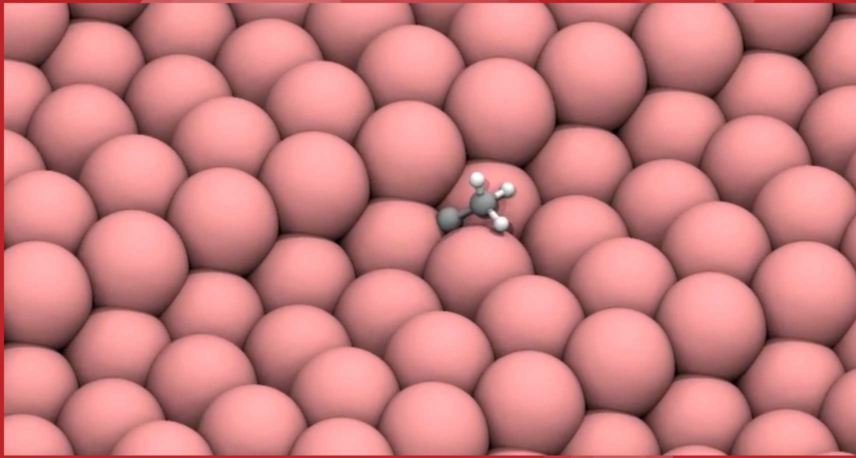
FACEBOOK AI Carnegie Mellon University

Open Catalyst Project

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



Muhammed Shuaibi
Abhishek Das

Team

FAIR


Abhishek Das


Siddharth Goyal


Anuroop Sriram


Janice Lan


Aditya Grover


Jure Zbontar


Nima Shoghi


Ammar Rizvi


Devi Parikh


Larry Zitnick

CMU Chemical Engineering


Zack Ulissi


Muhammed Shuaibi


Aini Palizhati

Javier Heras-Domingo


Brook Wander


Adeesh Kolluru


Richard Tran

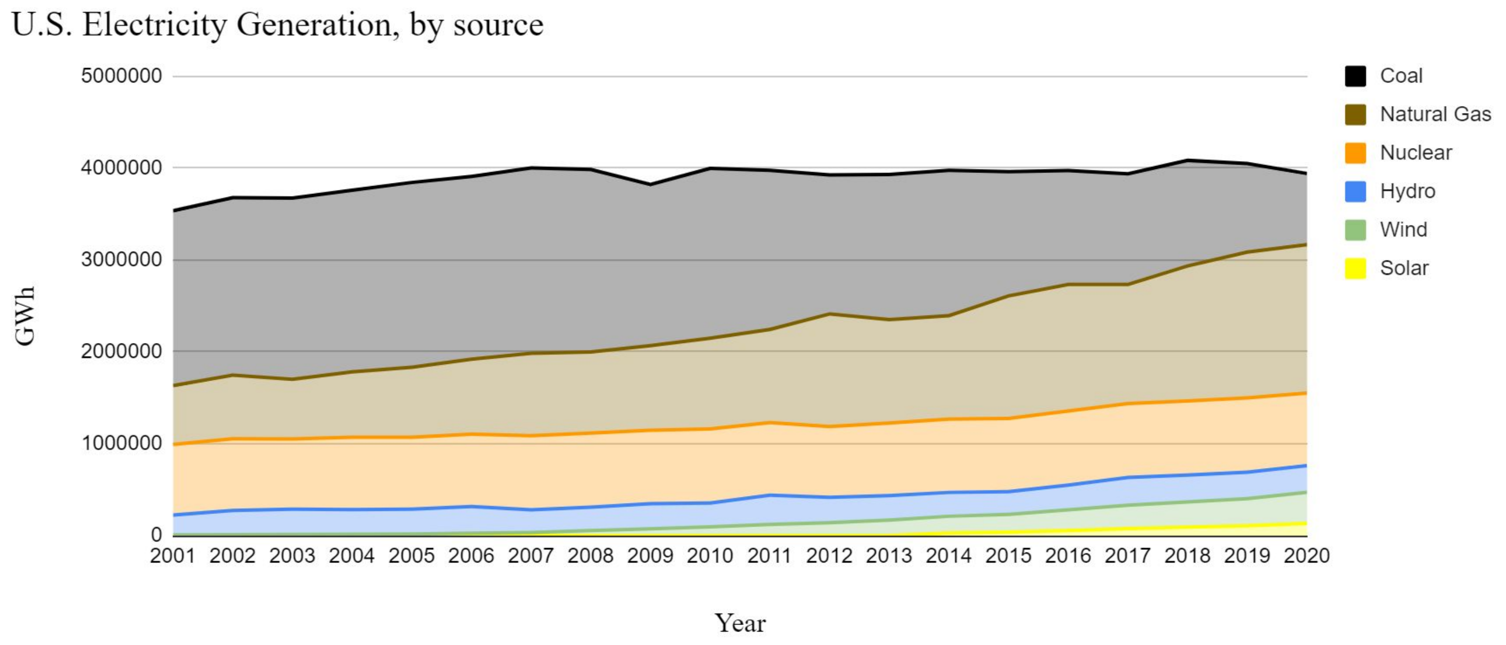
NERSC


Brandon Wood

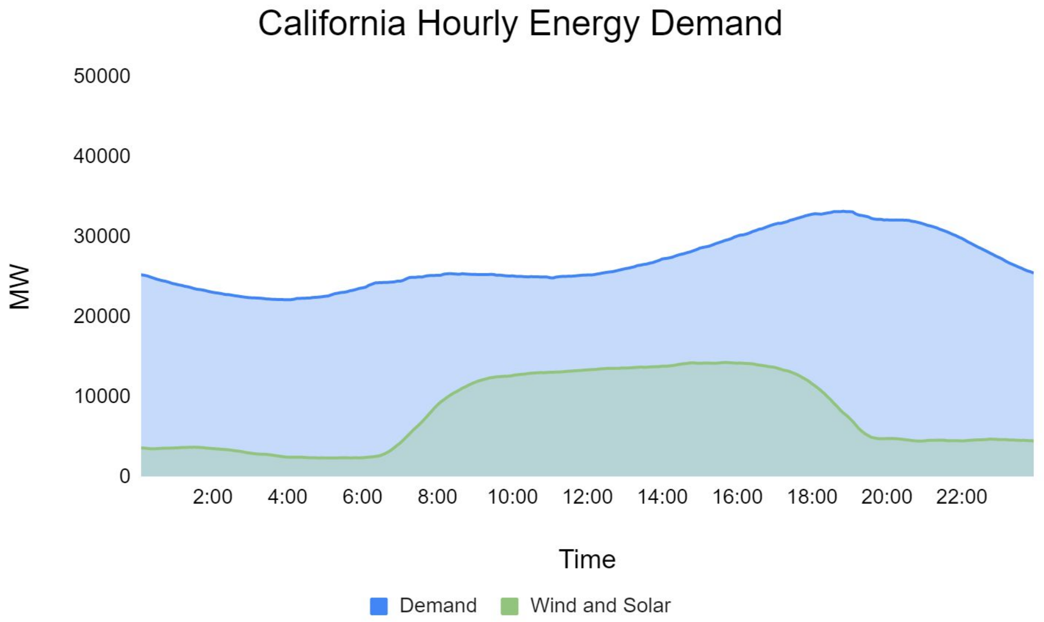
TU Munich


Johannes Klicpera

Decreasing costs of renewable technologies has led to an increase in their usage for U.S. electricity generation.

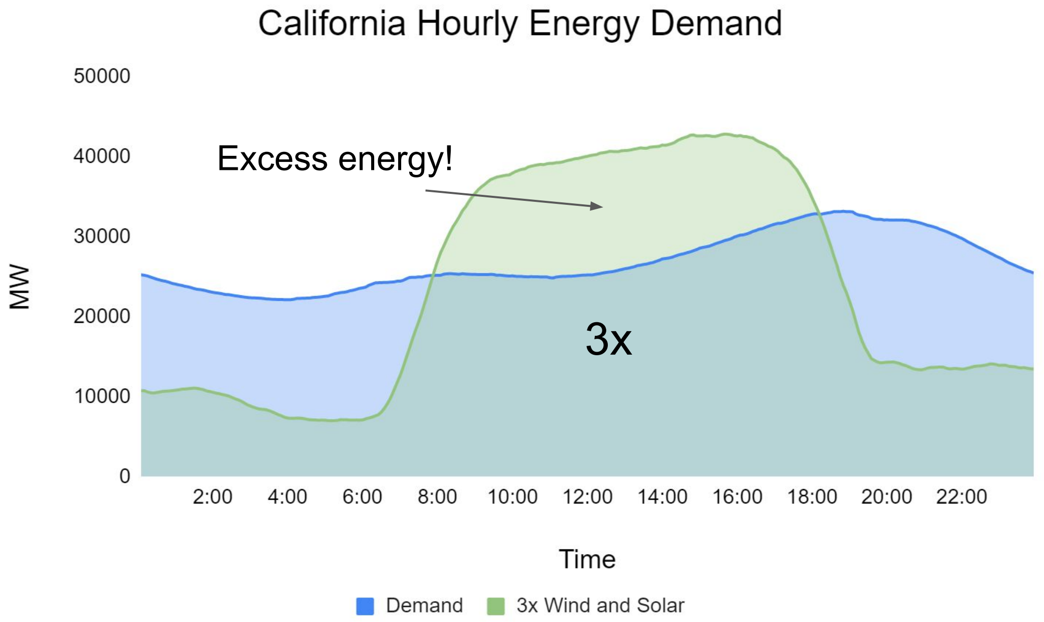


U.S. EIA. (2021). Electricity Data Browser.



California ISO. (2021). Today's Outlook.

As renewable technologies become more common, finding solutions for storing excess energy becomes critical.



[California ISO. (2021). Today's Outlook.]

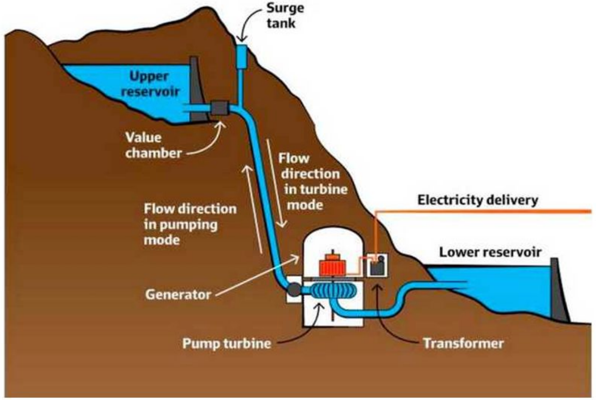
How do we store renewable energy?

Batteries

Tesla's 129 MWh installation ($50M)

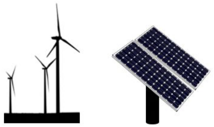
Total US Generation: 11,400,000 MWh (per day)

Pump water uphill



70-80% efficient

2% of US generating capacity



Excess generation

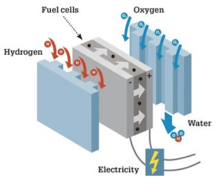
Storage

Excess demand

Electricity + $H_2O \rightarrow H_2 + O_2$

Hydrogen
H_2

$H_2 + O_2 \rightarrow$ Electricity + H_2O

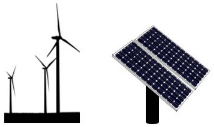


Fuel Cells

$H_2 + CO_2 \rightarrow CH_4 + H_2O$

Methane
CH_4

$CH_4 + O_2 \rightarrow$ Electricity + $H_2O + CO_2$



Excess generation

Storage

Electricity + $H_2O \rightarrow H_2 + O_2$

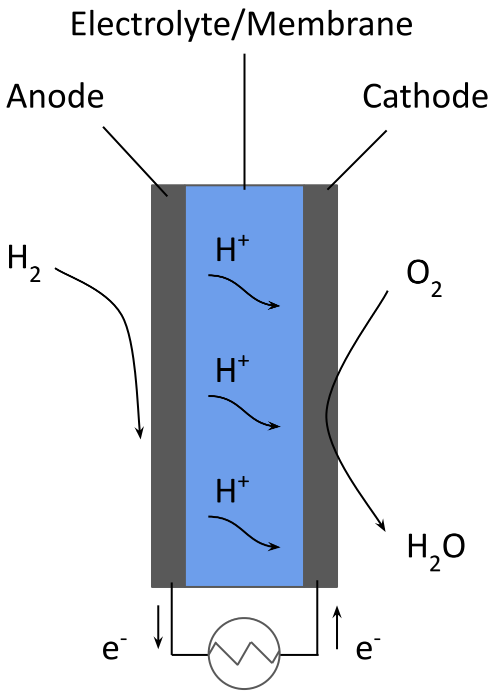
Hydrogen
H_2

$H_2 + CO_2 \rightarrow CH_4 + H_2O$

Methane
CH_4

Goal: to find efficient, economical **catalysts** that can drive these chemical reactions at high rates

Catalysts are vital components of the anode and cathode of an electrochemical fuel cell



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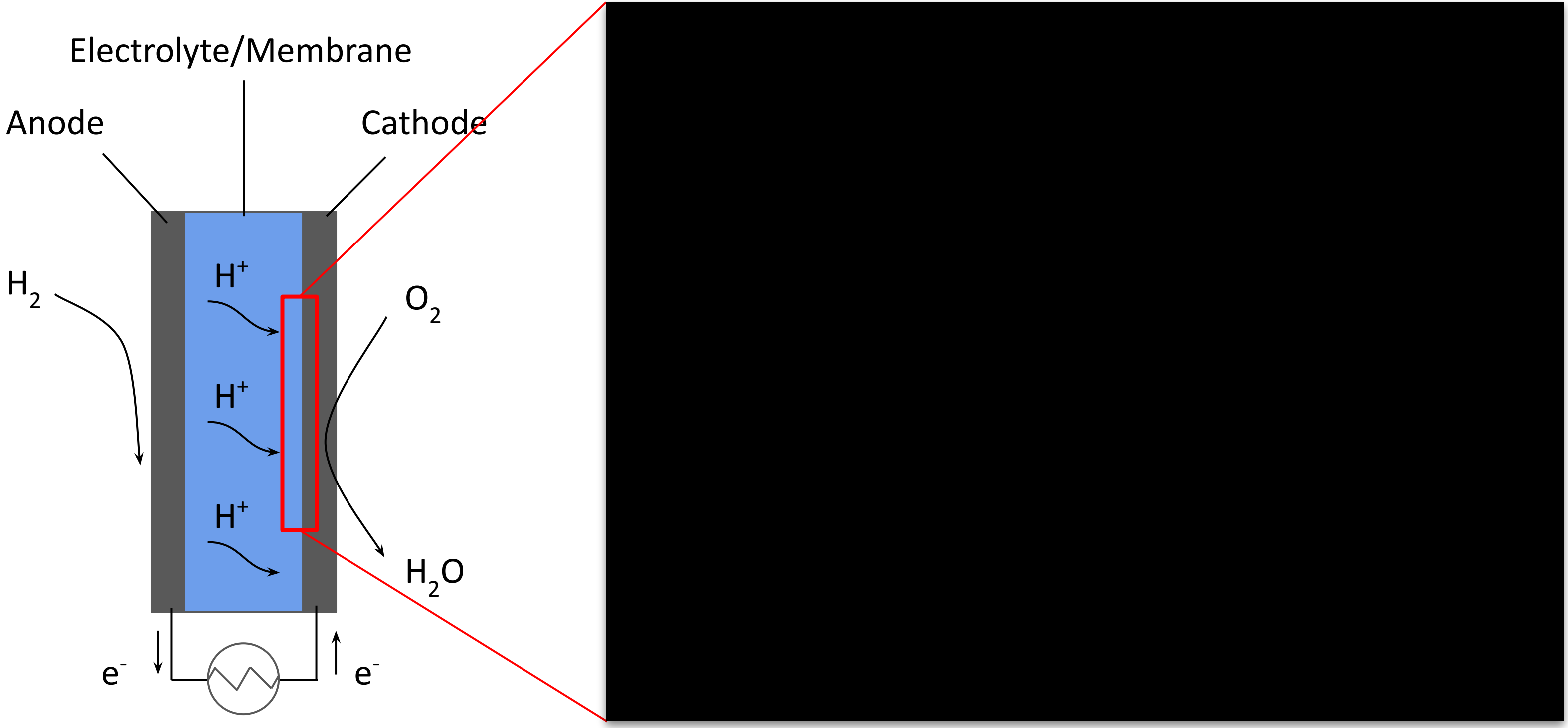
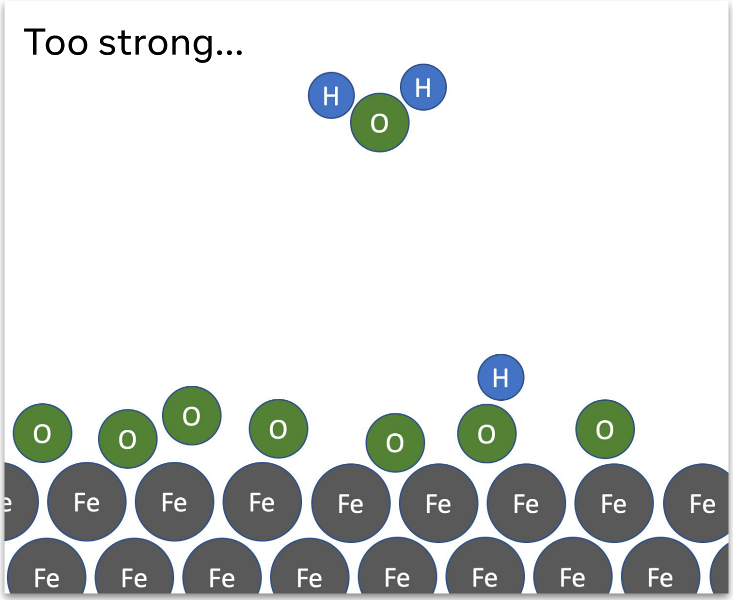
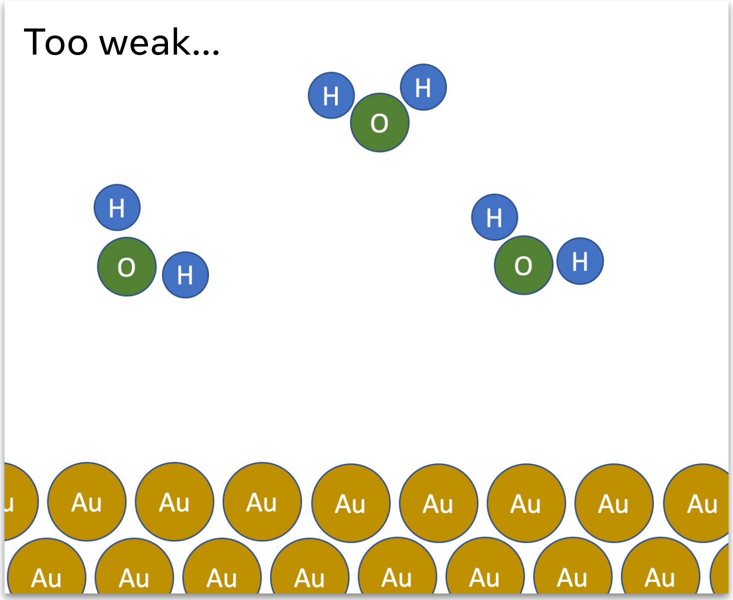


Goldilocks...





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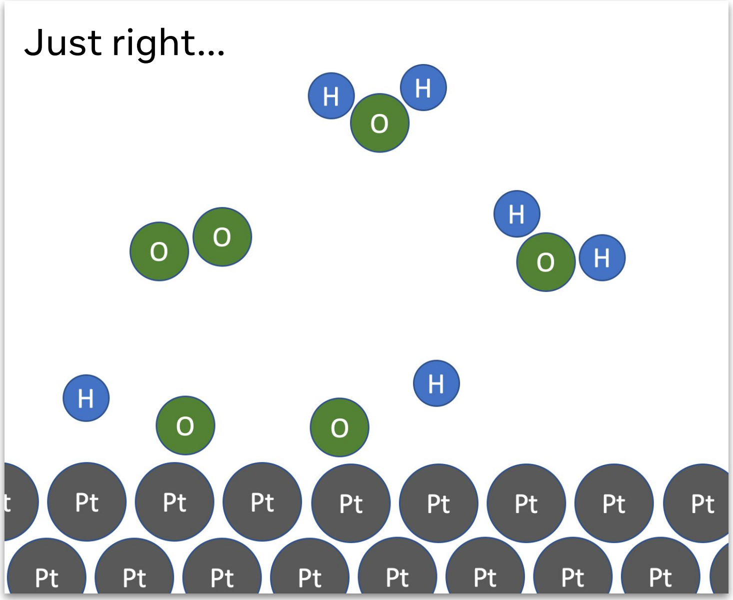
Just right...
H
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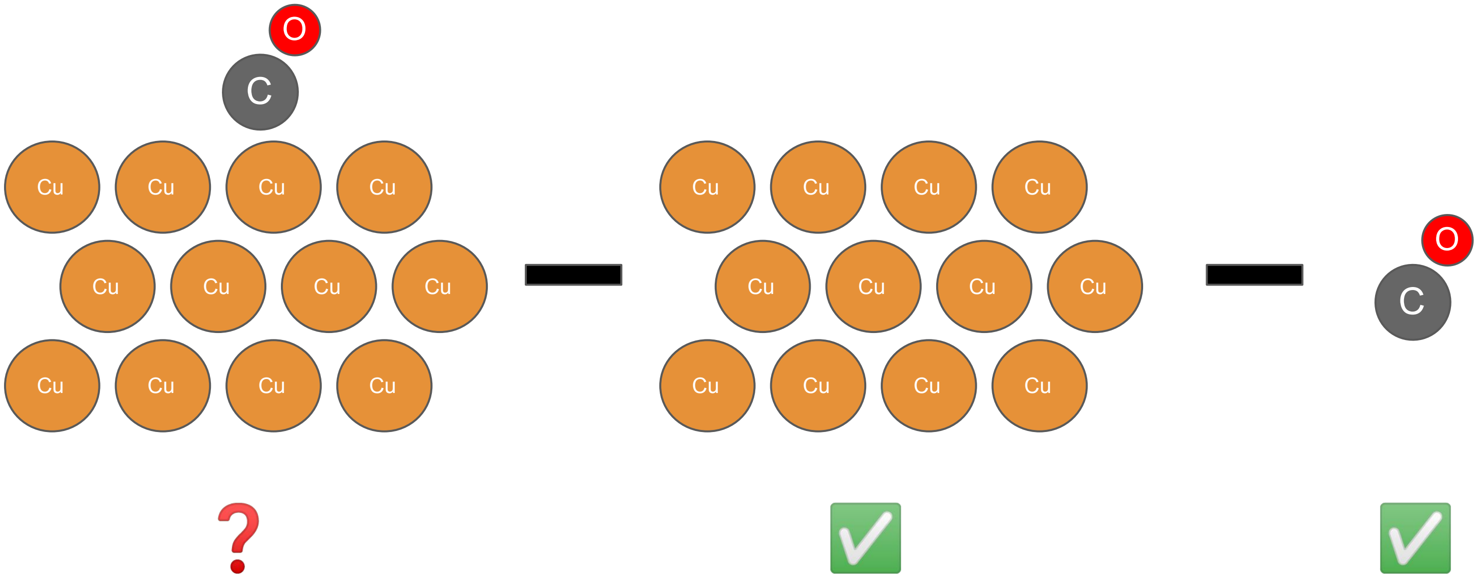
$$$

How are catalysts tested?

Adsorption energies are common descriptors to catalyst performance

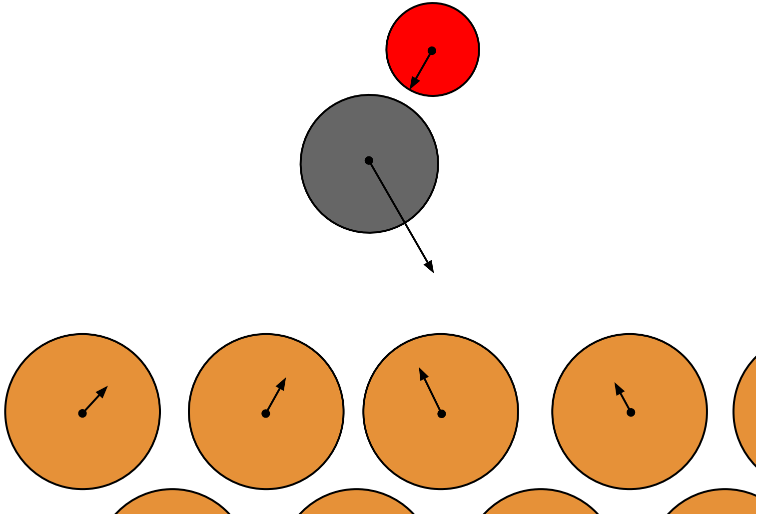
$$E_{ads} = E^{adslab}_{relaxed} - E^{slab}_{relaxed} - E^{adsorbate}$$



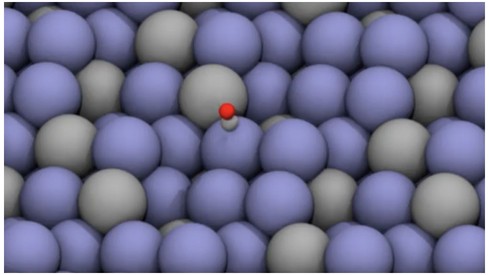
Quantum mechanical tools allows us to study atomic systems computationally

Density Functional Theory (DFT)

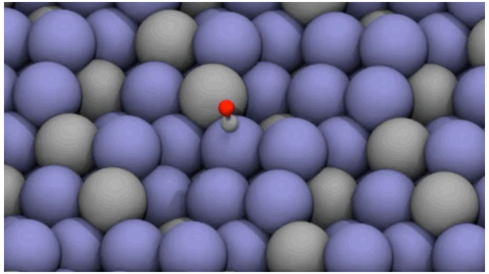
Computes system energy and
per-atom forces from first principles



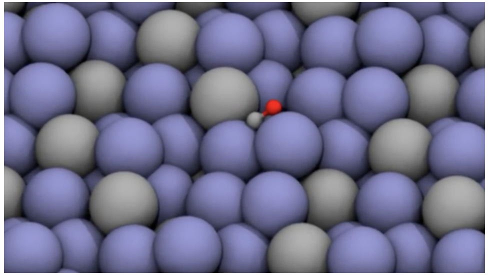
Relaxations are performed using DFT to arrive at the relaxed state



Initial state
High energy

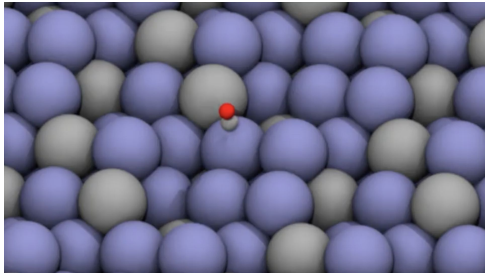


Adsorbate and catalyst atoms exert force on each other and move around

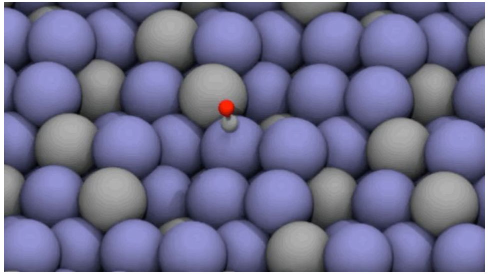


Relaxed state
Low energy

Relaxations are performed using DFT to arrive at the relaxed state



Initial state
High energy



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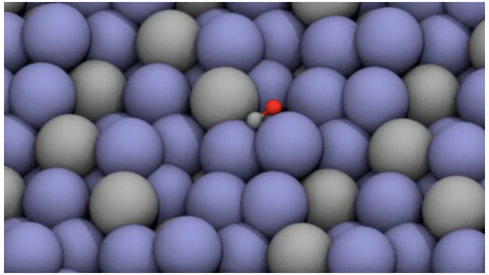
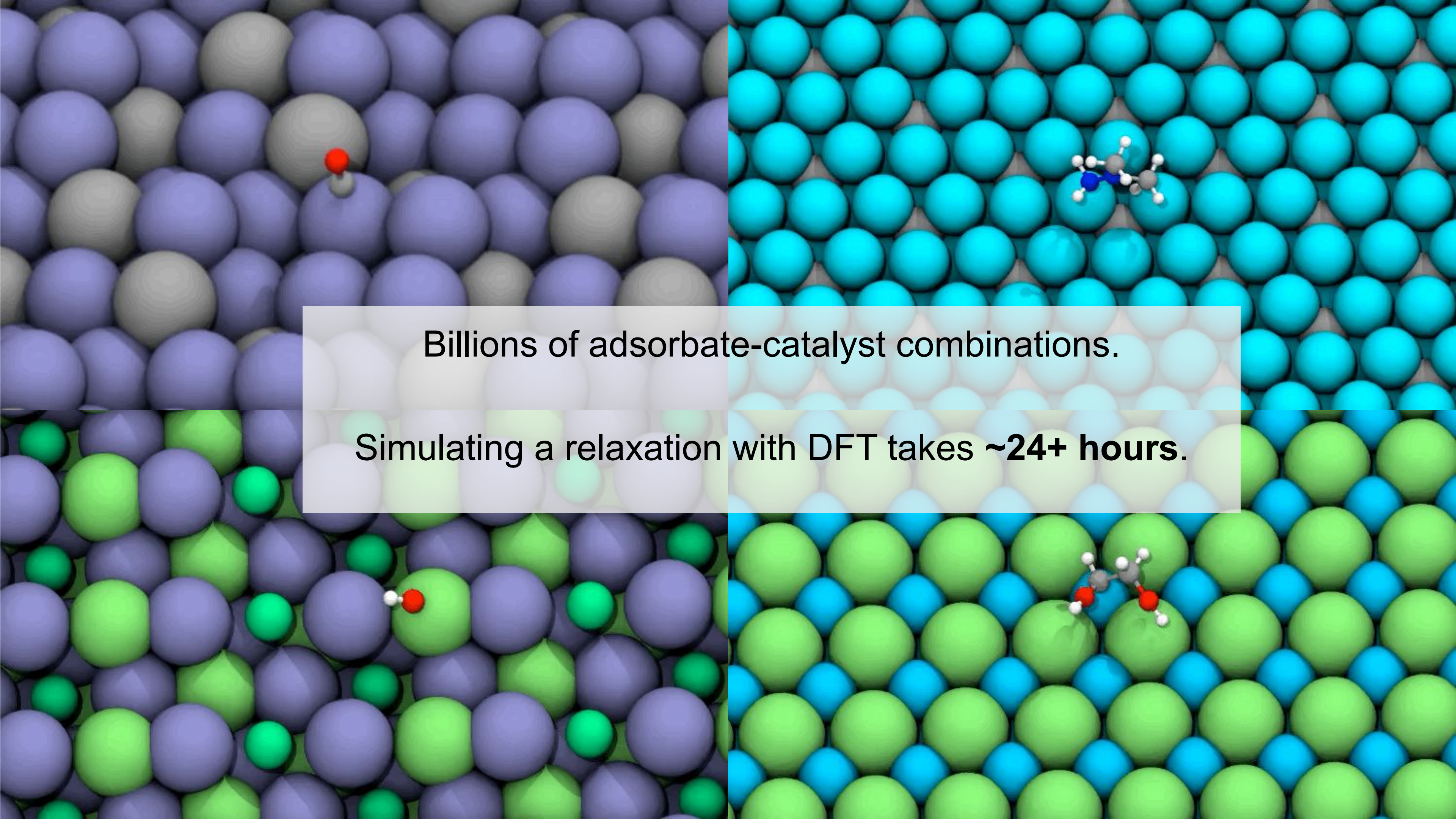


Relaxed state
Low energy

Can be used to determine reaction rate



Billions of adsorbate-catalyst combinations.

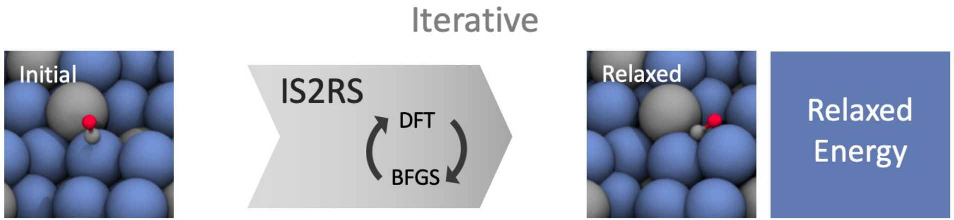
Simulating a relaxation with DFT takes **~24+ hours**.

Approximating DFT with ML

Tasks

- **S2EF:** Structure to energy and force. Black box replacement for DFT
- **IS2RS:** Initial state to relaxed state. Accelerate DFT with better initial guess
- **IS2RE:** Initial state to relaxed energy. Guess the final relaxed energy, which is what we usually want.

Tasks are interrelated



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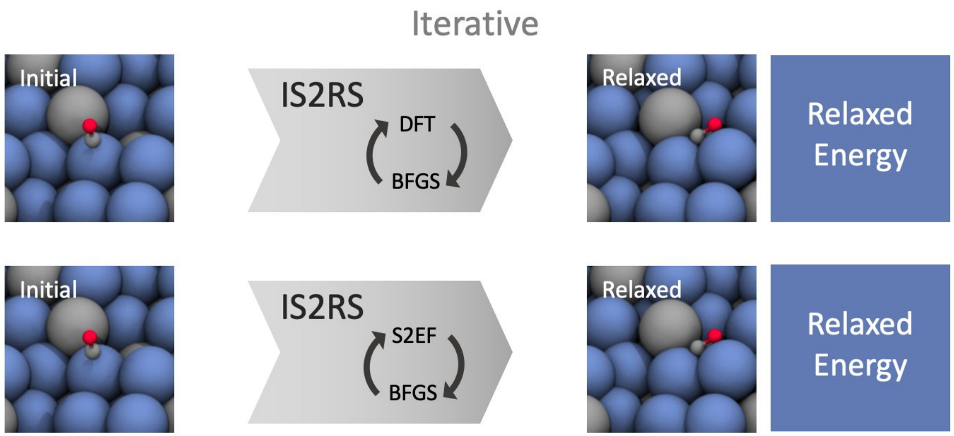

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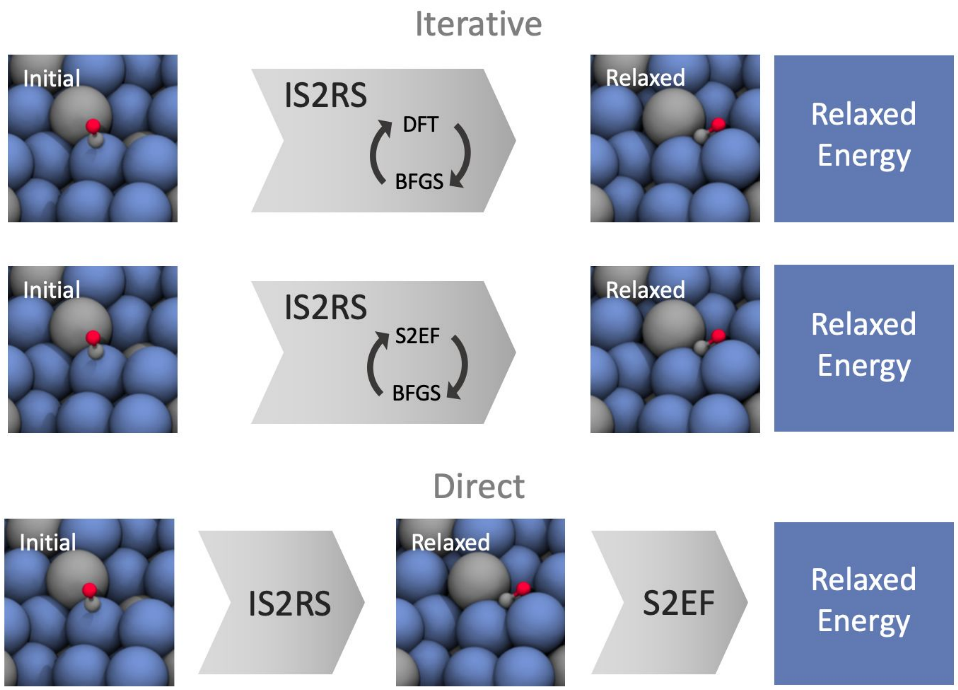

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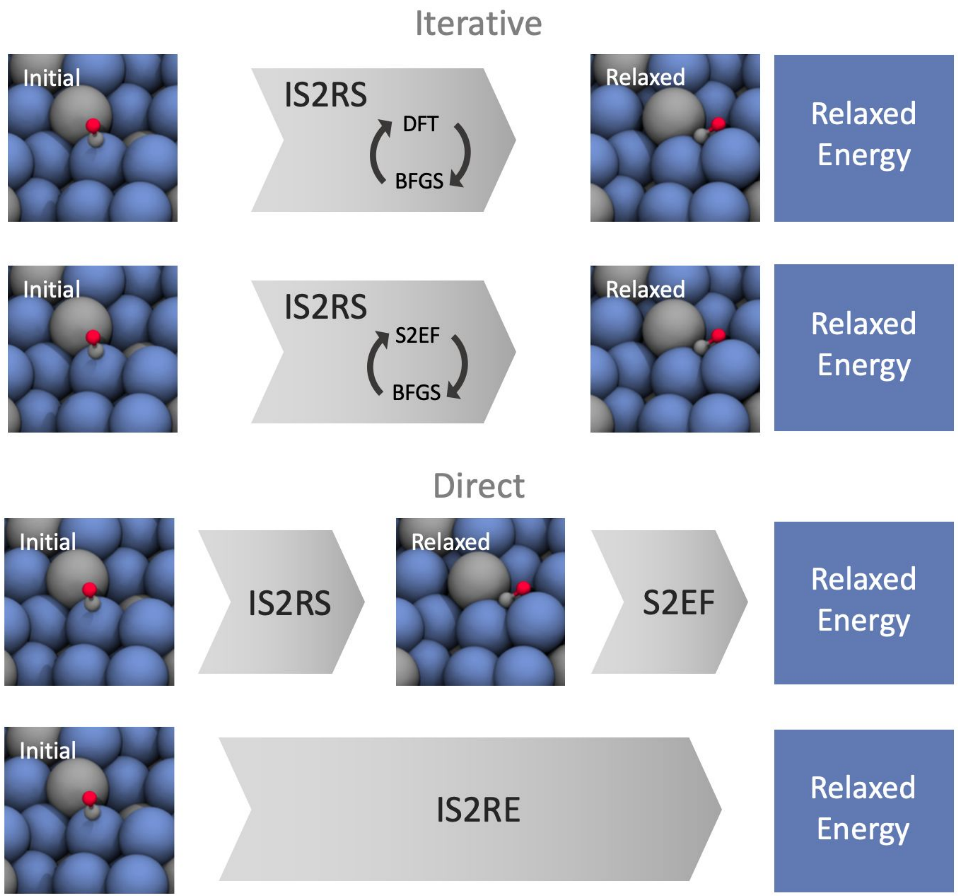
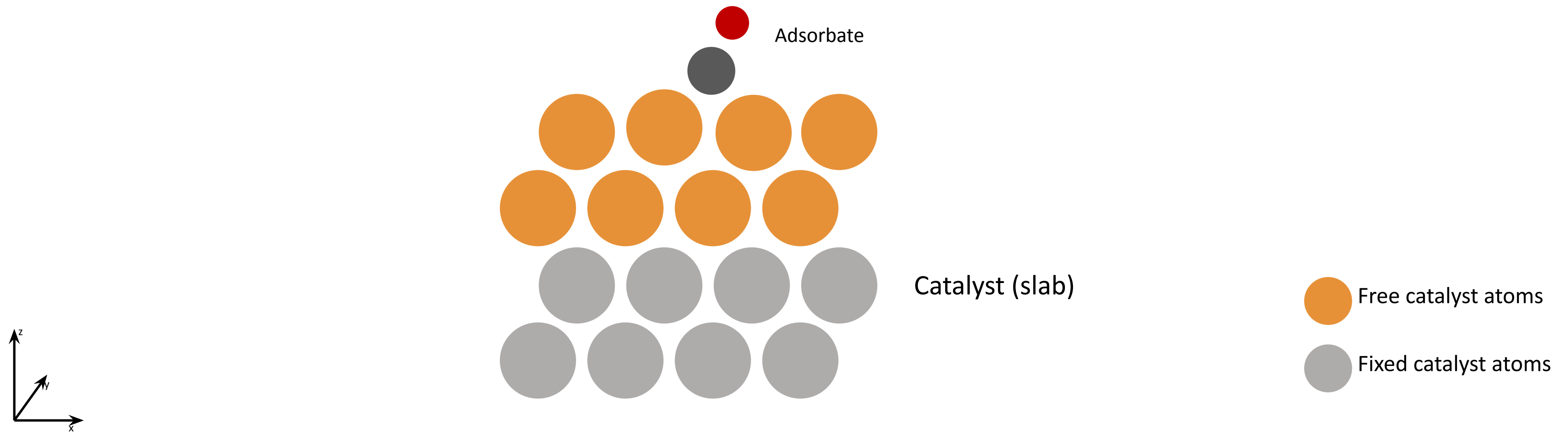


Atomic systems can be represented as graphs for use in graph neural networks (GNNs)



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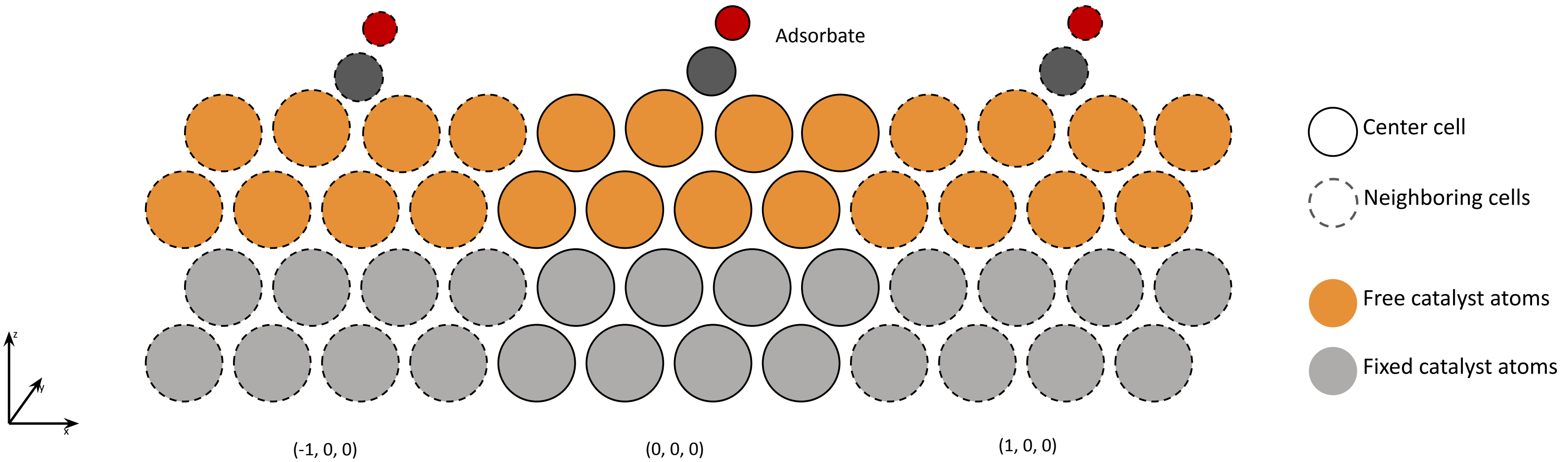

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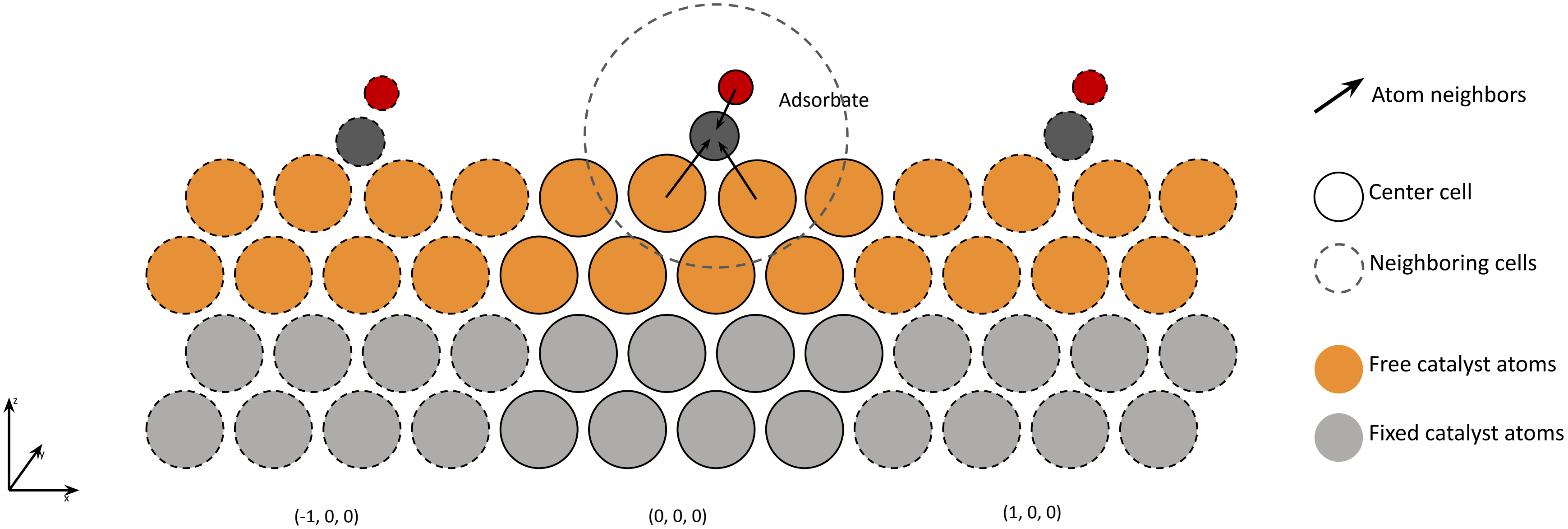

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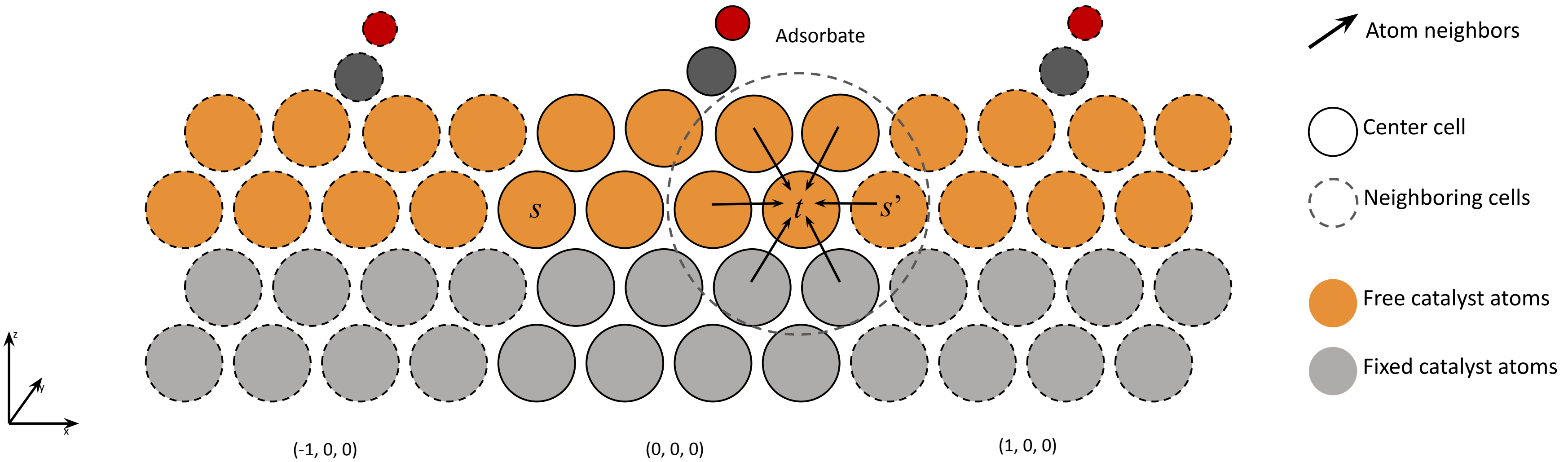
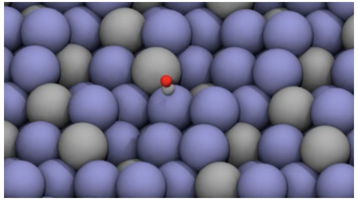
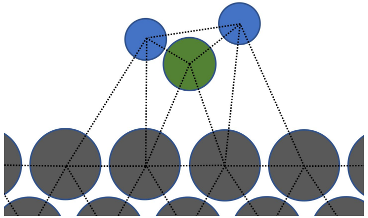


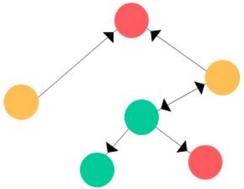
An ML surrogate to DFT (S2EF task) is the most general and widely applicable task



Inputs
3D atomic positions and atomic number



Construct graph
Node: atom
Edge: neighbors

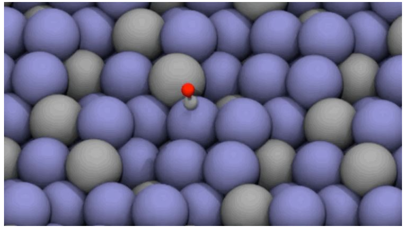


Graph neural network

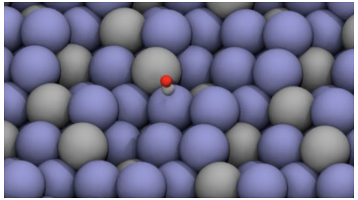
Outputs
3D atomic forces

Use predicted forces to recompute atomic positions

Till relaxation is complete
i.e. max force is close to 0



Direct property predictions can be 200x+ faster than iterative ML approaches



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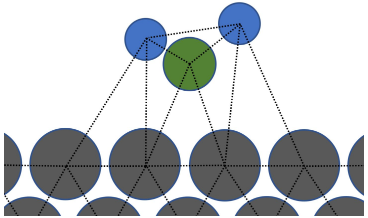

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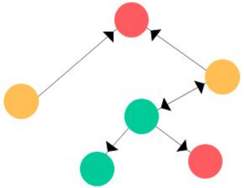


Graph neural network

Outputs
Relaxed energy

The Open Catalyst 2020 (OC20) Dataset

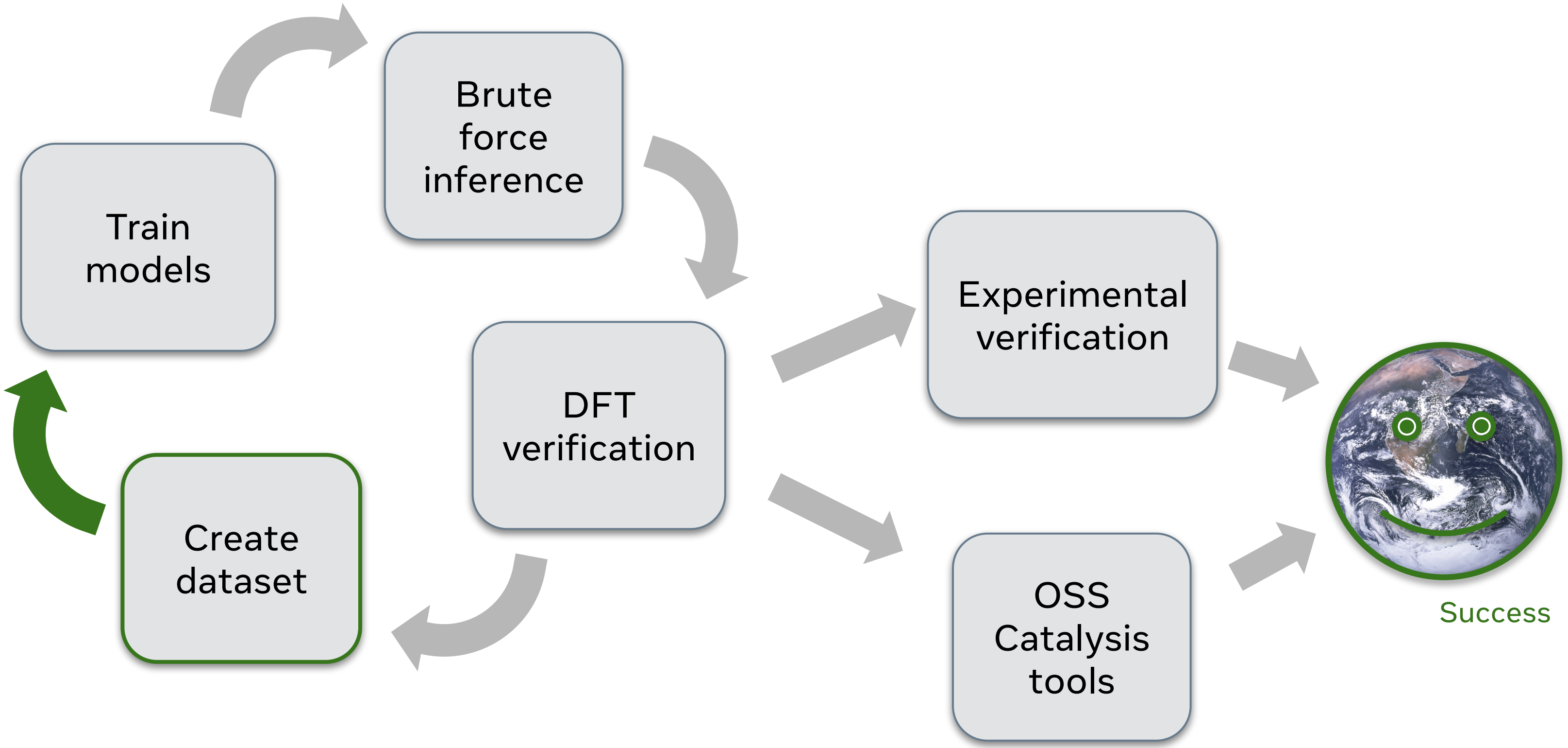
- 1.3M DFT relaxations for training and evaluation
- 130M+ training examples
- 55+ unique elements
- 70M+ hours of compute

- Publicly available at opencatalystproject.org.

Tutorial contents

1. Data visualization
2. Training models for OCP tasks:
    a. S2EF
    b. IS2RE
    c. IS2RS
3. Understanding modeling approaches
    a. Energy-centric
    b. Force-centric
4. Building your own model
5. Running OCP at the command line

Where are we headed



Resources

Tutorial:

https://colab.research.google.com/drive/1oGZcrakB4Pbj8Xq74lSvcRDUHw9L-Dh5#scrollTo=dzeHYa5GCxN7

Dataset, papers, code:

opencatalystproject.org
github.com/open-catalyst-project

Discuss:

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