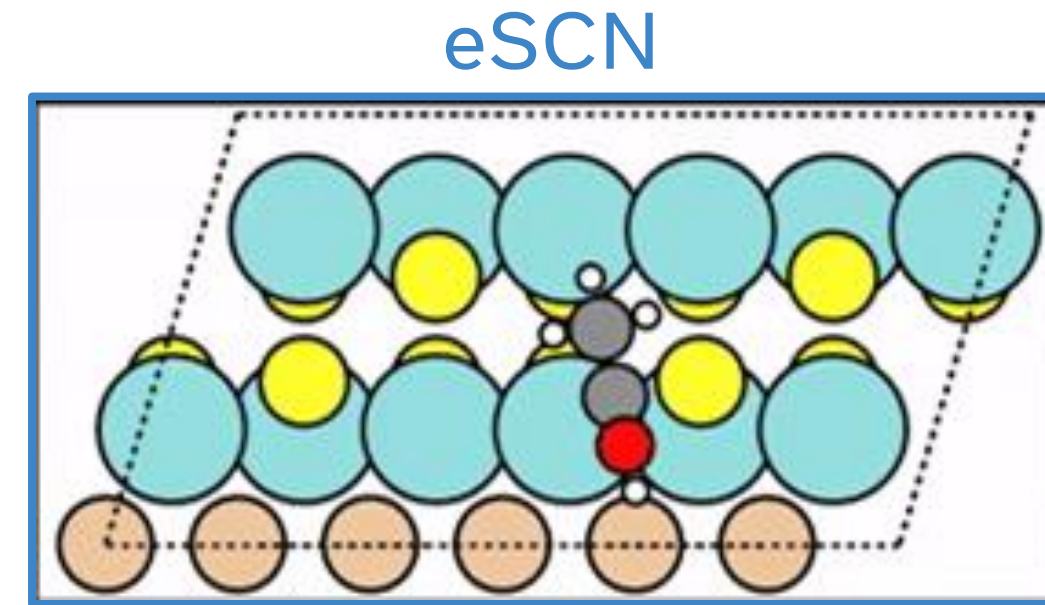
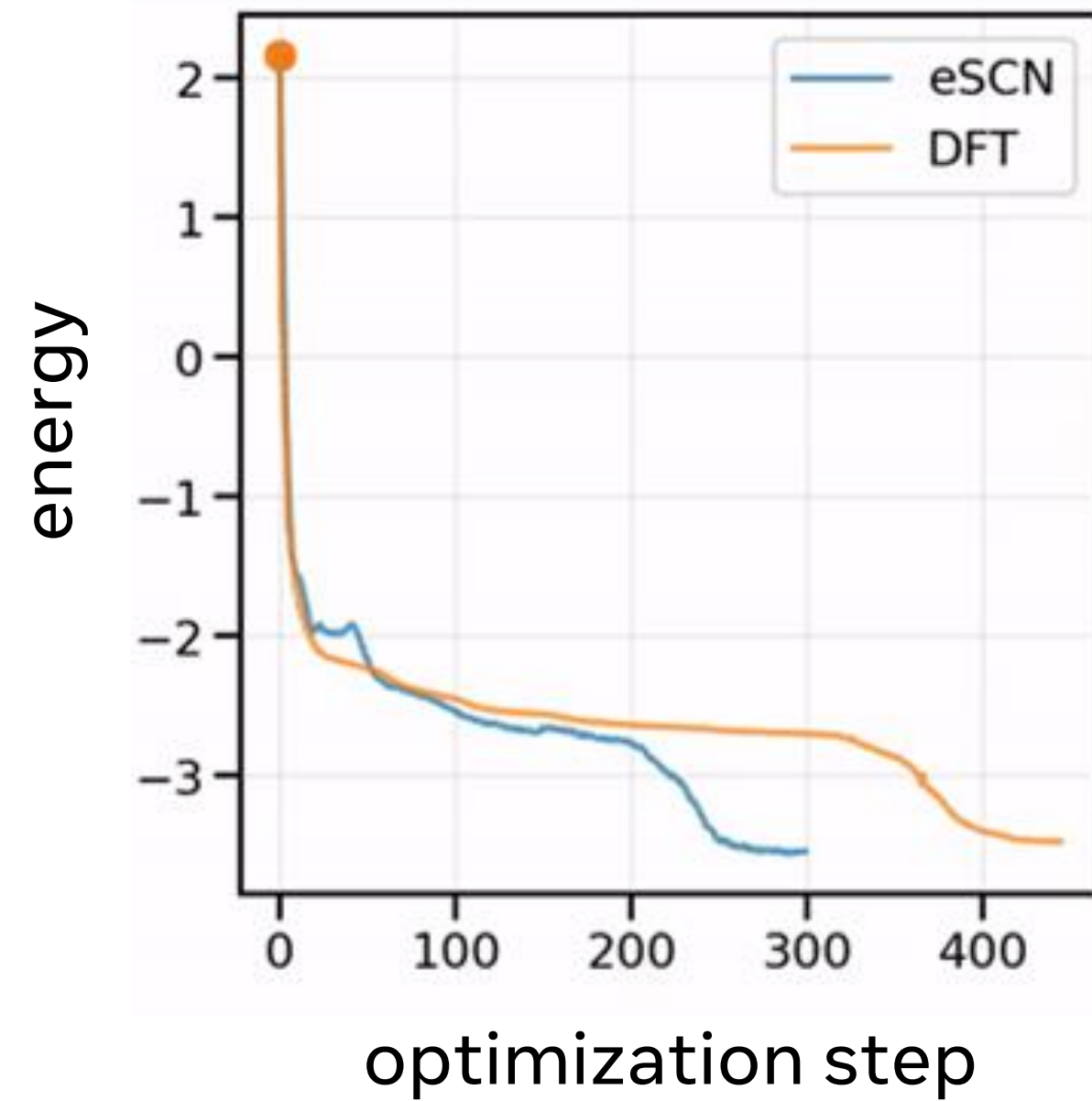
Results: Relaxed energy



Results: Relaxed energy



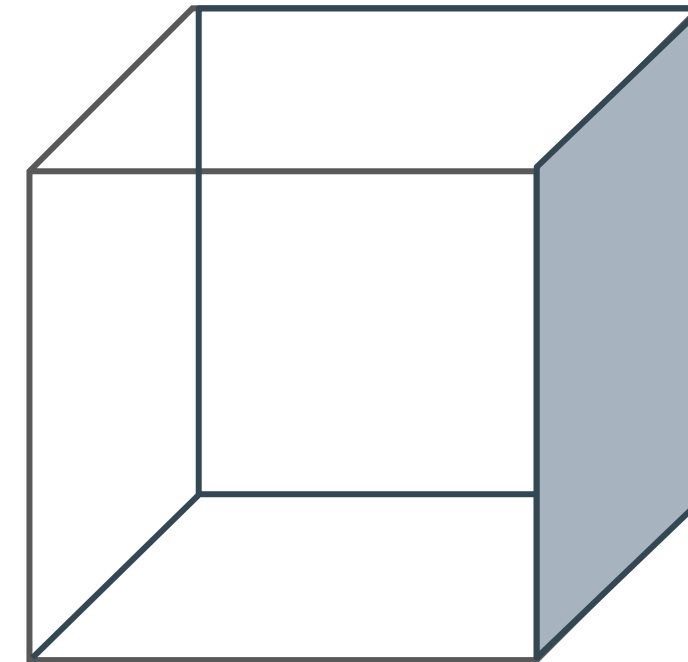
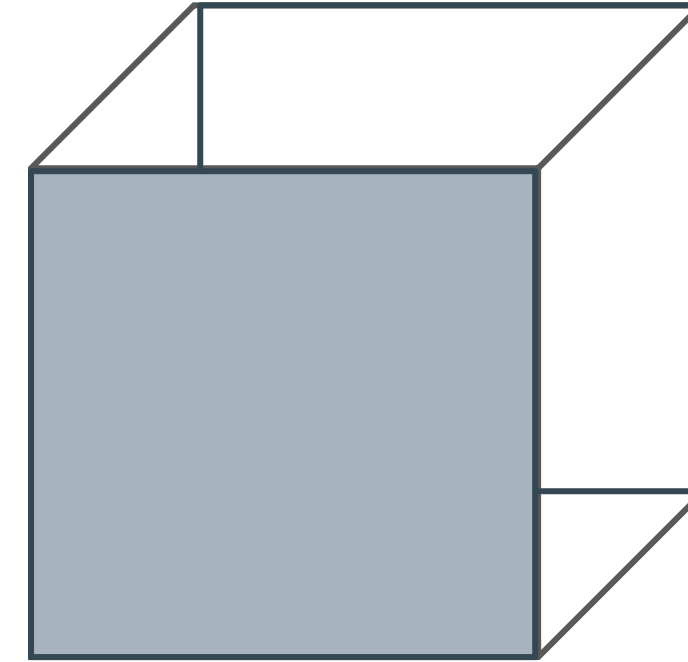
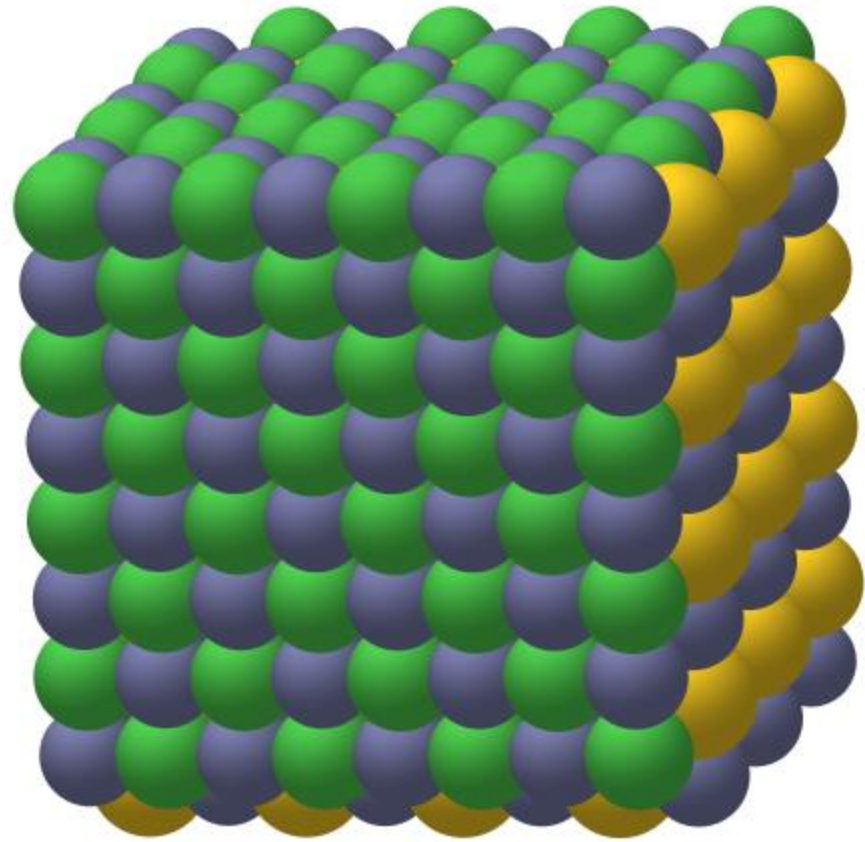
Relaxations



Screening a new material...

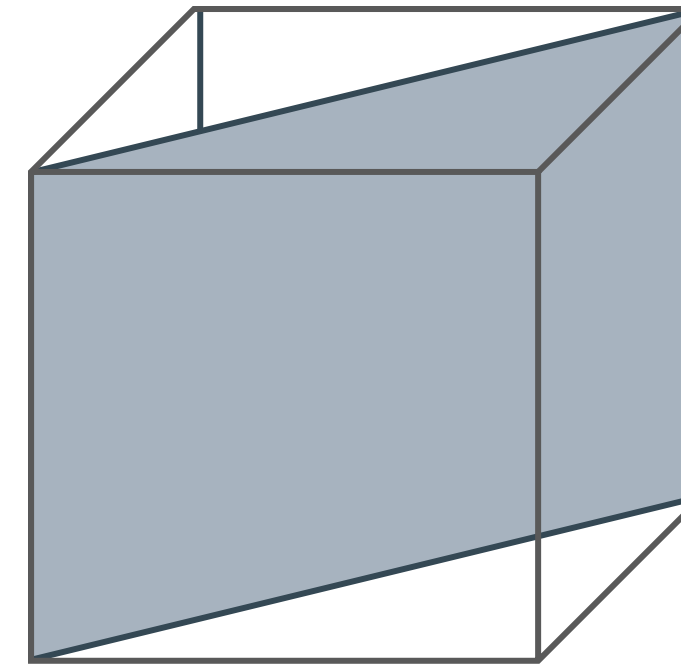
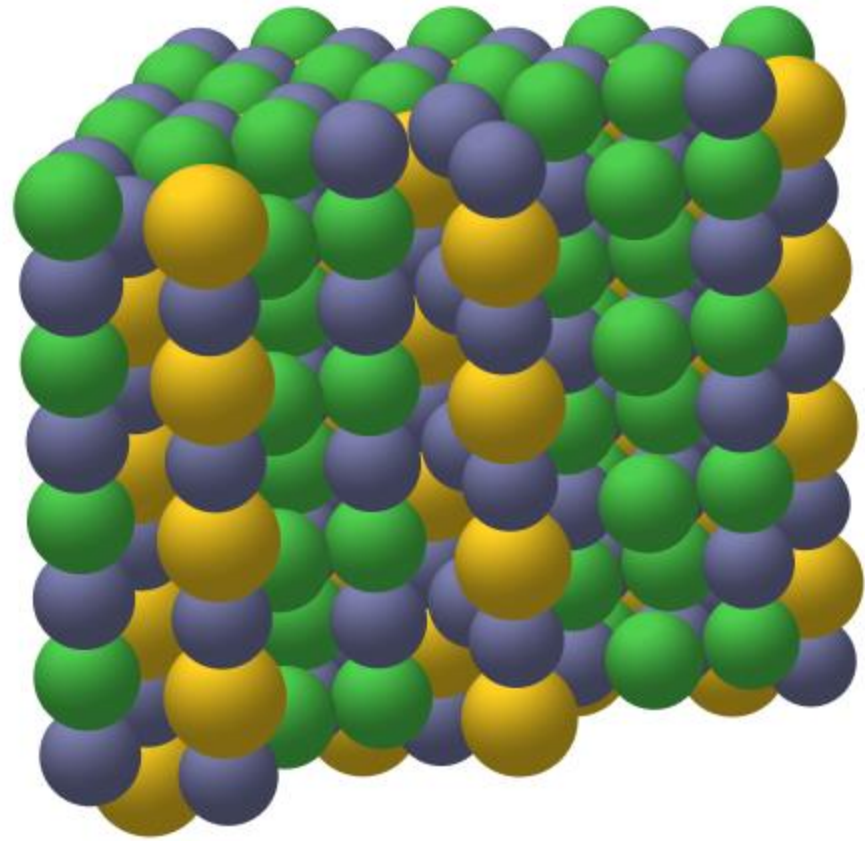
Bulk materials

How do you slice the material?



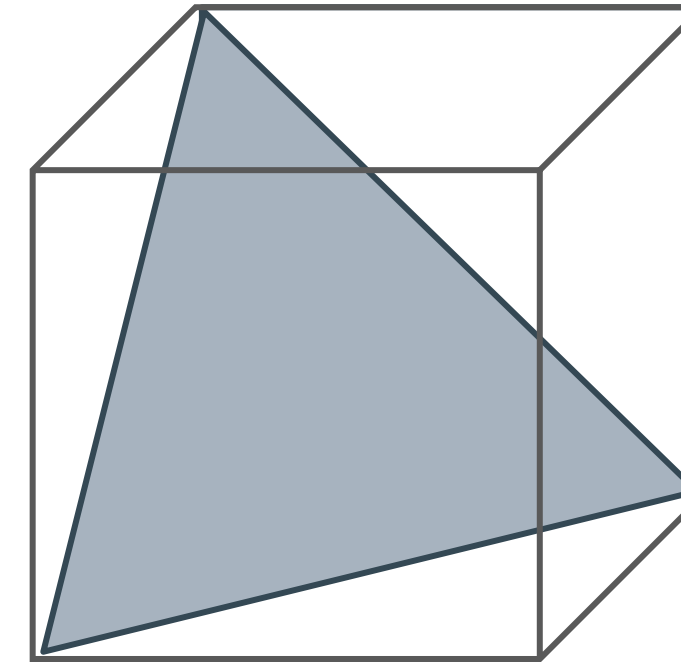
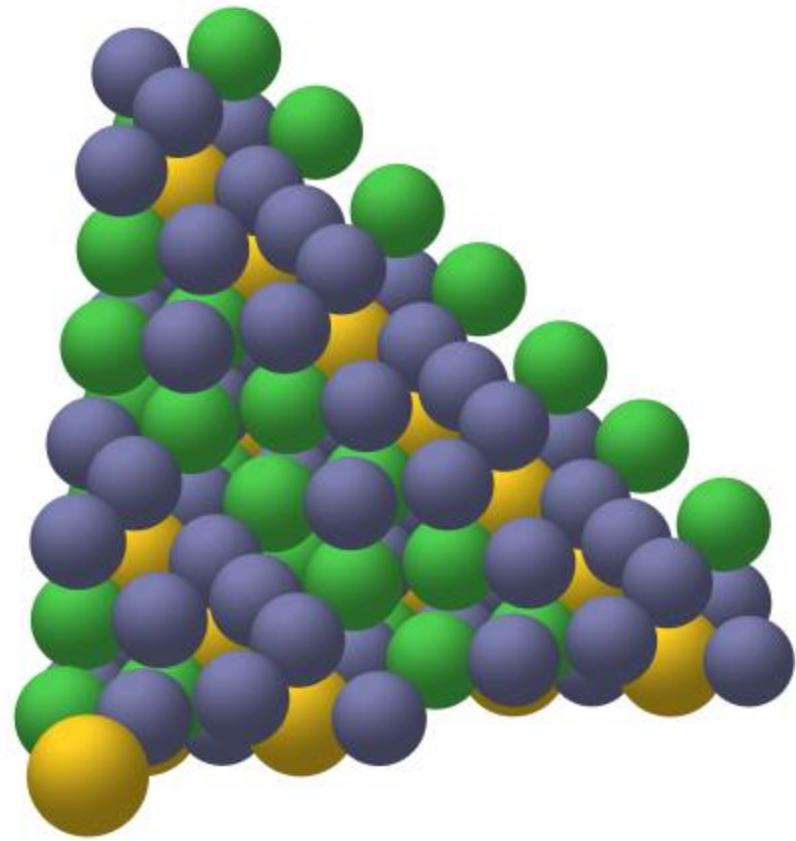
Bulk materials

How do you slice the material?



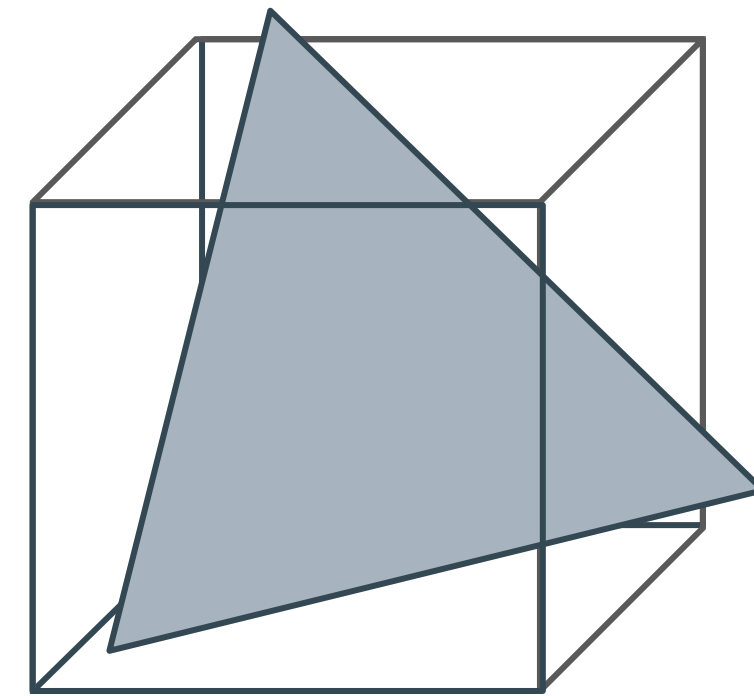
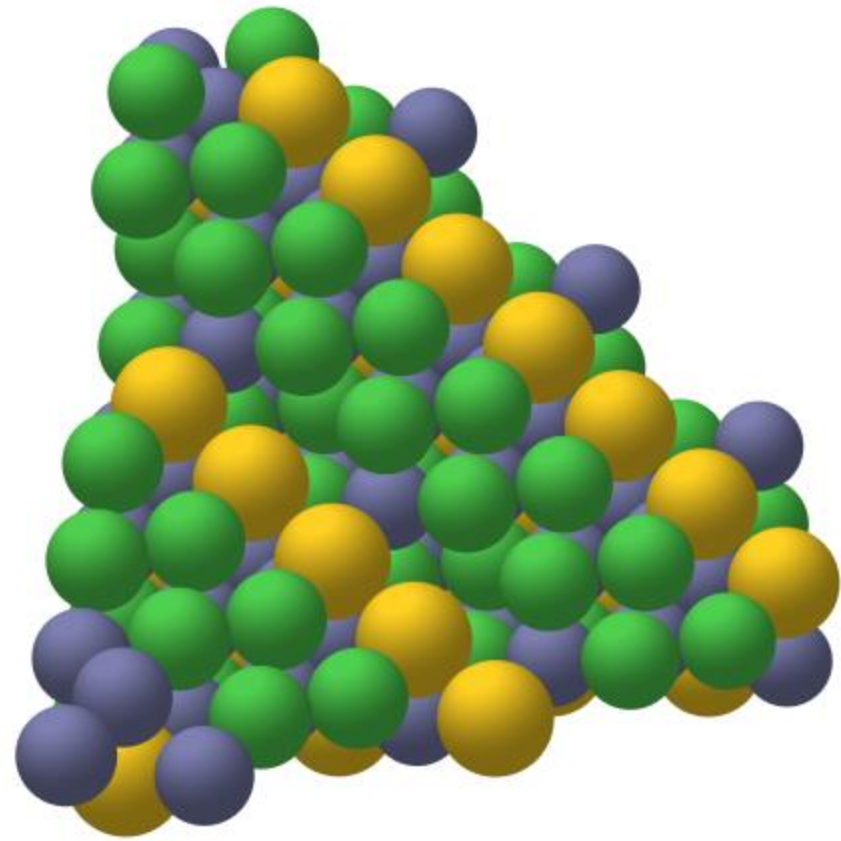
Bulk materials

How do you slice the material?



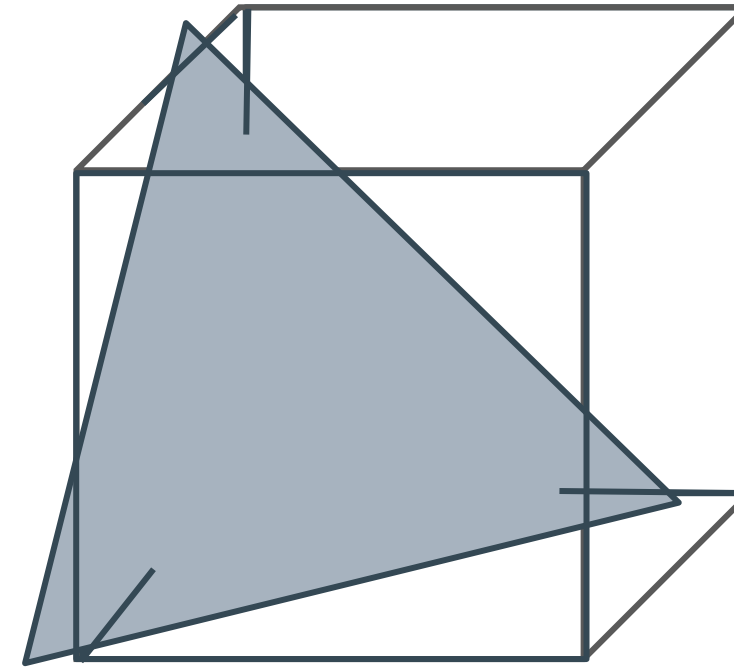
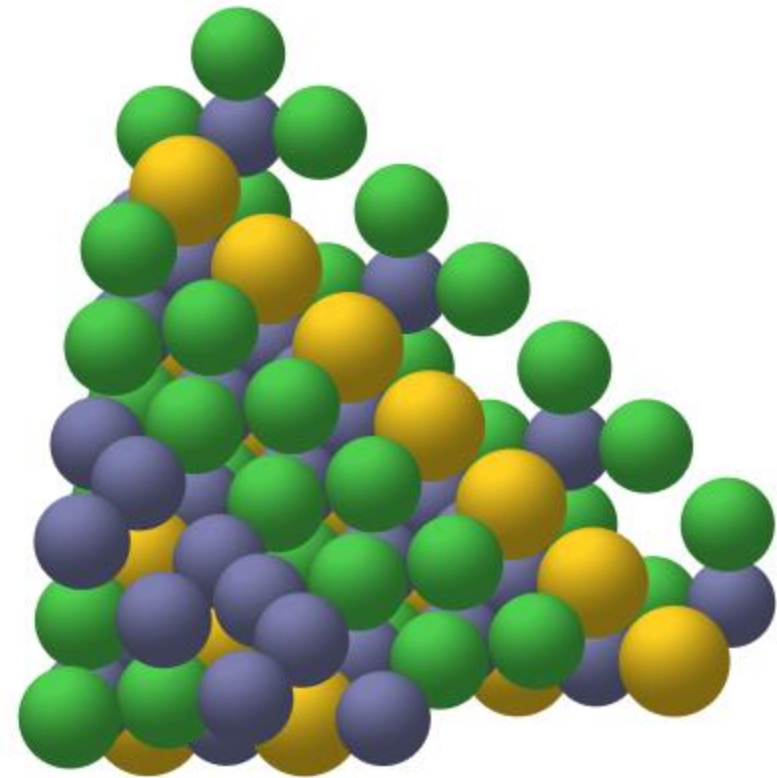
Bulk materials

How do you slice the material?



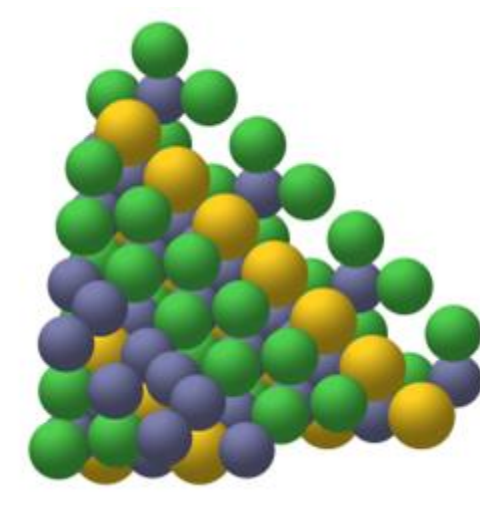
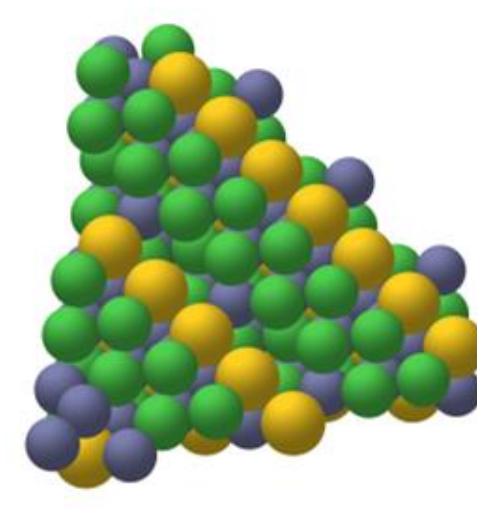
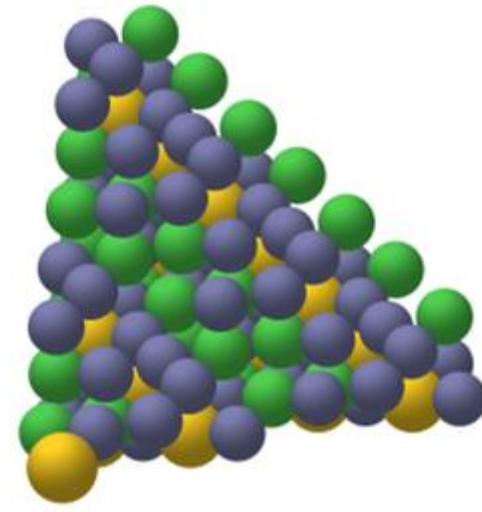
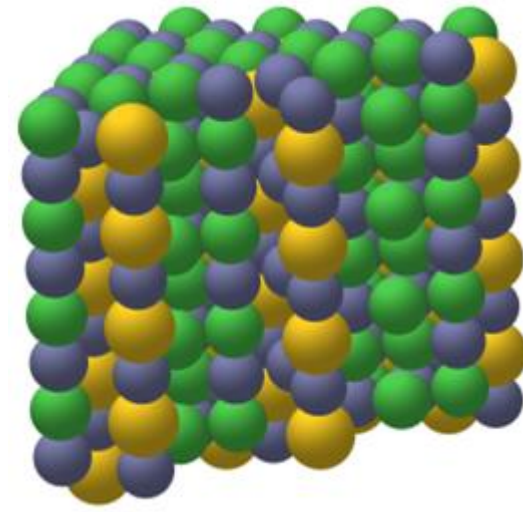
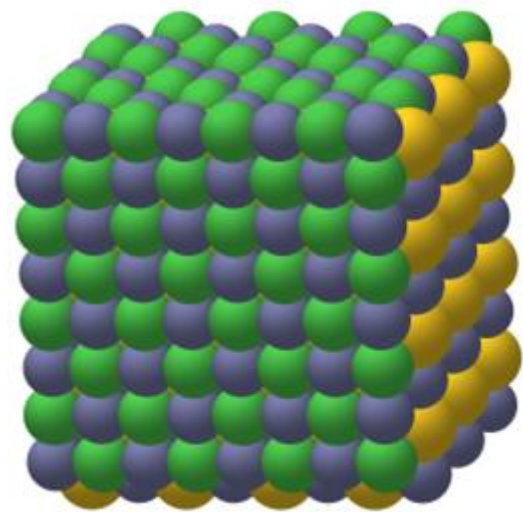
Bulk materials

How do you slice the material?



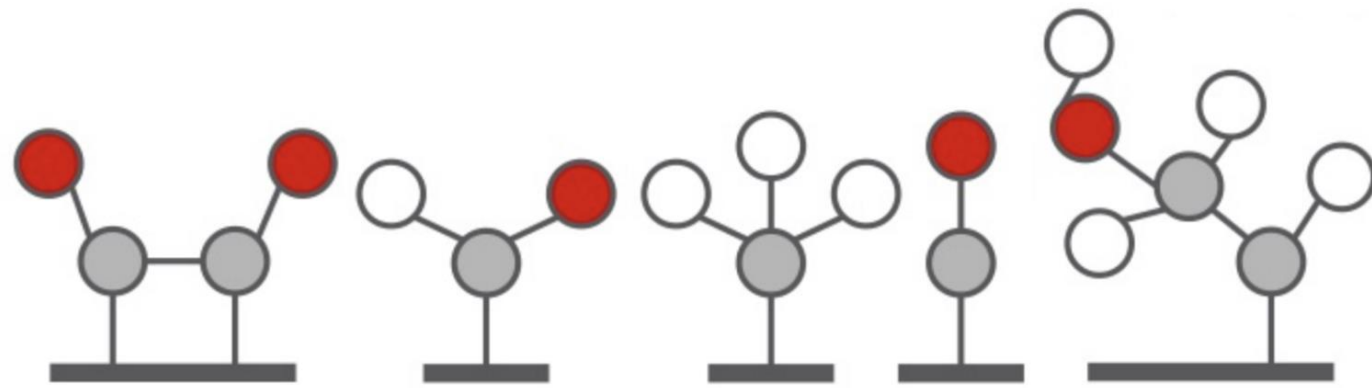
Bulk materials

~90 possible slices!

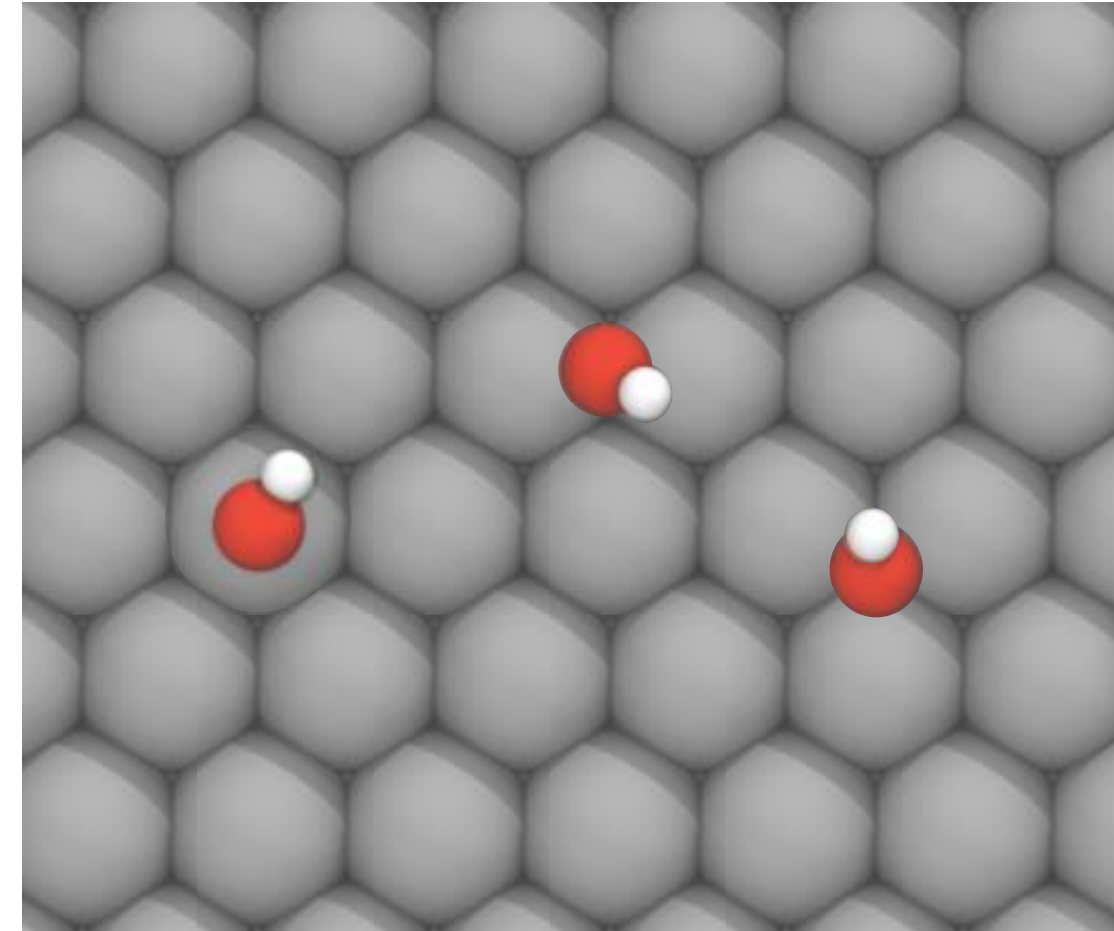


Adsorbates

~5 adsorbates of interest

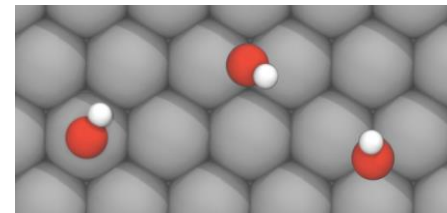
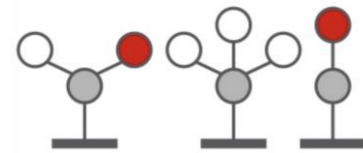
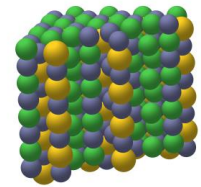


~100 different initial placements
for each adsorbate.



How many relaxations do we need?

90 slices x 5 adsorbates x 100 placements = 45,000 relaxations!



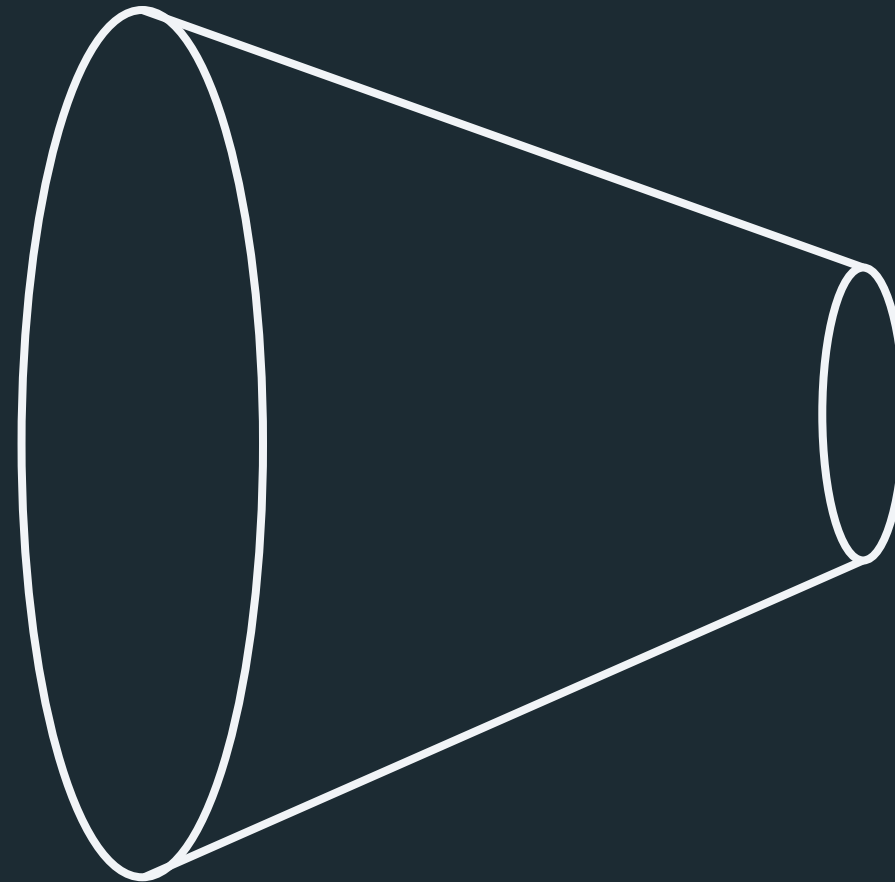
DFT = 120 CPU* years!

ML + DFT = 2.5 GPU days + 70 CPU* days

How many known materials are there?

Materials Project

155k



Stable in reaction conditions

6k

Generative AI!

Make-A-Video



Sailboat sailing on a sunny day in a mountain lake, highly detailed

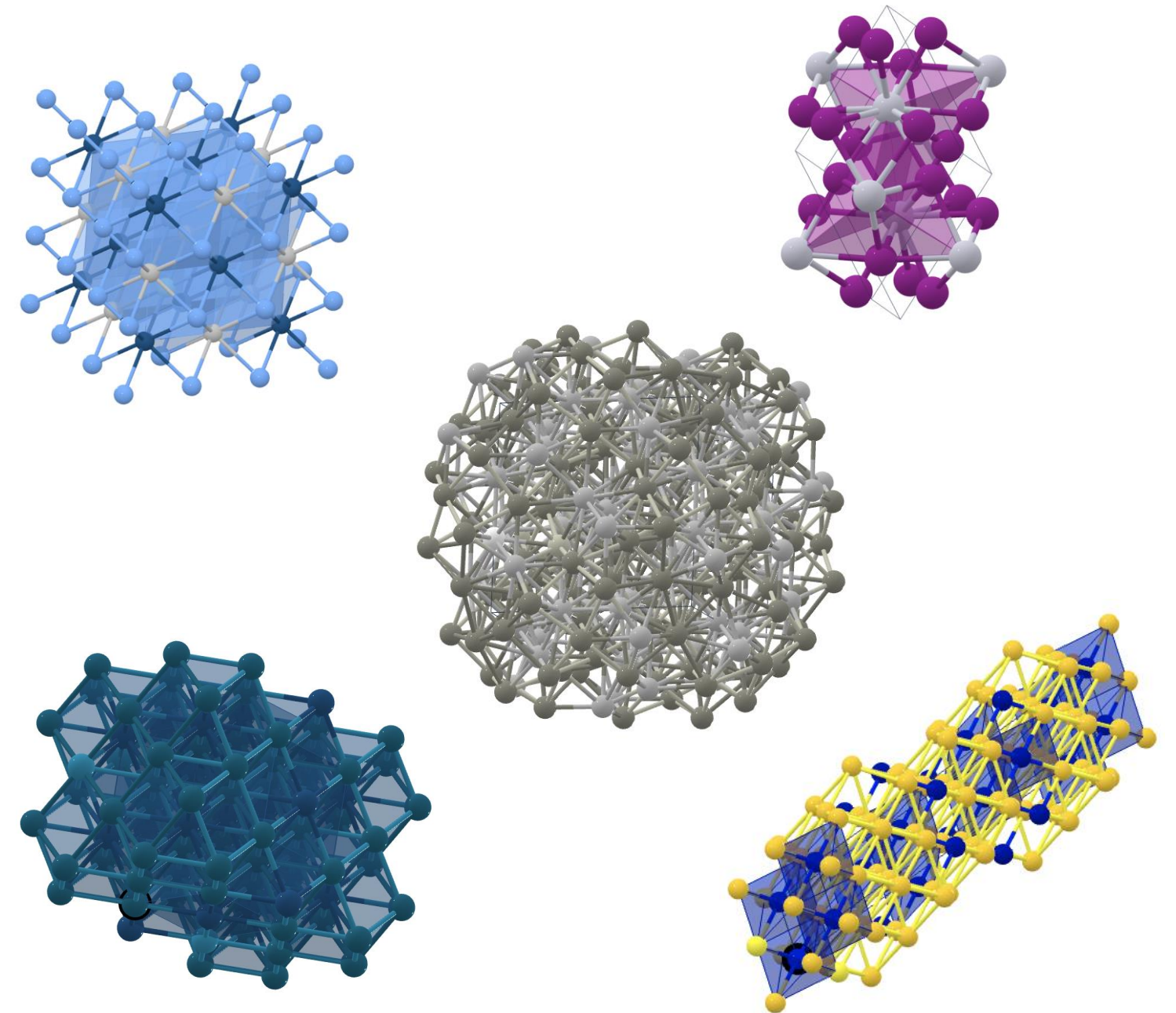


A confused grizzly bear in calculus class



A ballerina performs a beautiful and difficult dance on the roof of a very tall skyscraper; the city is lit up and glowing behind her

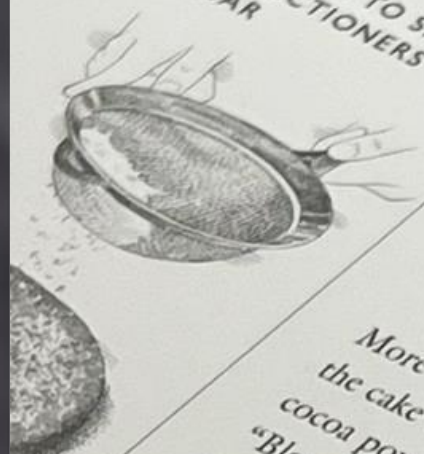
<https://makeavideo.studio/>



<https://materialsproject.org/>



BEST WAY TO SIFT CONFECTIONERS' SUGAR



WHY THIS RECIPE WORKS
This easy wartime cake made with just a few ingredients (flour, sugar, cocoa powder, baking soda, vanilla, and mayonnaise, a stand-in for butter and eggs) had a lot of good things going for it, but chocolate flavor wasn't one of them. We changed that.

DEEPEN THE CHOCOLATE FLAVOR
More than a half-cup of cocoa would turn the cake dry and chalky so we supplement the cocoa powder with a little melted chocolate. "Blooming" the cocoa powder in hot water intensifies its flavor, and using hot coffee instead of water enriches the flavor even more. Chopping the dark chocolate fine means we can melt it in the hot coffee as well—no need for an extra pan.

ACCENT THE CHOCOLATE WITH COFFEE
A full cup of coffee adds moisture and brightens the chocolate flavor in this cake. Coffee also serves to give the chocolate a rich, deep flavor.

WHY THE MAYO
As for the mayonnaise—we won't be using it to make the cake richer by adding fat or eggs and we learned the hard way that emulsifiers like salt and vanilla. Stir mayonnaise into the batter until combined.

1. Adjust oven rack to middle position and heat oven to 350 degrees. Grease 8-inch square baking pan, line with parchment paper, and grease parchment and flour pan.

2. Whisk flour, sugar, baking soda, and salt together in large bowl. In separate bowl, combine cocoa and chocolate. Pour hot coffee over cocoa mixture and let sit, covered, for 5 minutes. Gently whisk mixture until combined, and vanilla. Stir mayonnaise into mixture until combined. Pour batter into prepared pan.

Easy Chocolate Cake

EASY CHOCOLATE CAKE
SERVES 8

Choose a high-quality chocolate for this cake. Instead of confectioners' sugar, the cake can be served with Whipped Cream (page 348).

- 1½ cups (7½ ounces) all-purpose flour
- 1 cup (7 ounces) sugar
- ½ teaspoon baking soda
- ¼ teaspoon salt
- ½ cup (1½ ounces) Dutch-processed cocoa powder
- 2 ounces bittersweet chocolate, chopped
- 1 cup brewed coffee, hot
- ¾ cup mayonnaise
- 1 large egg, room temperature
- 2 teaspoons vanilla extract
- Confectioners' sugar (optional)

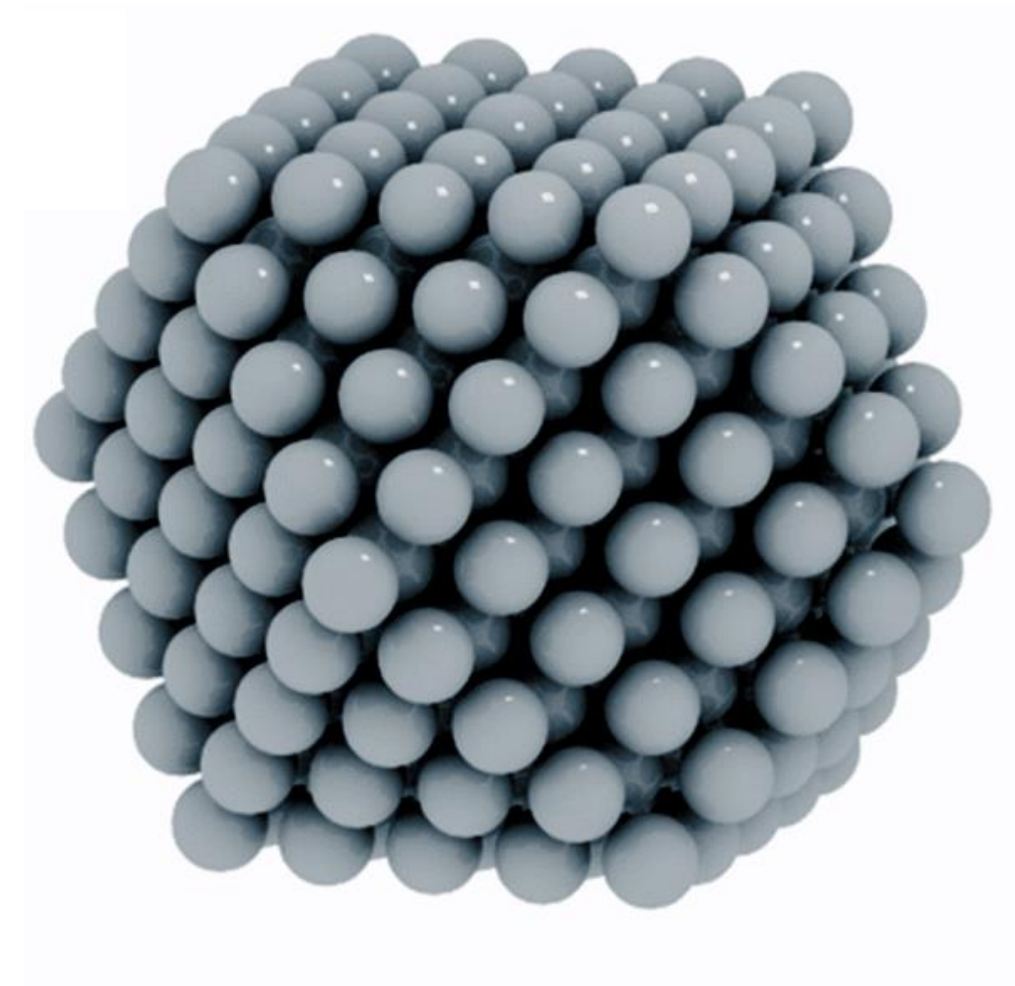
ADD
apple snack.
But applesauce
apple flavor is
applesauce mak
fresh apples
other

You pour in 20% platinum and 80% copper what do you get?

Which crystal structure?

Which facets?

Does it create a uniform material?





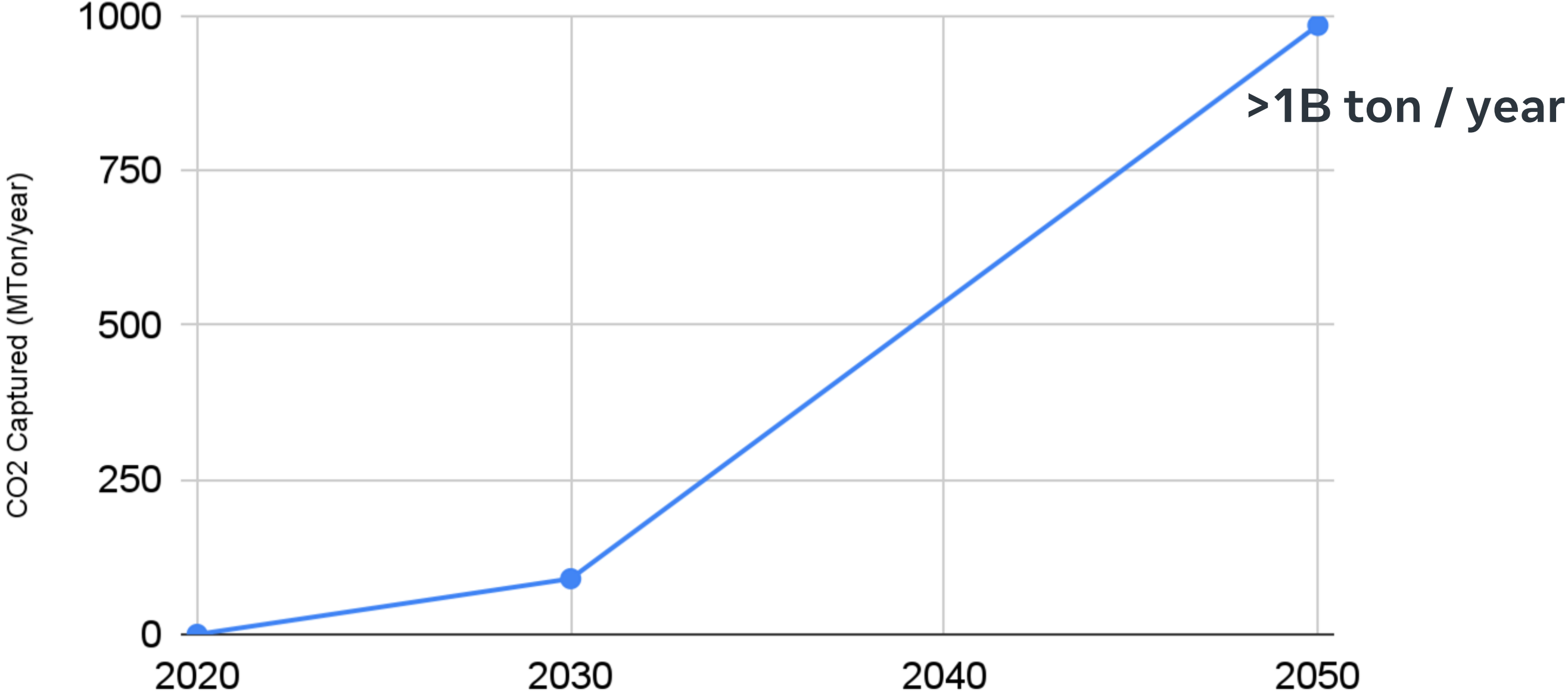
UNIVERSITY OF
TORONTO



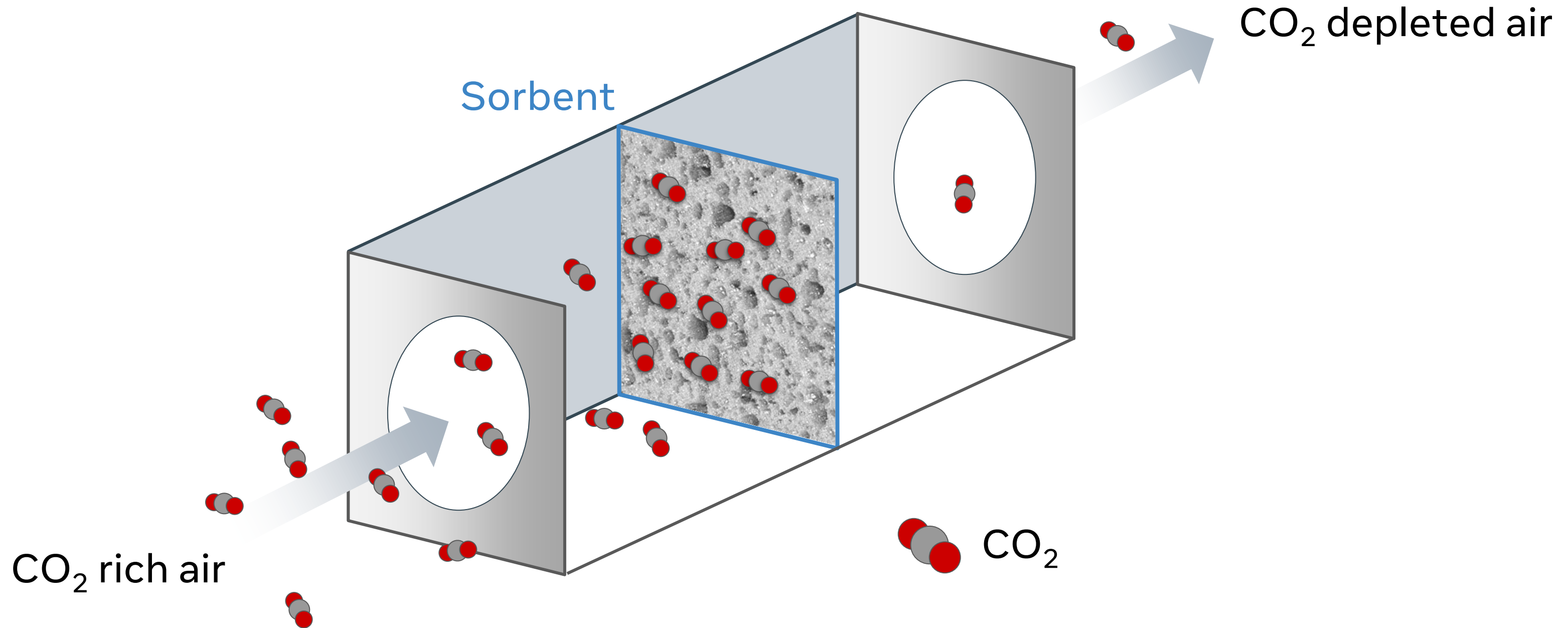
Direct Air Capture

Direct Air Capture

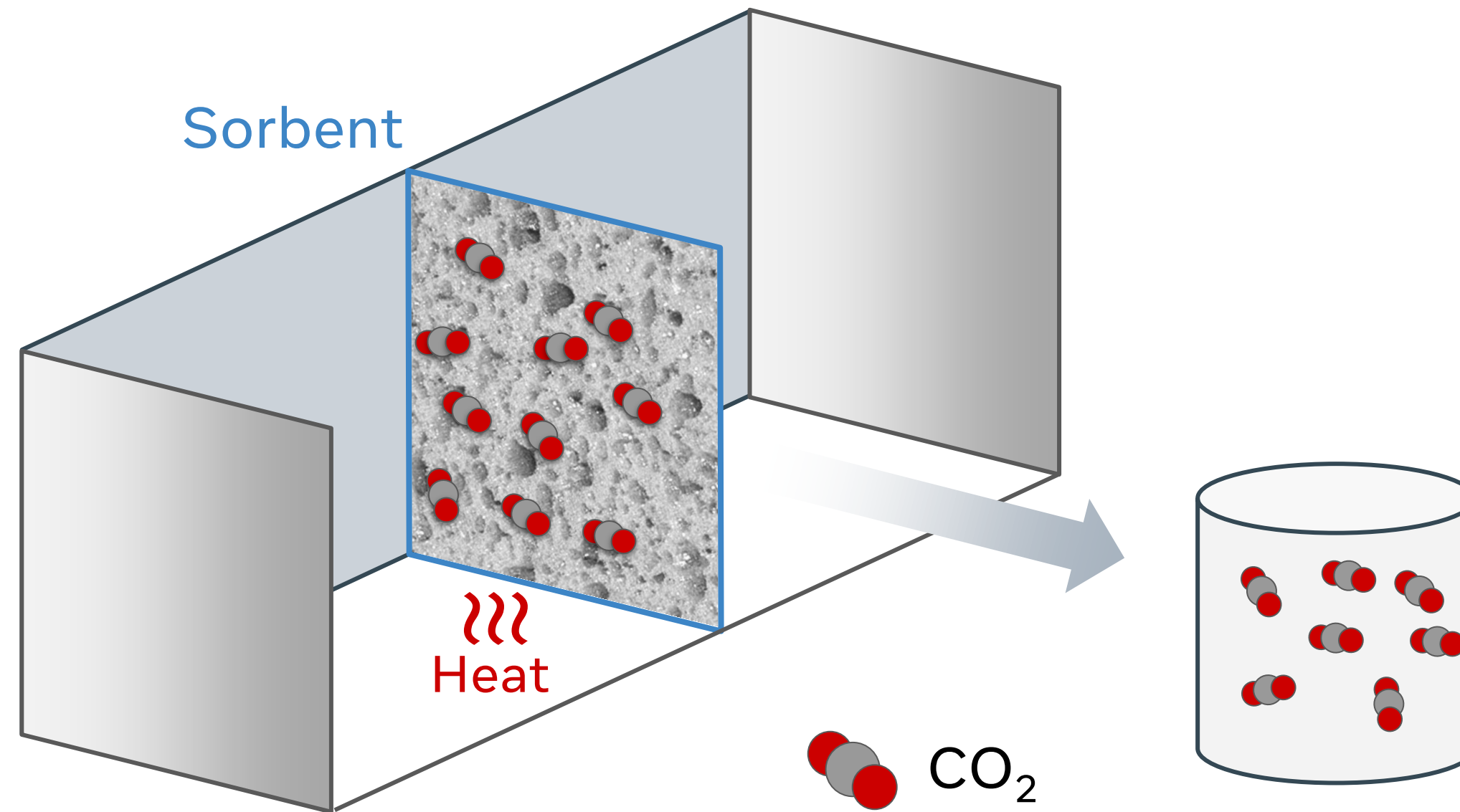
IEA Net Zero by 2050



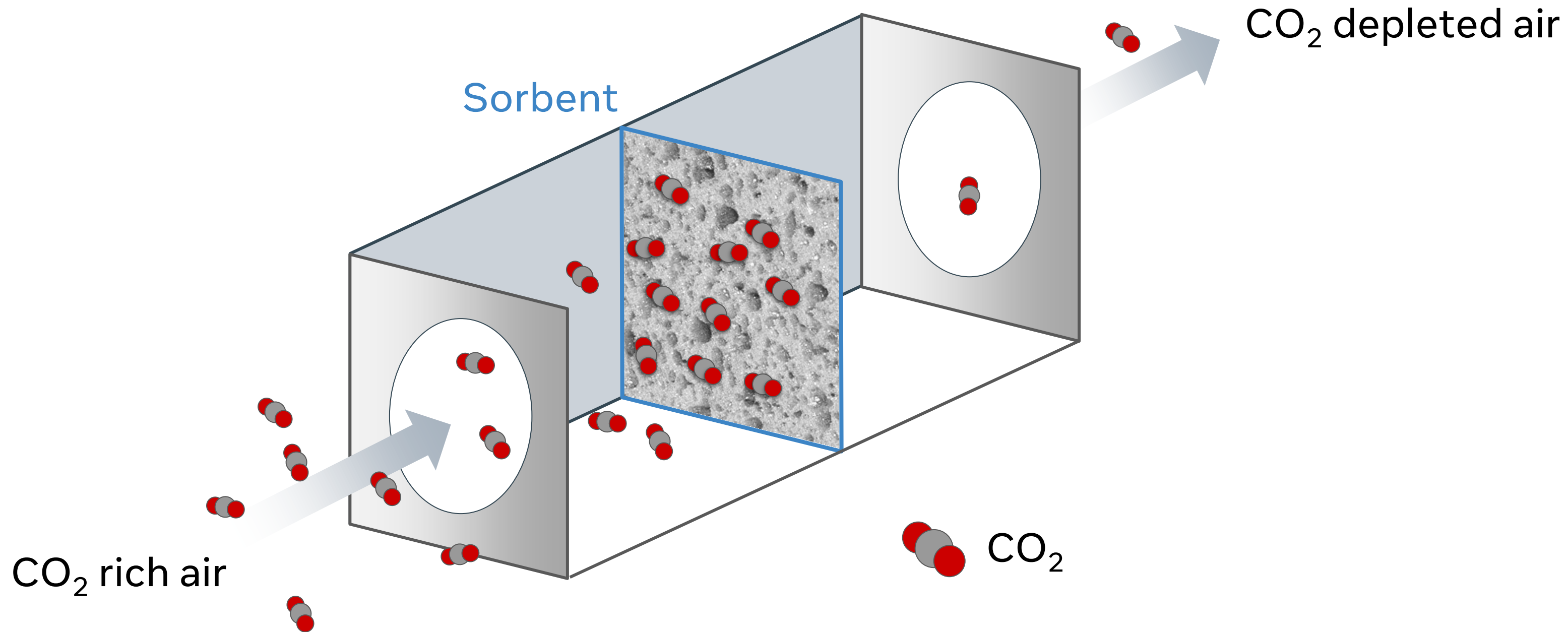
OpenDAC



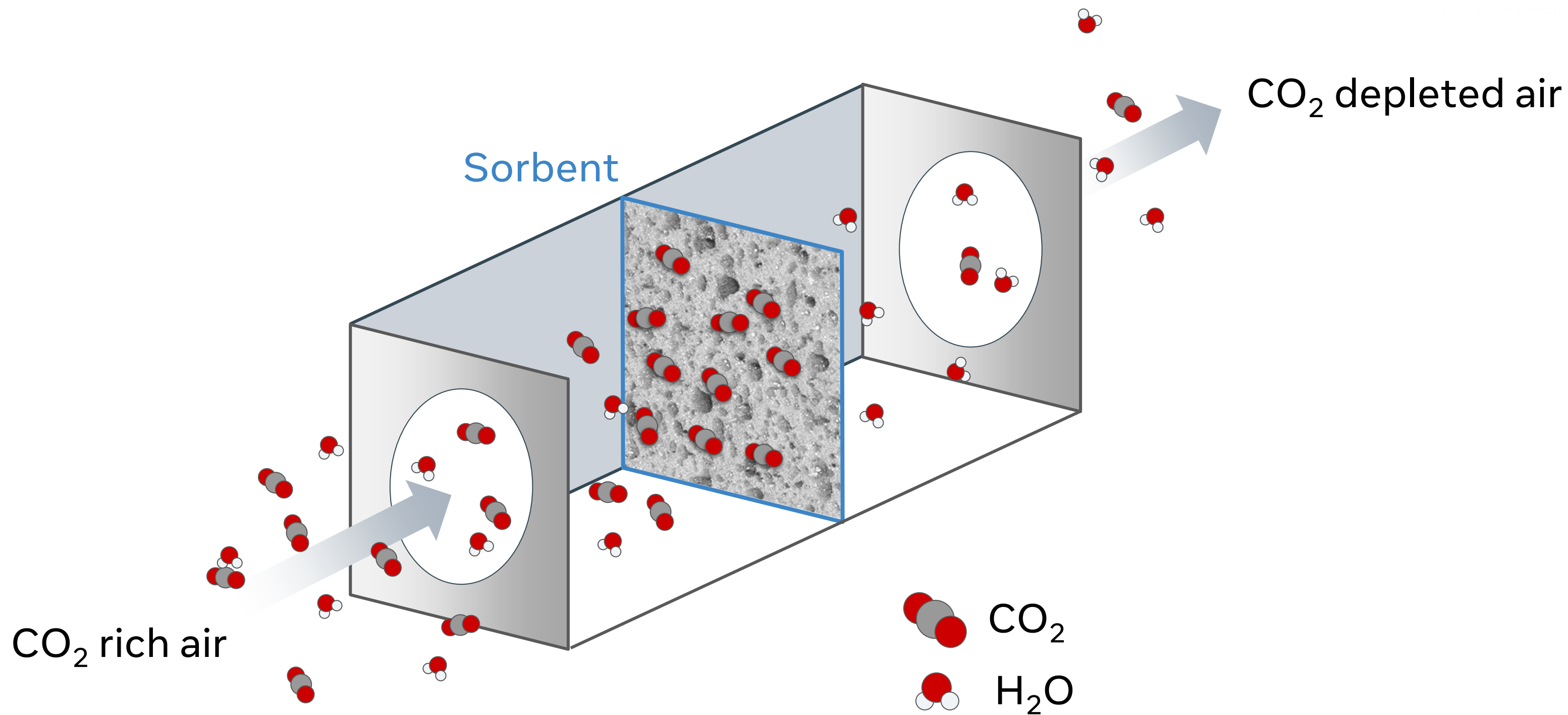
OpenDAC



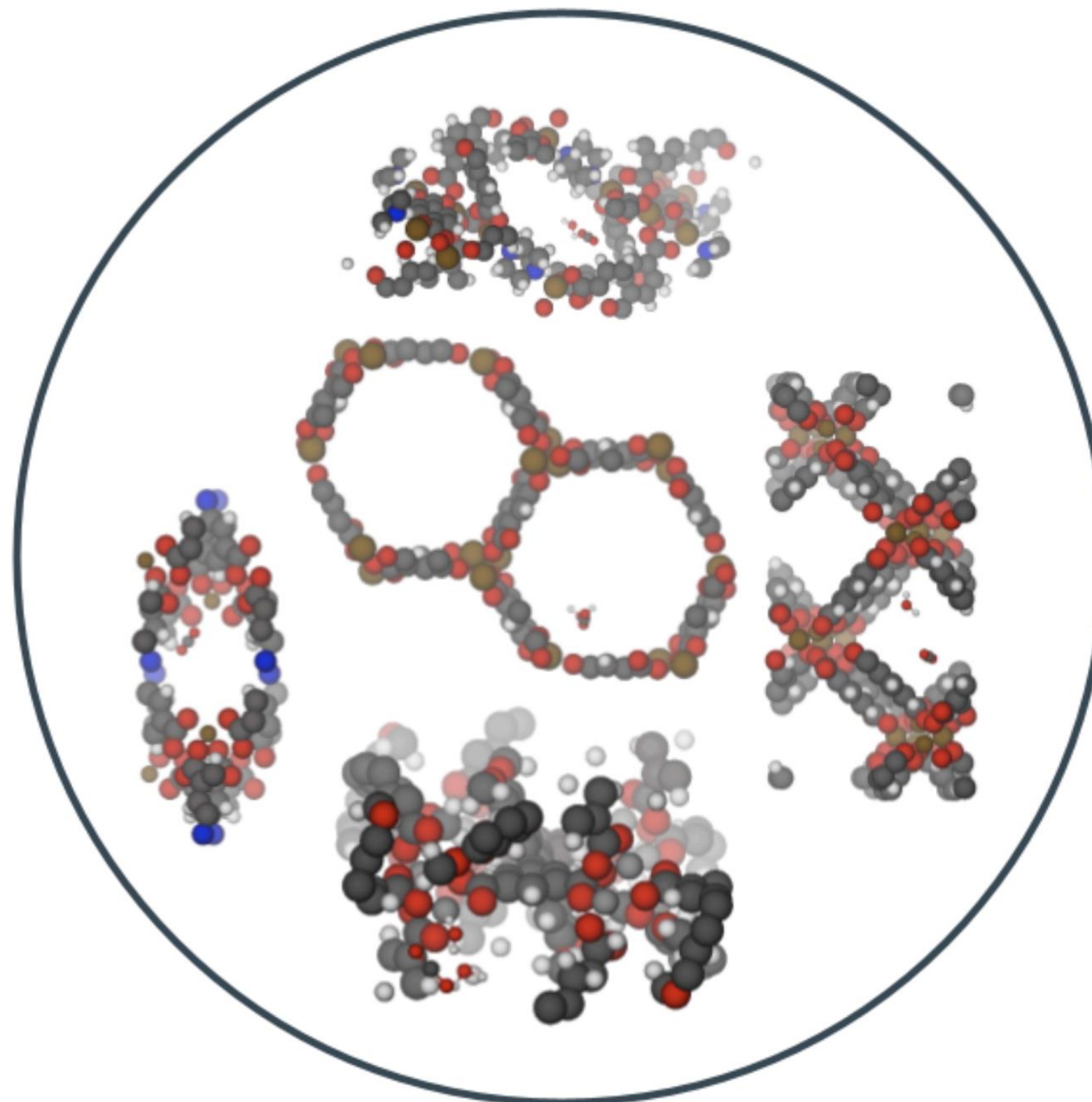
OpenDAC



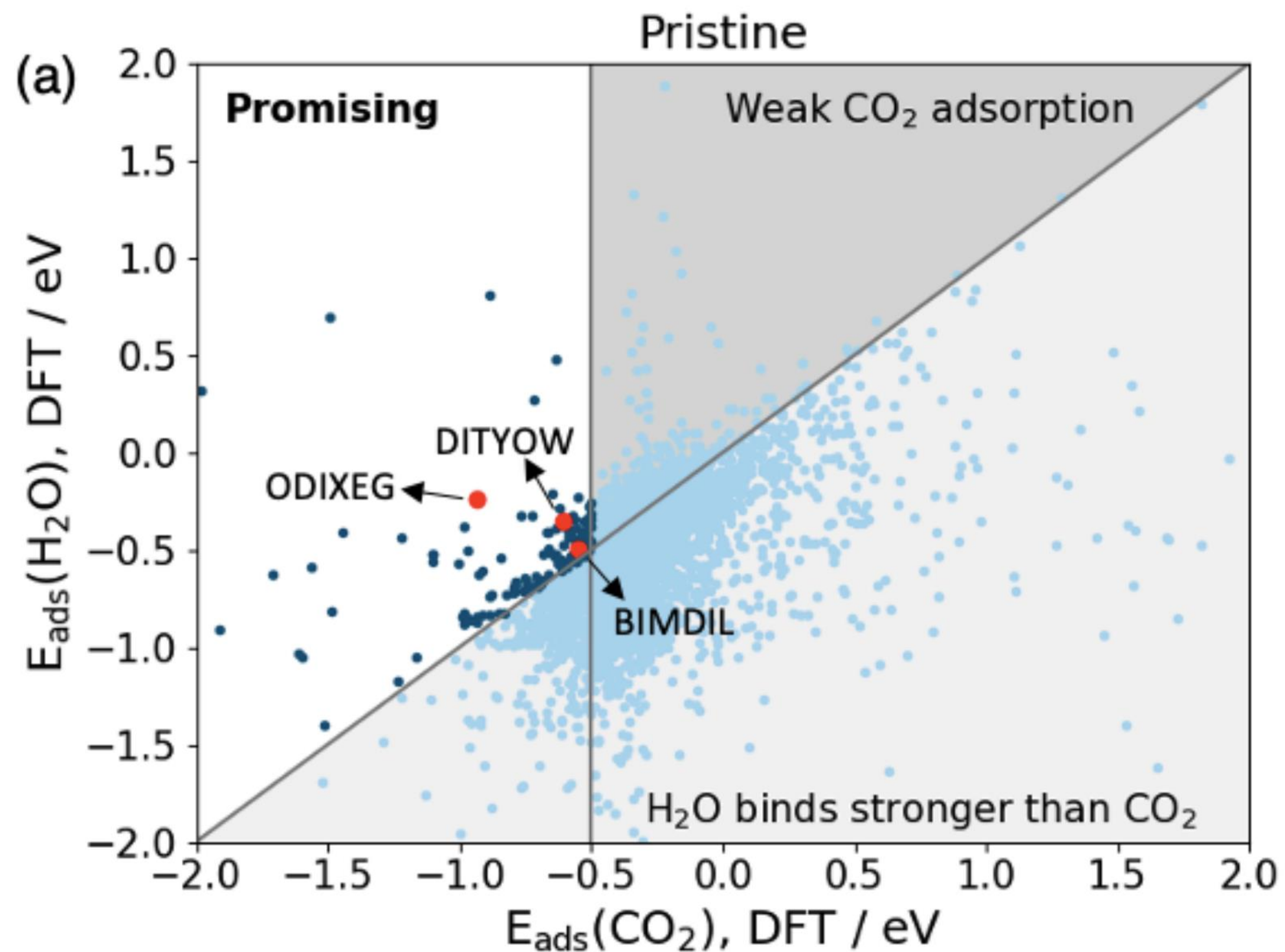
OpenDAC



OpenDAC23



OpenDAC23



AI Datacenters

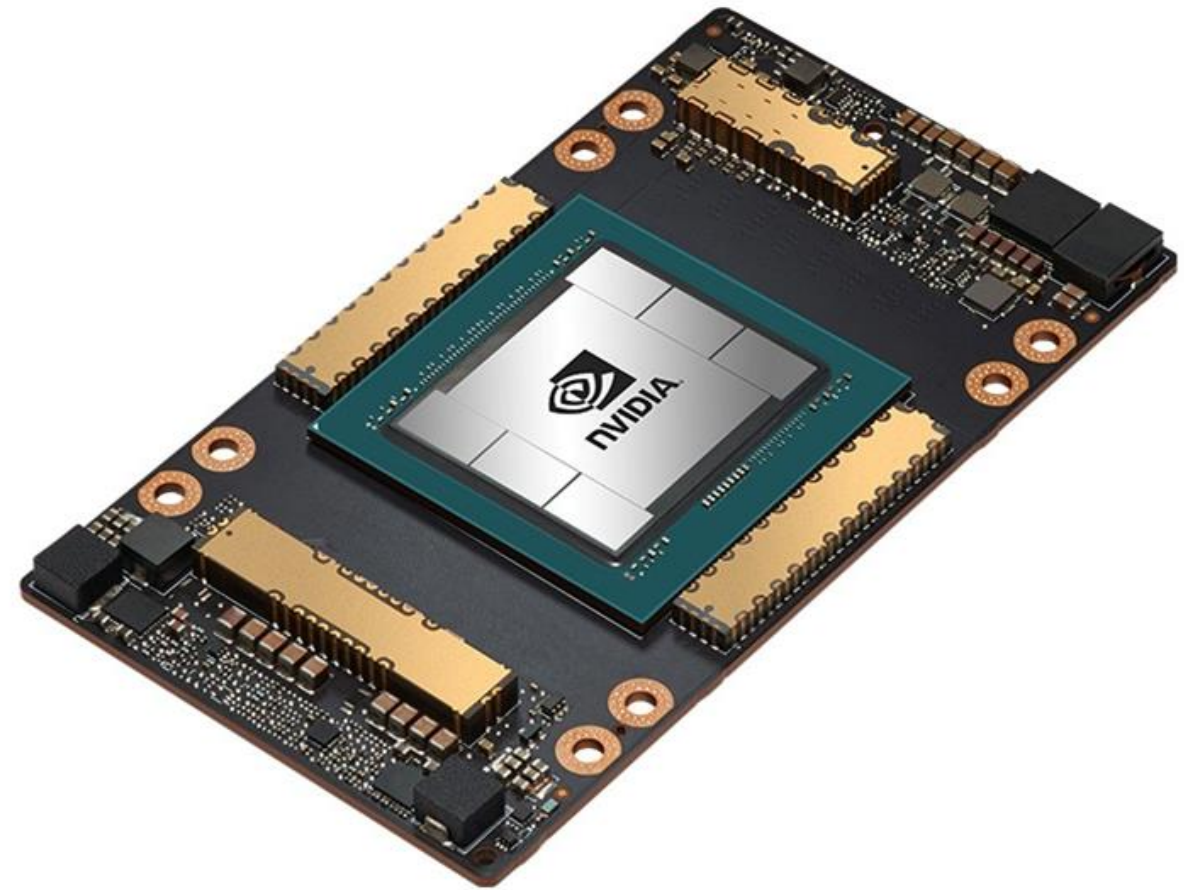
What if we interacted with AIs for 1 billion hours per day?

Let's assume it takes one A100 to power an AI.

An A100 requires 400W plus a PUE of 1.1...

...results in 160 TWh of power required per year.

A100



160 TWh (scenario 1)

0.5% of the world's electricity

Roughly doubles the power required by datacenters worldwide.

@ \$0.08 per kWh = \$12.8 Billion

0.86 pounds of CO₂ are emitted per kWh in the US

70 million metric tons of CO₂ per year

@ \$200 per ton = \$14 Billion

160 TWh (scenario 2)*

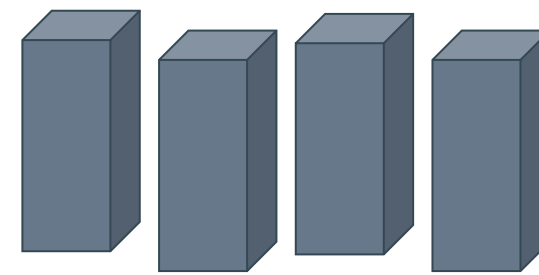
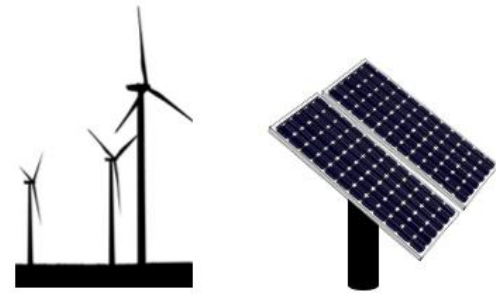
@ \$0.02 per kWh for solar = \$3.2 Billion

0 pounds of CO₂ are emitted per kWh of solar power in the US

\$26.8 Billion vs. \$3.2 Billion
(scenario 1) (scenario 2)

*only runs for ~8 hours a day

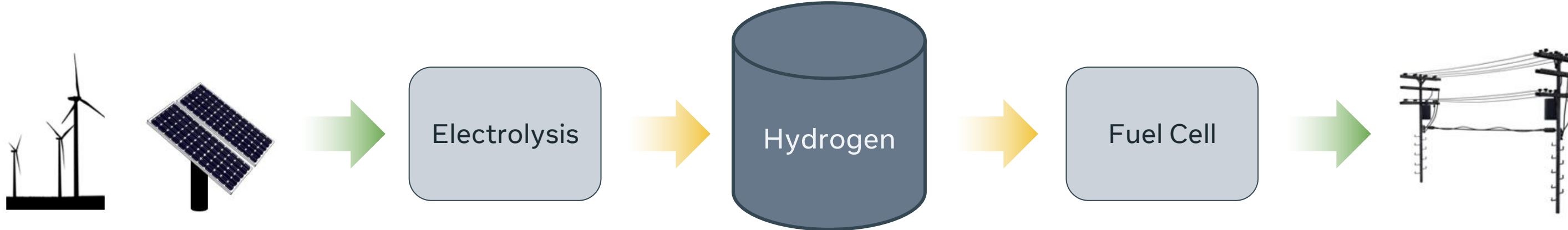
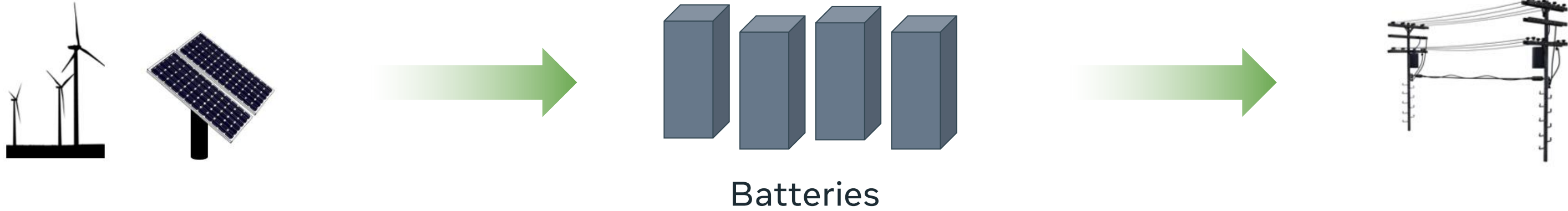
Renewable energy storage



Batteries

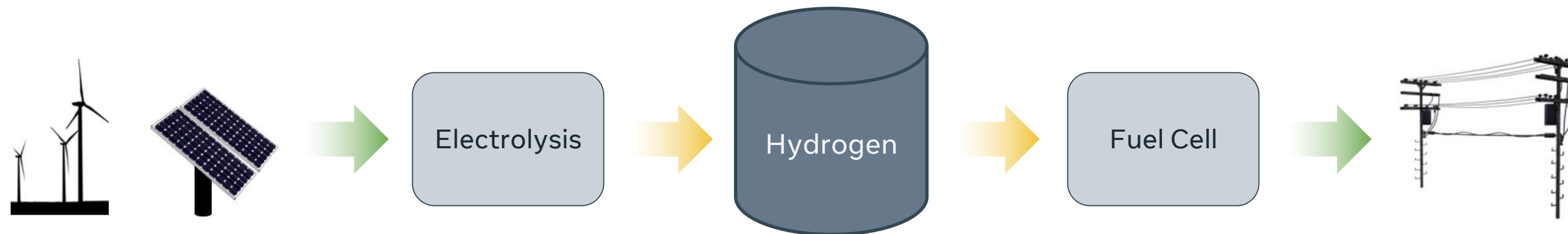
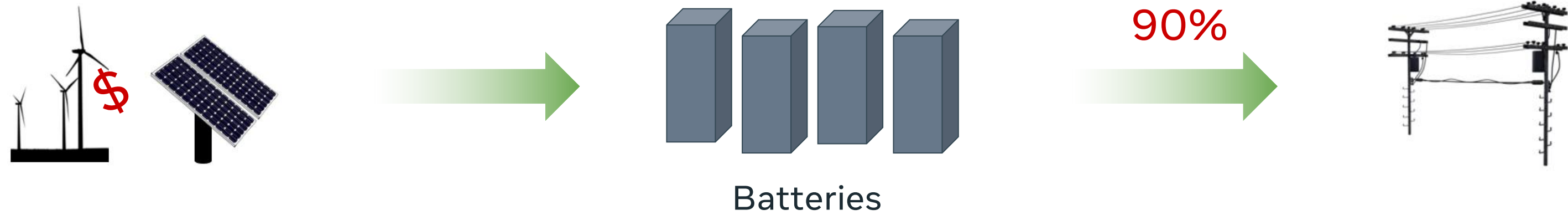


Renewable energy storage

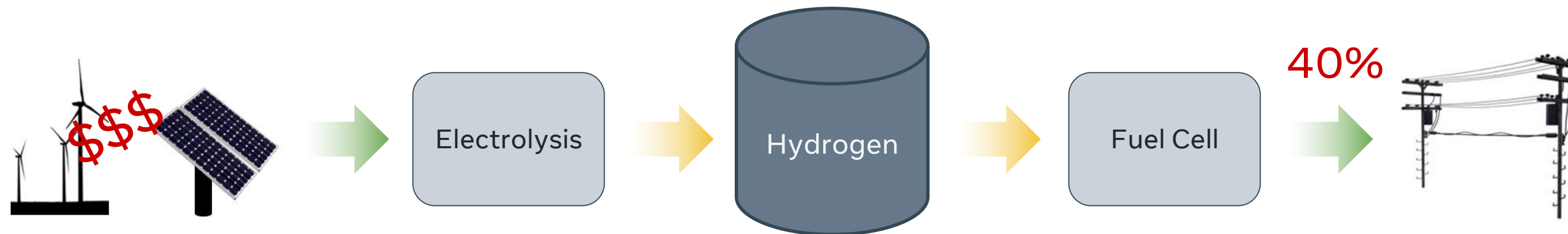
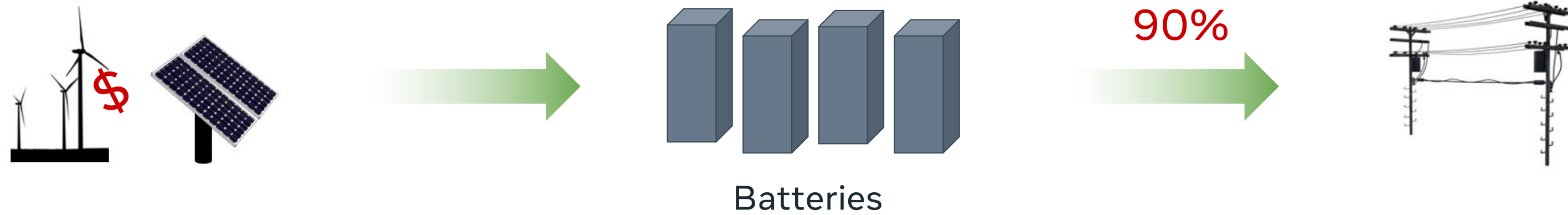


Scenario A (high electricity costs)

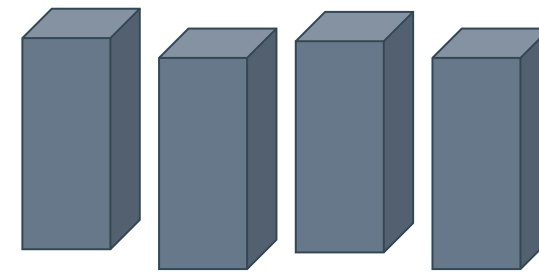
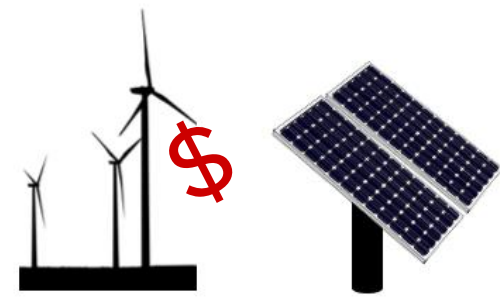
Scenario A (high electricity costs)



Scenario A (high electricity costs)

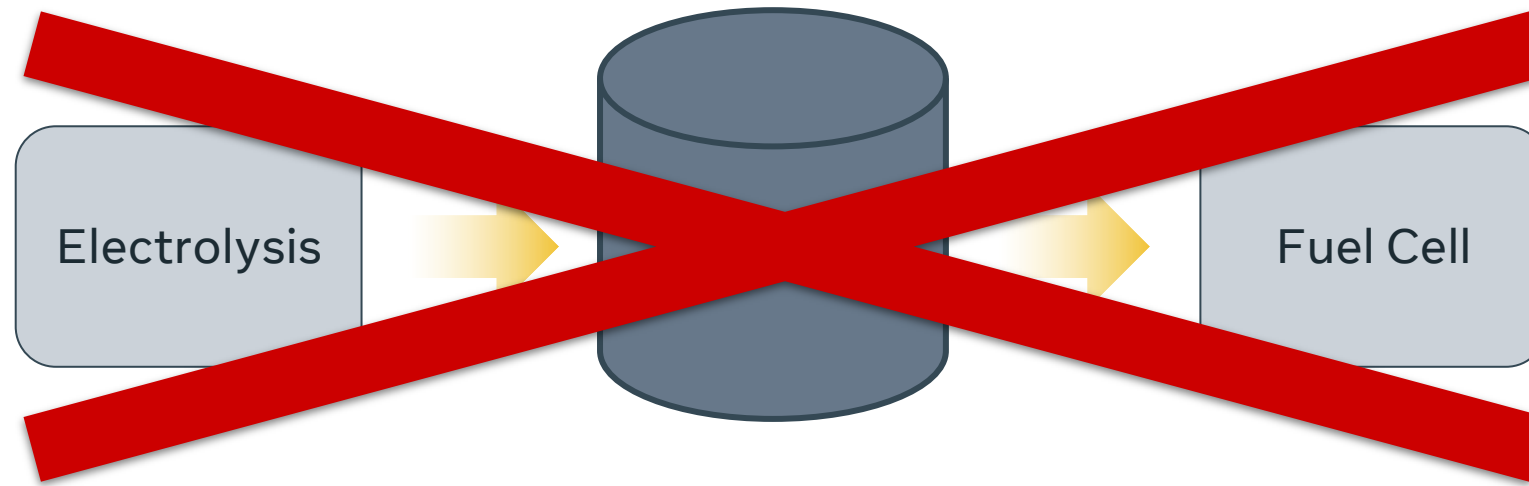
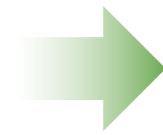
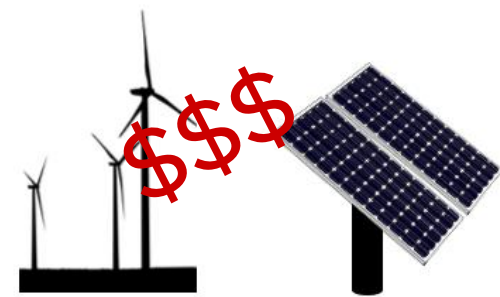


Scenario A (high electricity costs)

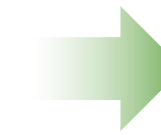


Batteries

90%

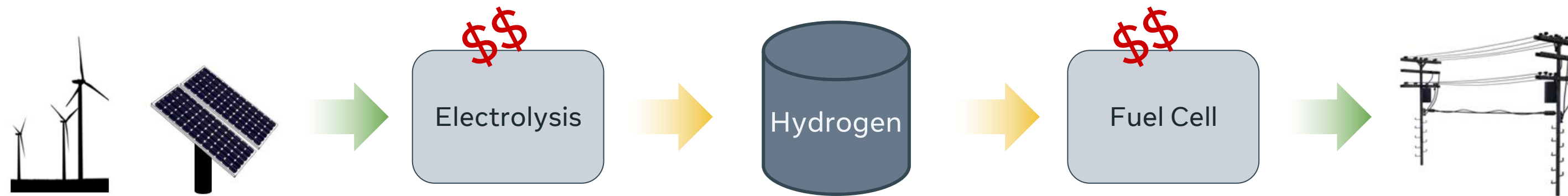
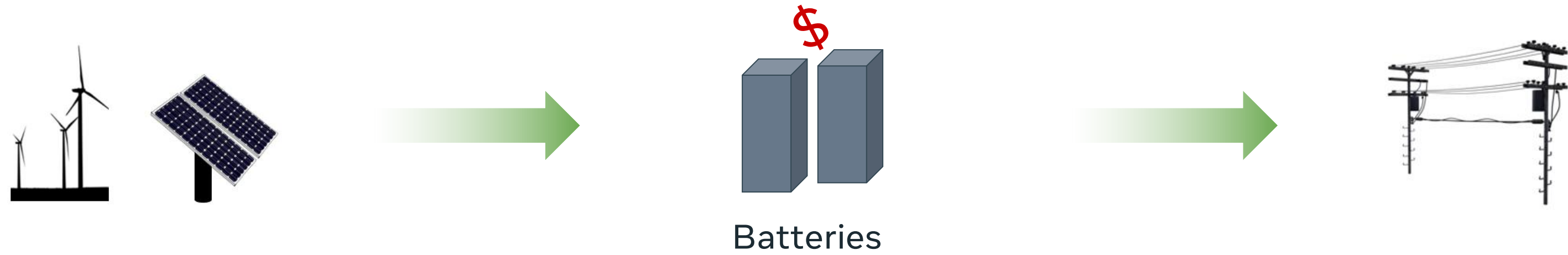


40%

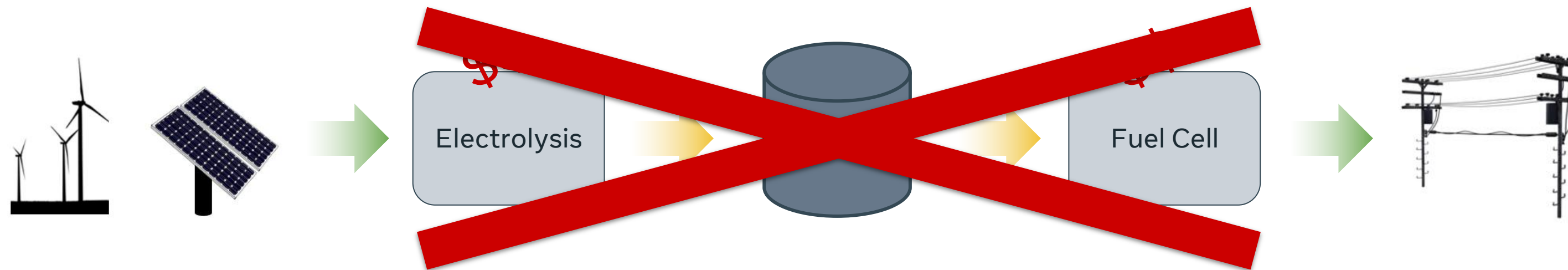
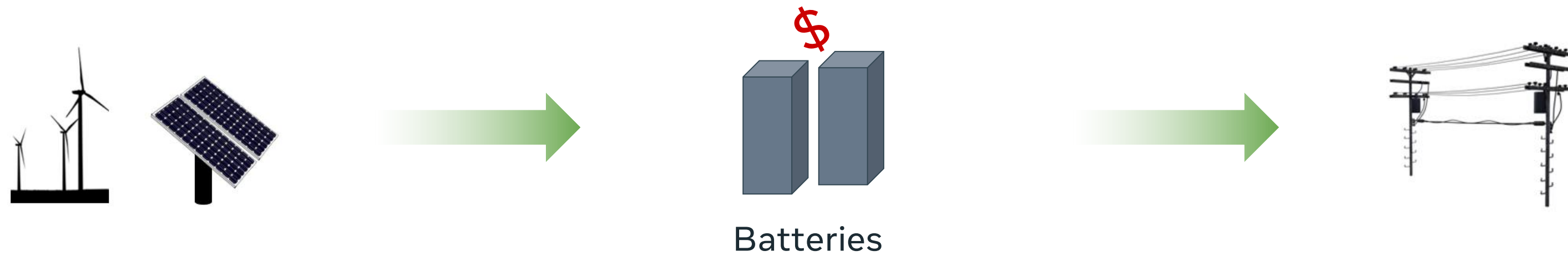


Scenario B (low electricity costs, short-term storage)

Scenario B (low electricity costs, short-term storage)

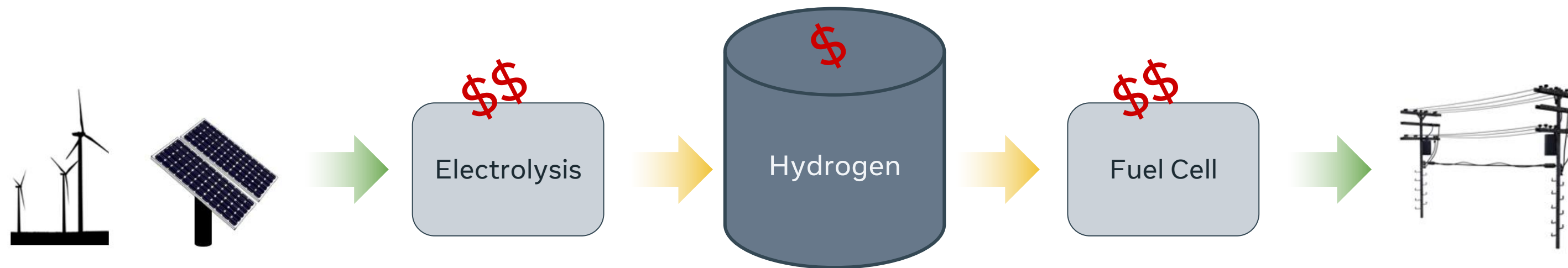
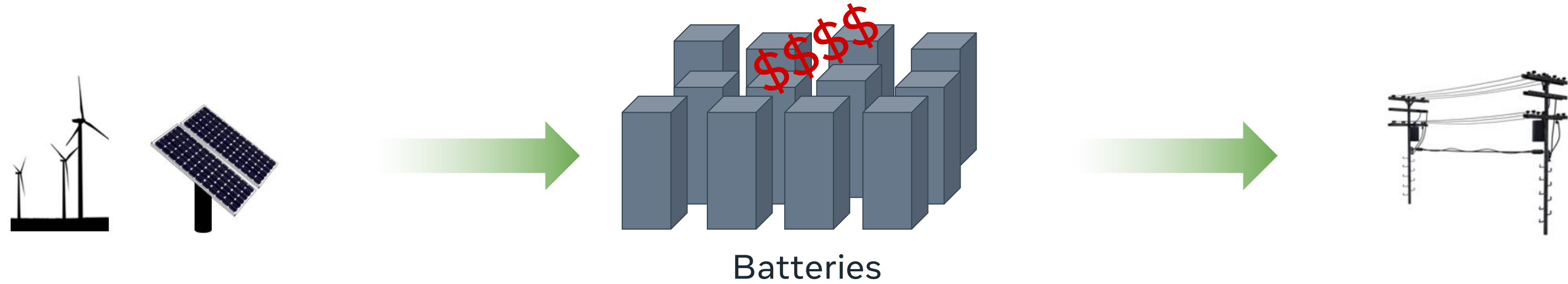


Scenario B (low electricity costs, short-term storage)



Scenario C (low electricity costs, long-term storage)

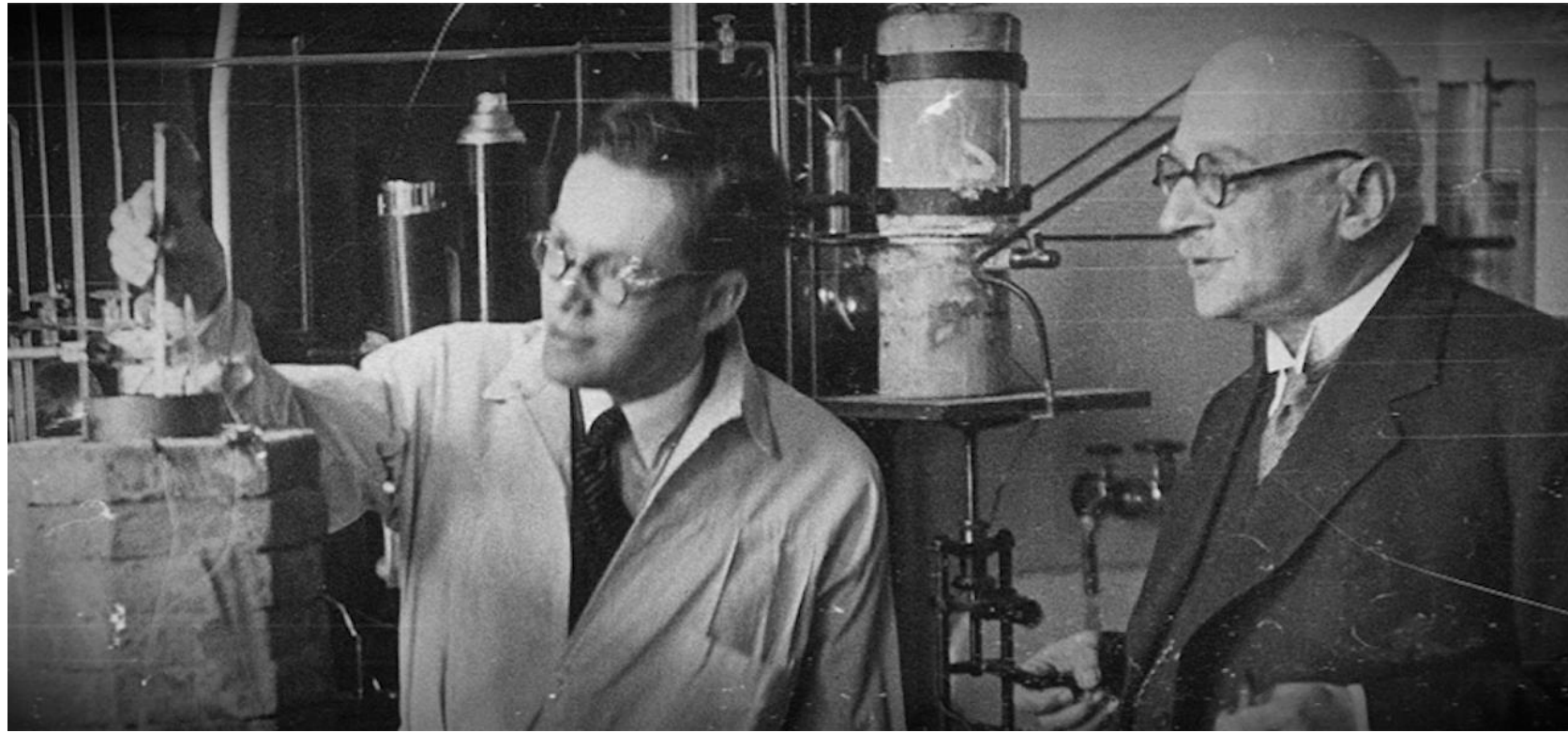
Scenario C (low electricity costs, long-term storage)



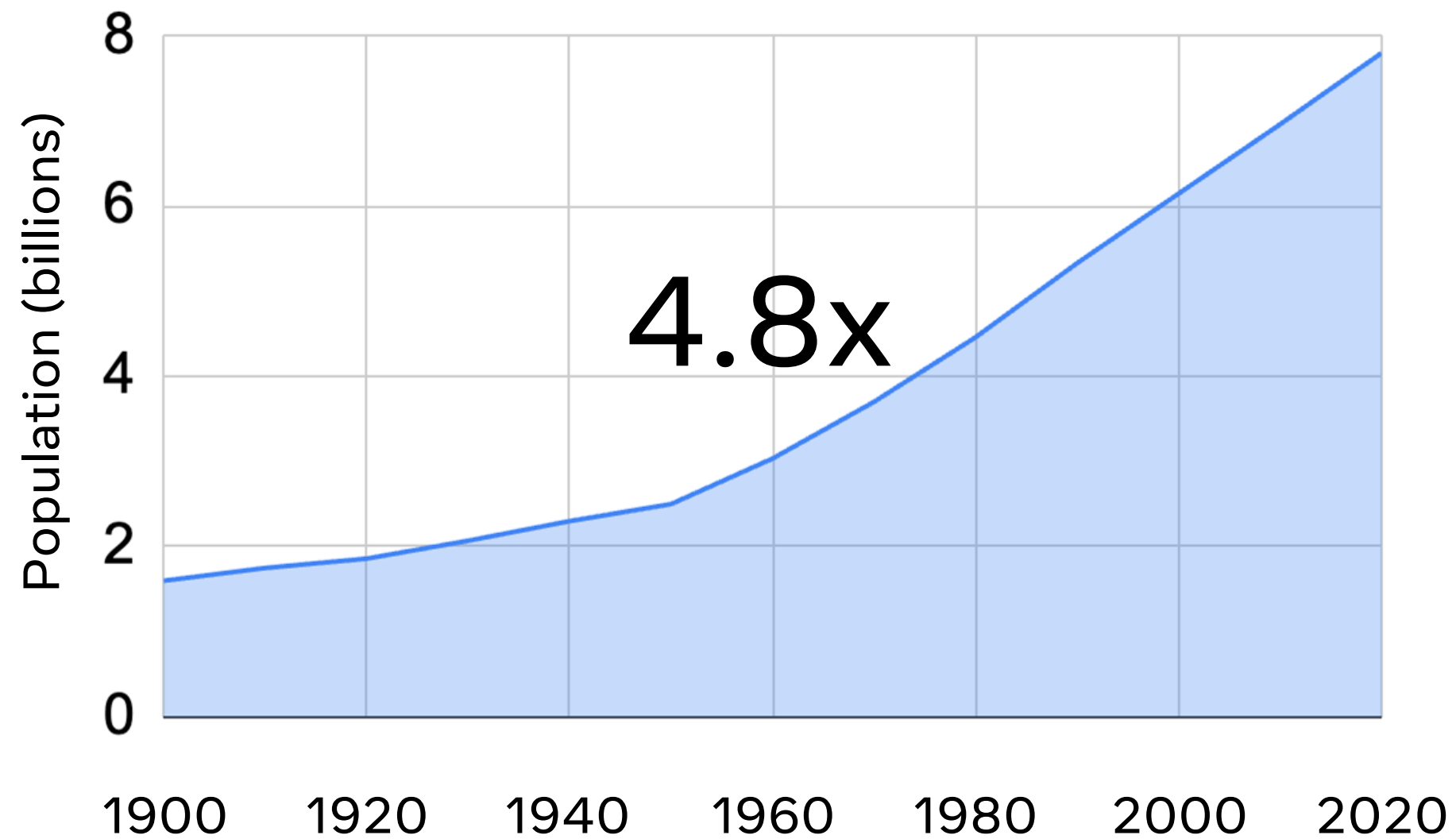
More areas...

1. Batteries
2. Proteins
3. Drug discovery
4. Hazardous waste cleanup
- 5....



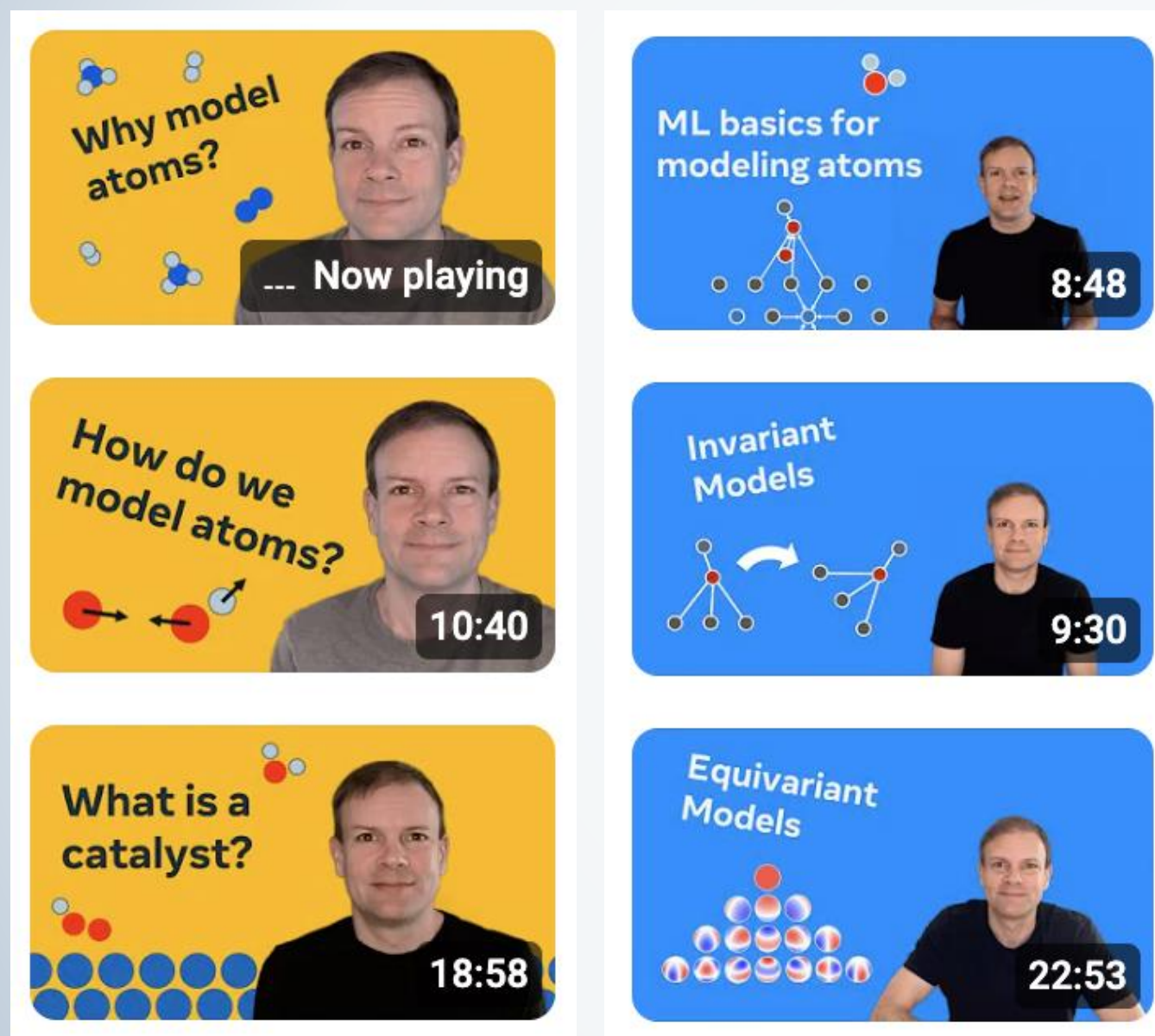


Helped keep Germany supplied with munitions during World War I.

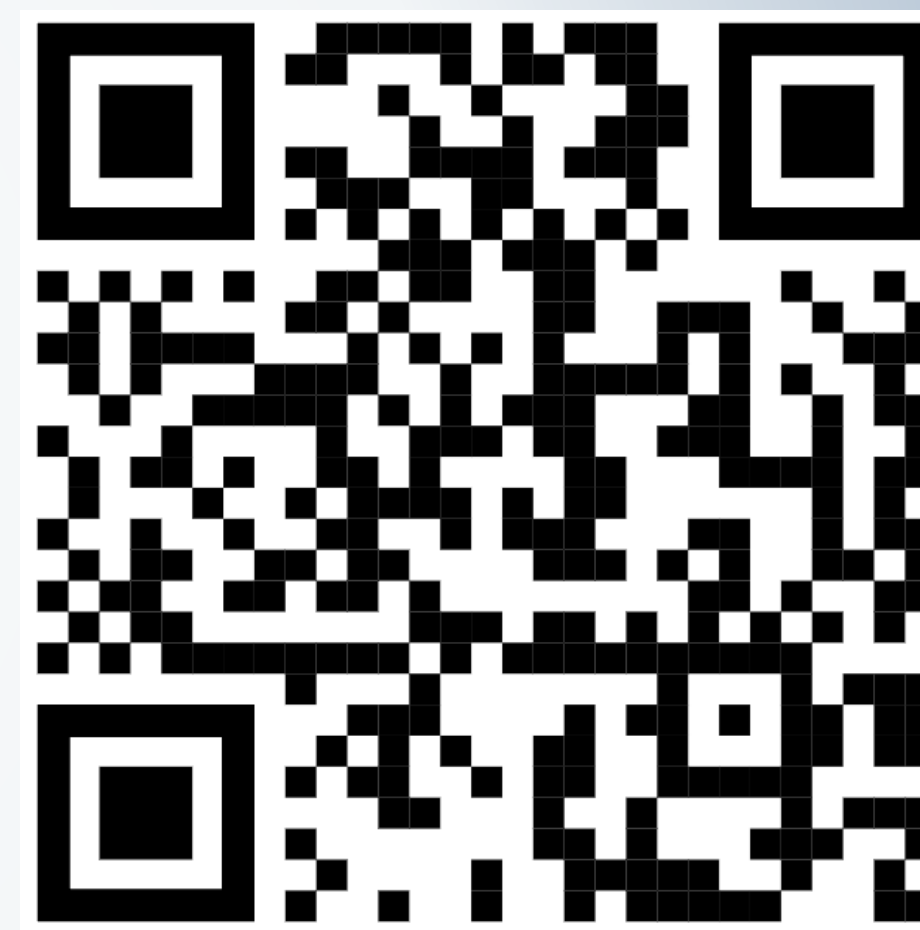


The overuse of ammonia fertilizers has led to ocean dead zones.

Thanks!



Open Catalyst YouTube



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