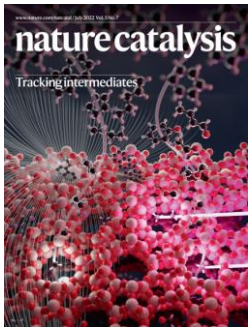
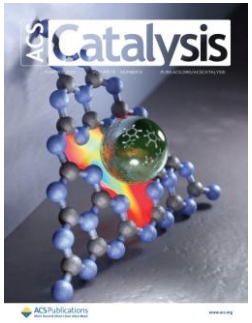
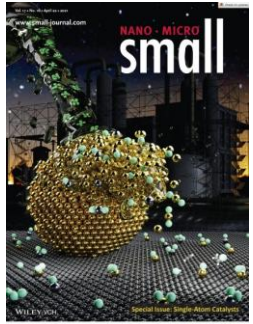
About me
Edvin Fako

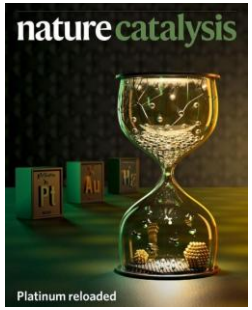
Professionally

2025 | Postdoc @ LIAC
2021-25 | Scientist @ BASF
2016-21 | Lopez's Group @ ICIQ



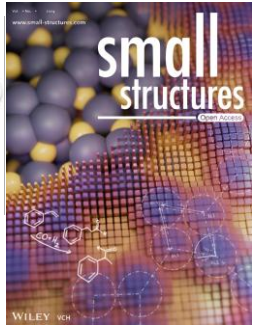


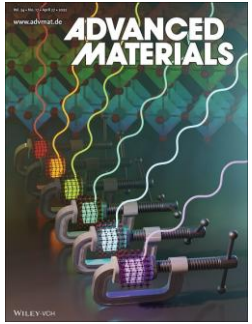




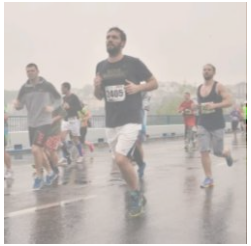
Blender for Science: Import and render chemical structures - part 1
7.4K views • 4 years ago

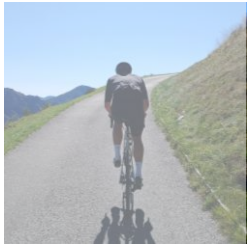
Blender for Science: Modelling and Materials - part 2
1.6K views • 4 years ago

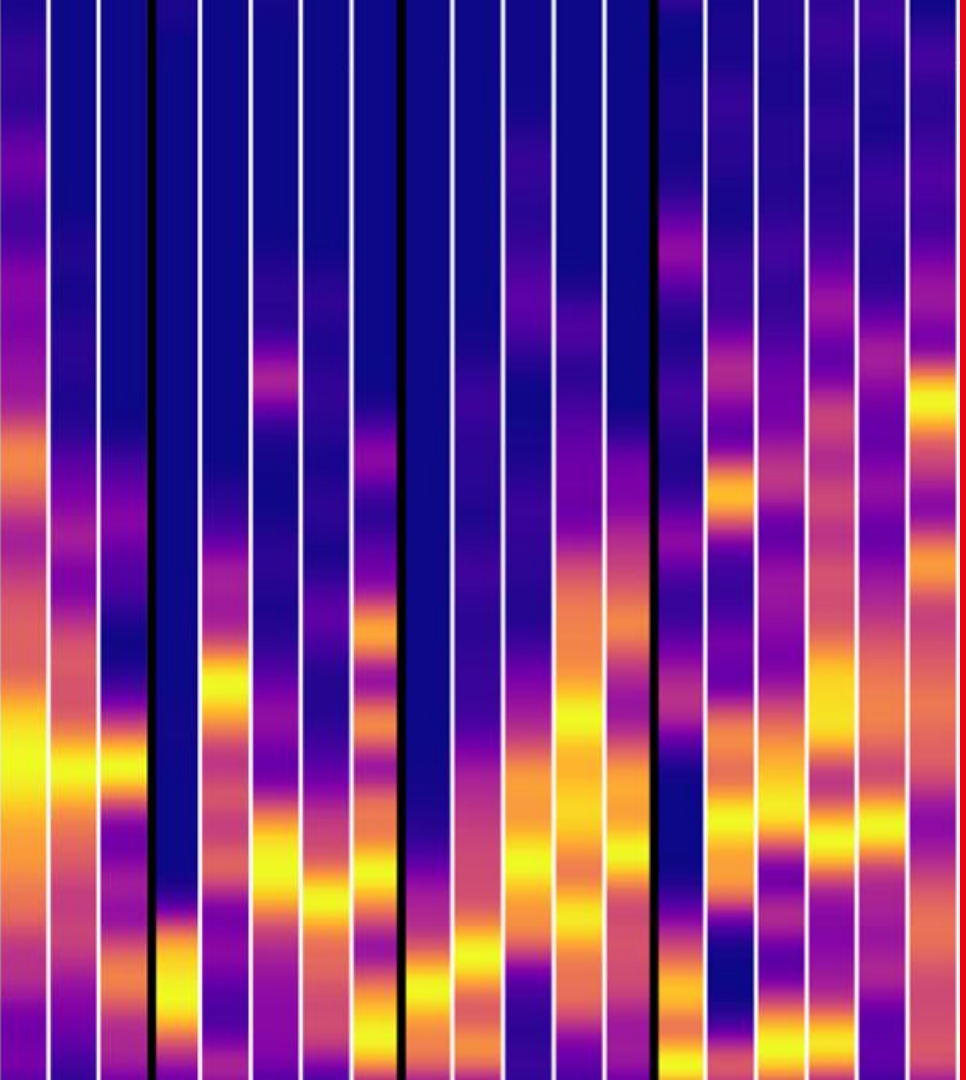




Privately







Edvin Fako

How Computational Methods and Data Shape AI for Discovery

of Functional Materials

Lausanne 07.05.2025

EPFL LIAC

Outline

Edvin Fako

- What are functional materials?
- Parallels between drug (molecule) and heterogeneous catalyst discovery
- Materials as catalysts: How do materials facilitate chemical reactions?
- Descriptor versus dynamic approaches
  - Descriptors in surface science
  - Dynamic approaches in surface science
- MLIPs: Where do we stand?
- How to sample fragments on a surfaces?

GOAL: **Motivate and empower you to generate and explore data!**

What are functional materials?

ChatGPT

Functional materials are materials that have specific properties and functions beyond just their structural or mechanical uses. They are designed to respond to external stimuli—such as temperature, electric or magnetic fields, light, or chemical environments—in predictable and useful ways.

Key Features:

- **Responsive**: They change their properties in response to external conditions.
- **Active Role**: Unlike passive structural materials, functional materials are active participants in a system's performance.

- Piezoelectric Materials
- Ferro/Thermoelectric Materials
- Shape Memory Alloys (SMAs)
- Electrochromic Materials
- Photovoltaic Materials
- **Heterogeneous Catalysts**
- …

Why do we care?

Why do we care?

The **BASF site in Ludwigshafen, Germany**, is the **largest integrated chemical complex in the world** operated by a single company. It's often referred to as **BASF's headquarters and flagship site**.

~6 raw materials coming in

~ 65 000 products going out

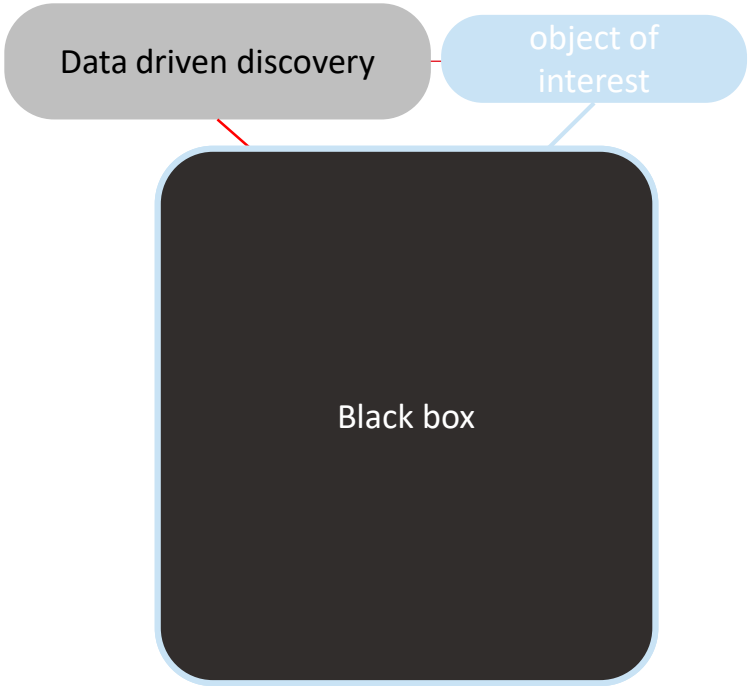
Why do we care?

~ 39 000 people working

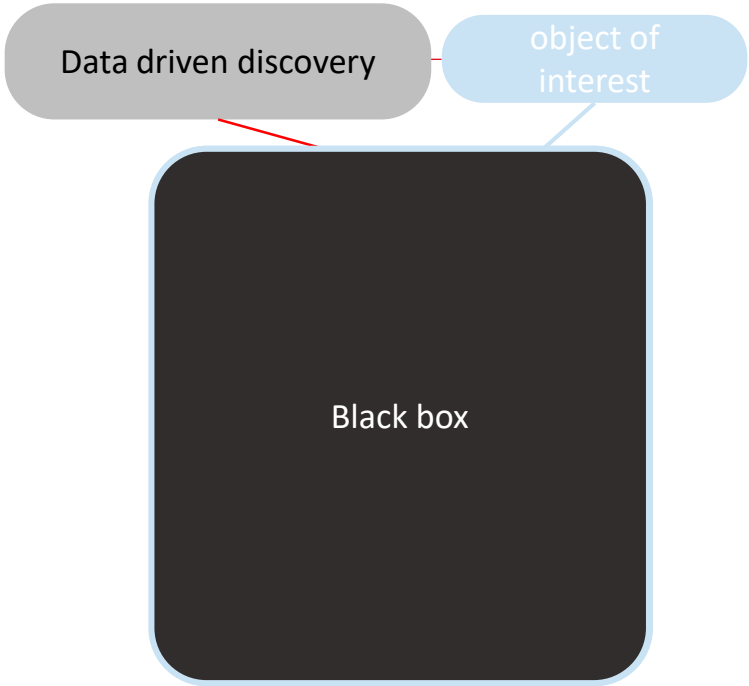
~ 200 plants

~ 2 power plants

Parallels between drug and heterogeneous catalyst discovery

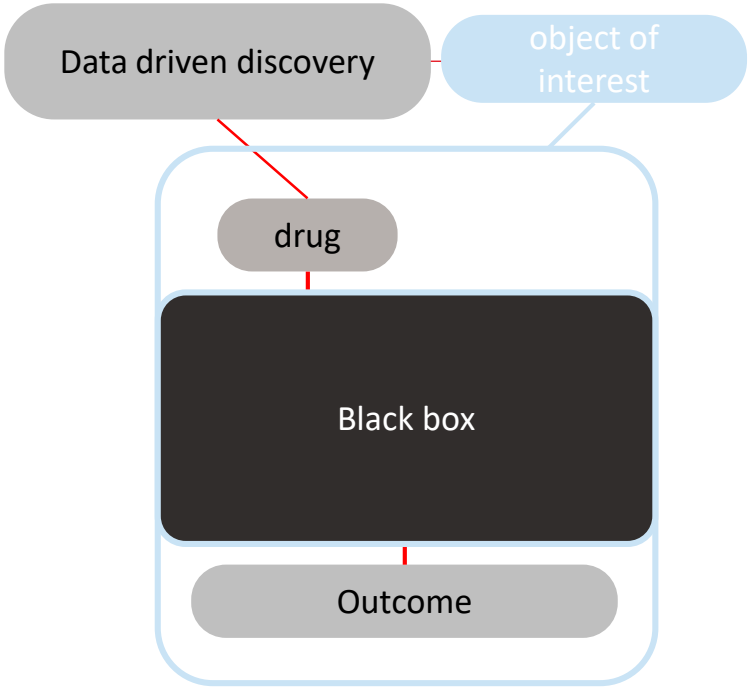


Drug



Catalyst

Parallels between drug and heterogeneous catalyst discovery



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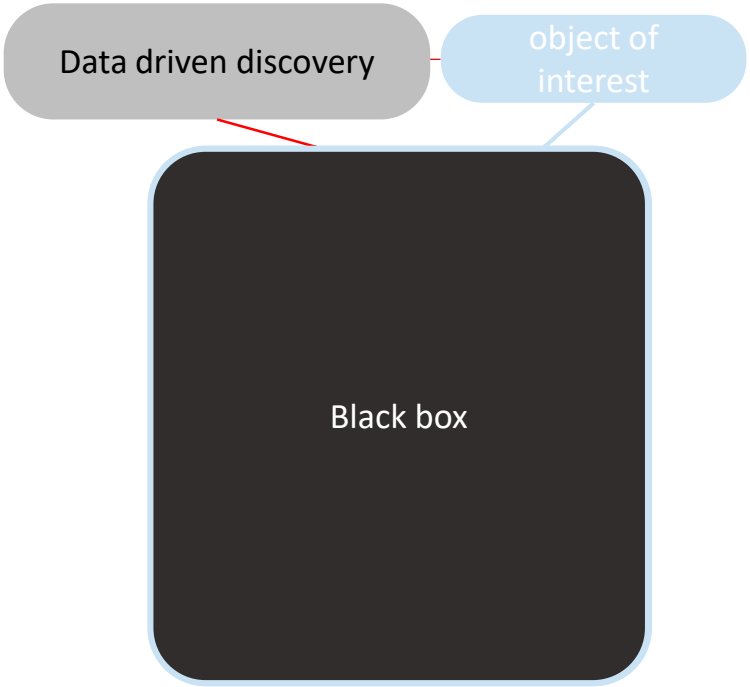

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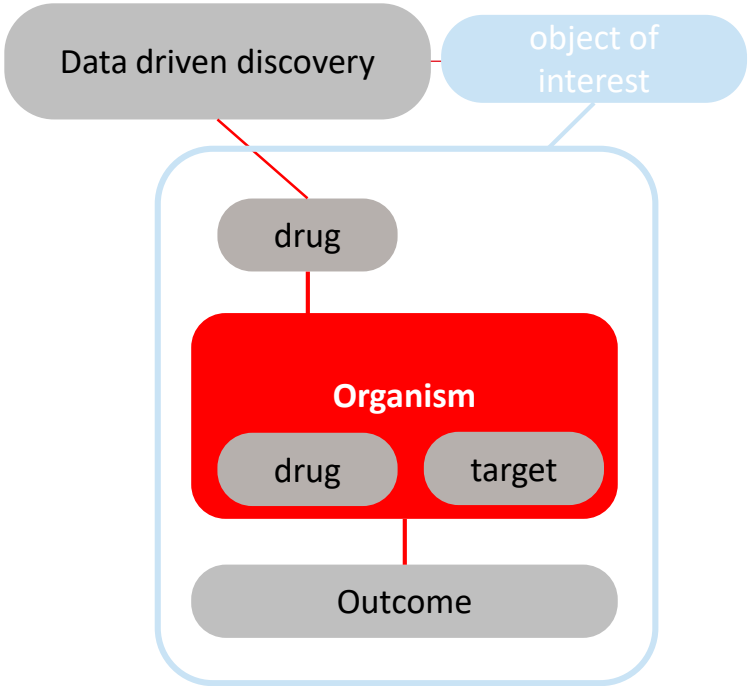

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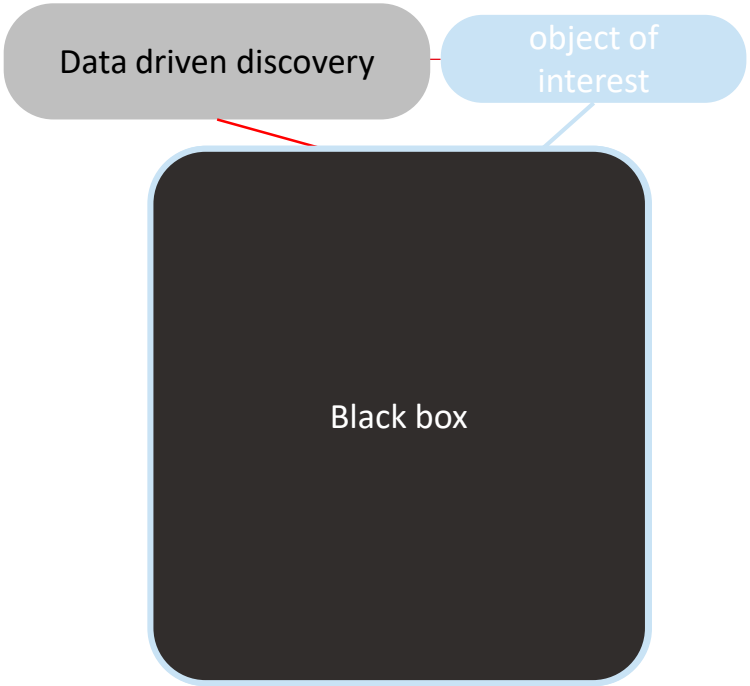

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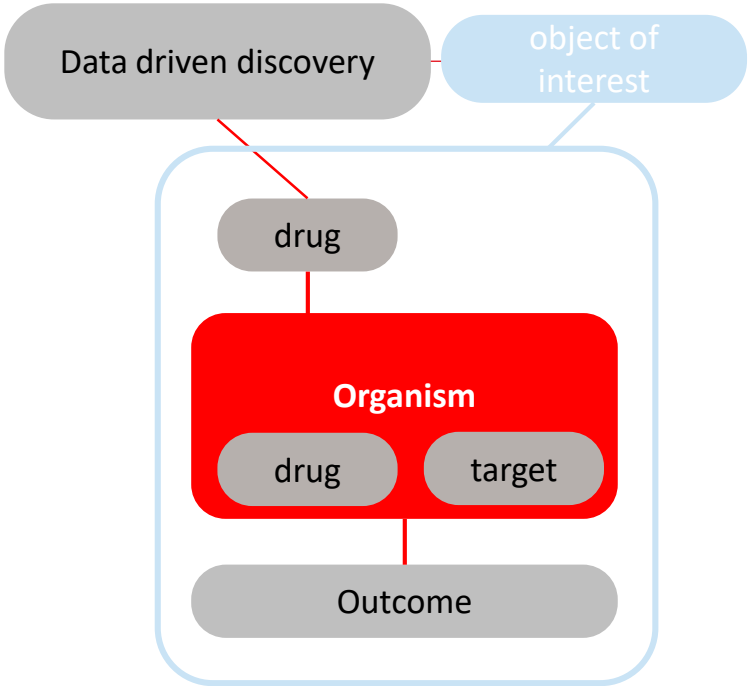

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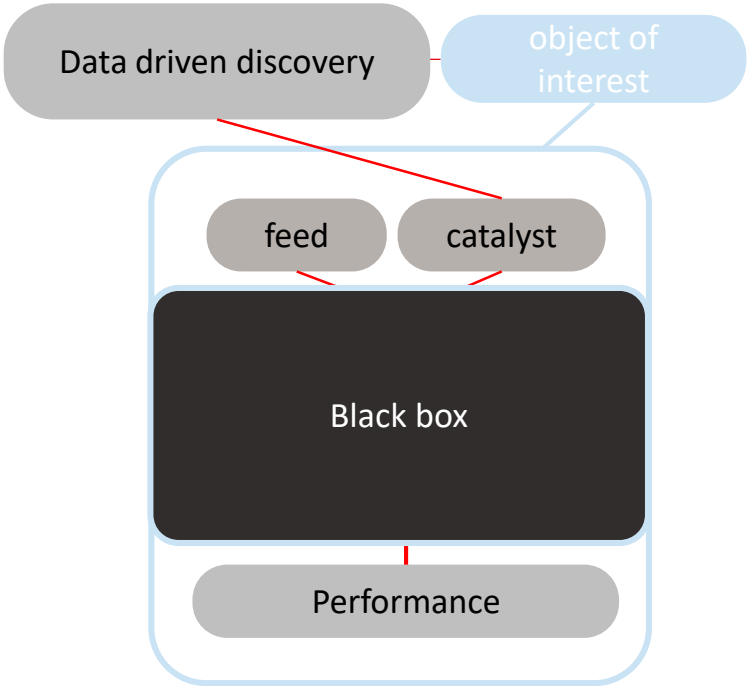

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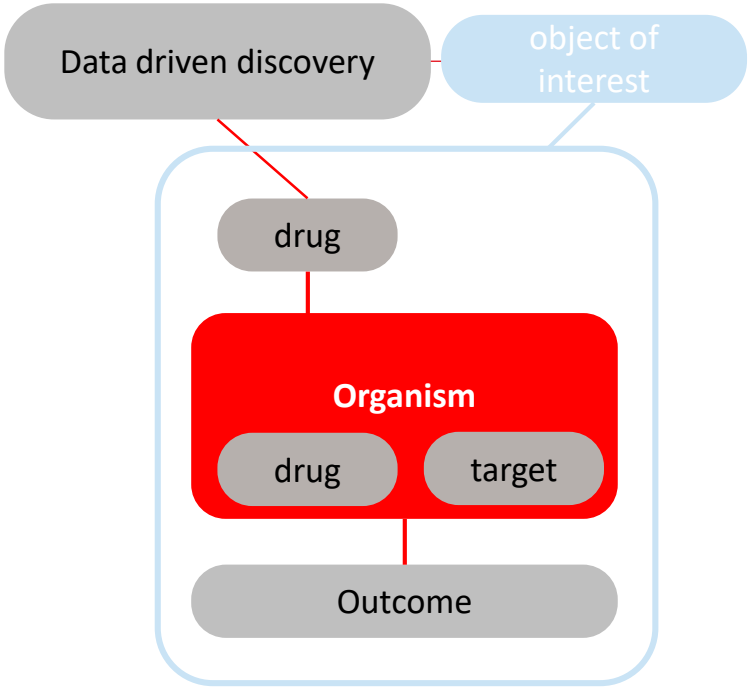

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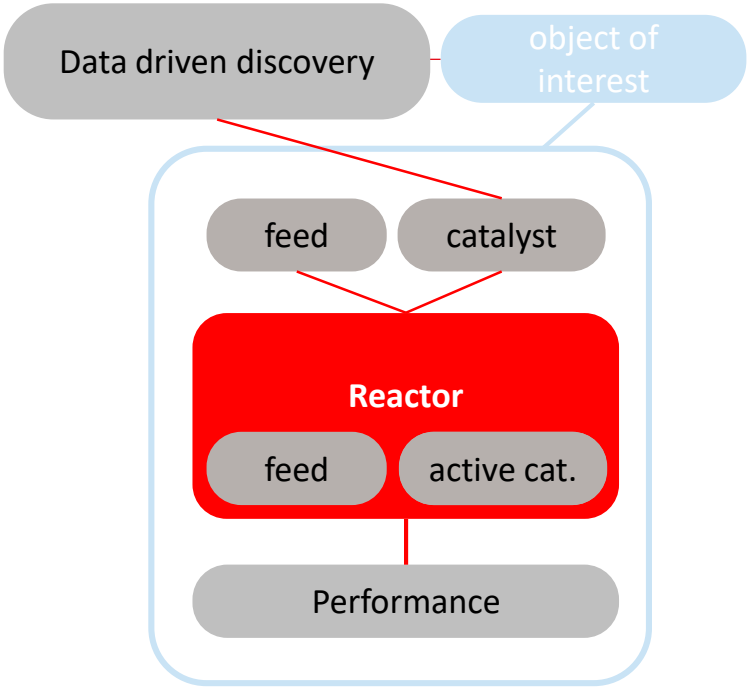

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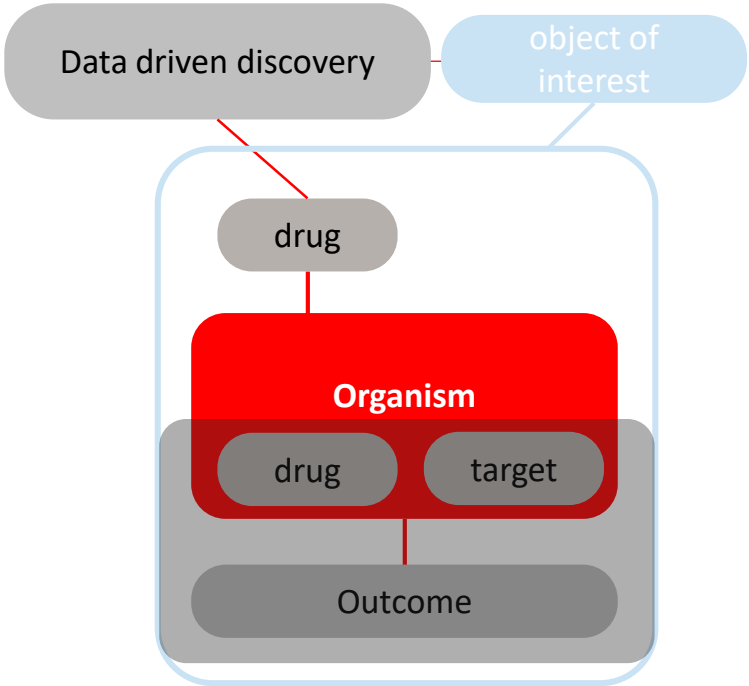

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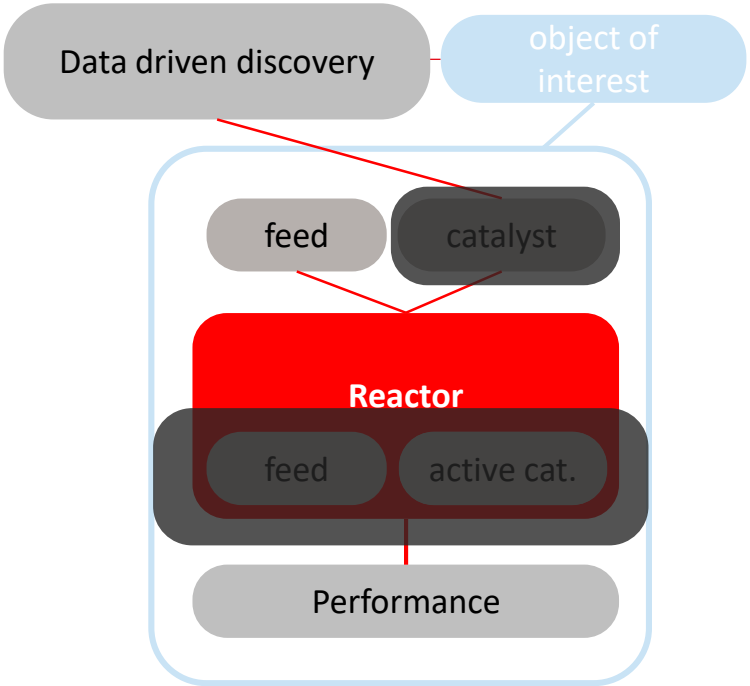
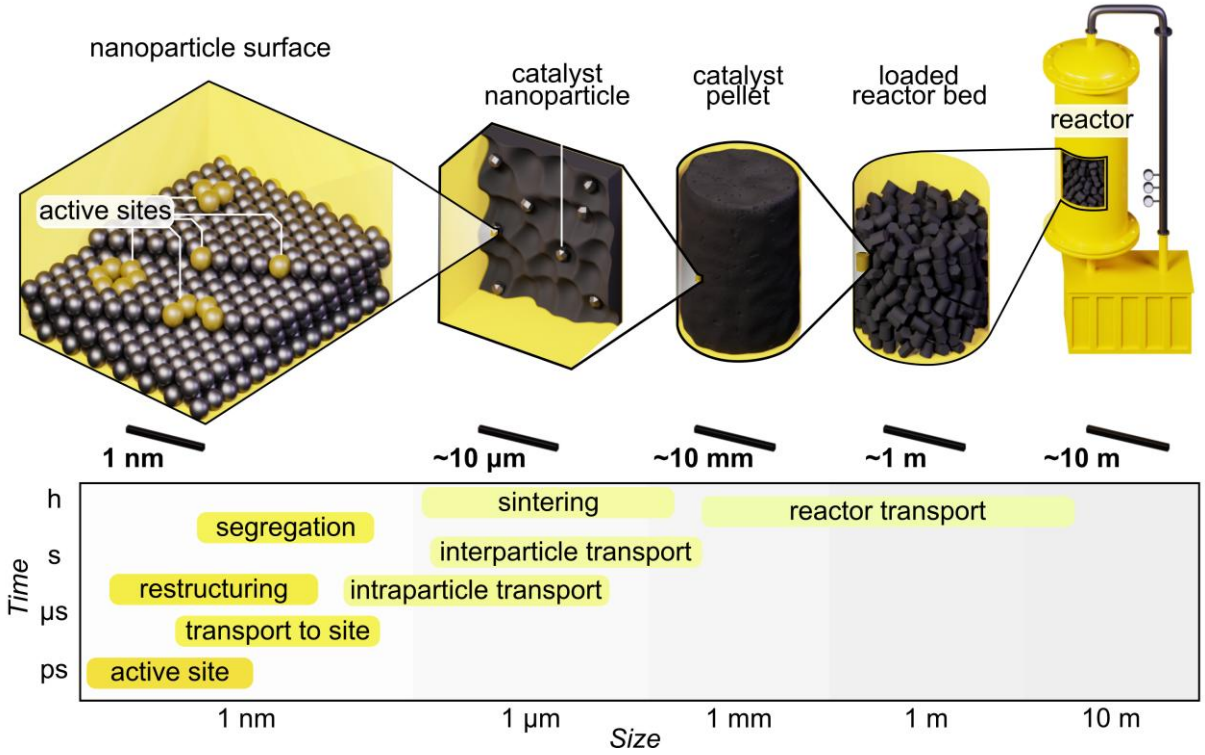


Catalyst

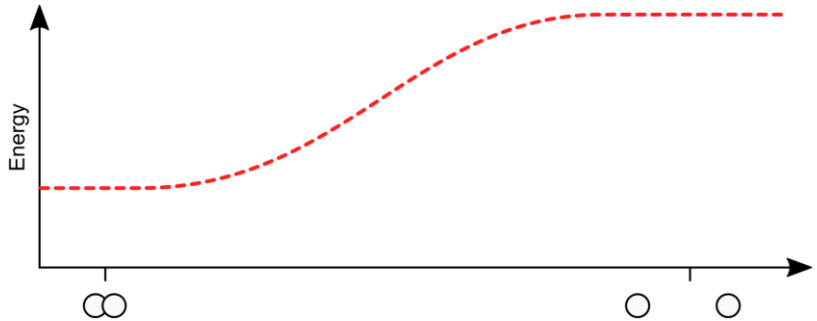
Heterogeneous Catalysis

Edvin Fako



Heterogeneous Catalysts

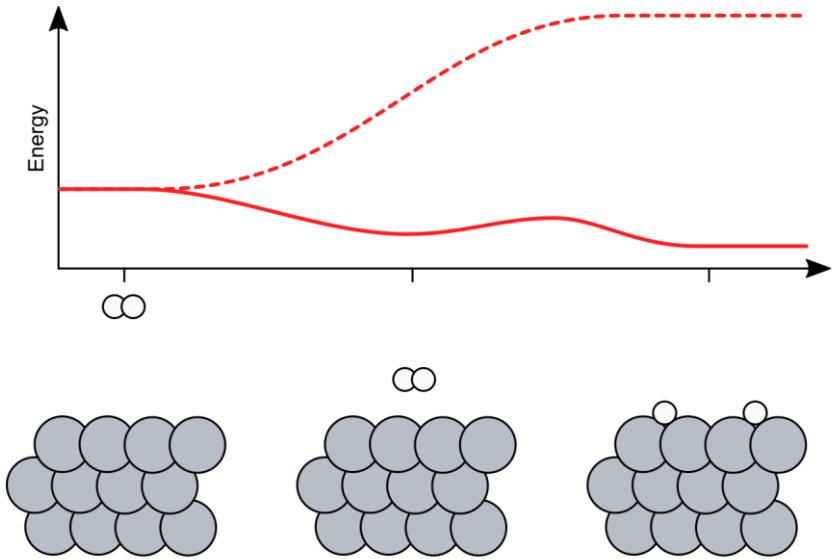
Edvin Fako



Even a simple H-H bond is very hard to simply pull apart…

Heterogeneous Catalysts

Edvin Fako



Here is how the same profile looks if a metal surface is near by…

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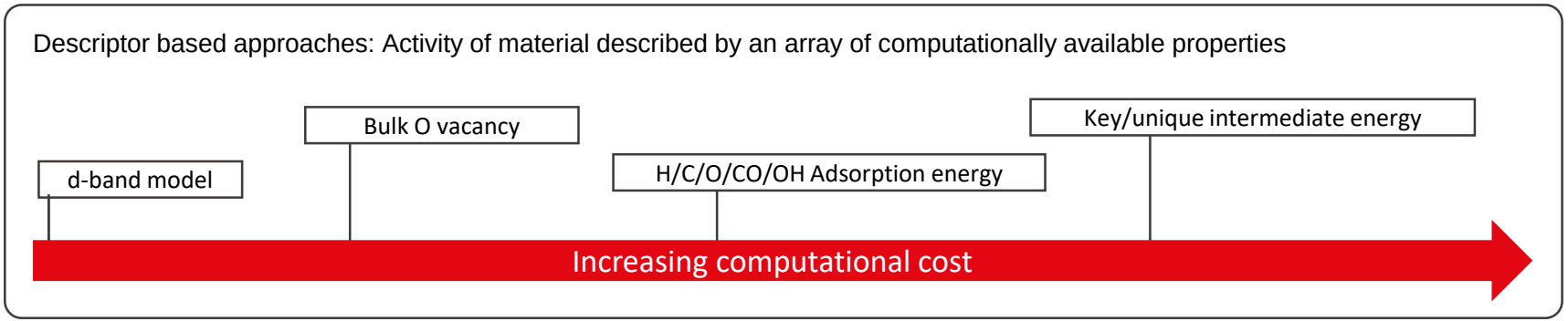
Descriptor versus dynamic approaches

- Approaches of tackling complexity in heterogenous catalysis



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Descriptor versus dynamic approaches

- Approaches of tackling complexity in heterogenous catalysis

Descriptor based approaches: Activity of material described by an array of computationally available properties

d-band model

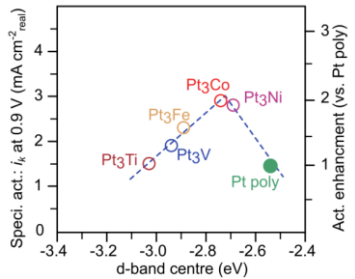
Bulk O vacancy

H/C/O/CO/OH Adsorption energy

Key/unique intermediate energy

Increasing computational cost

Single bulk calculation required



Stamenkovic et al. Nature Materials, 2007, 6, 241–247

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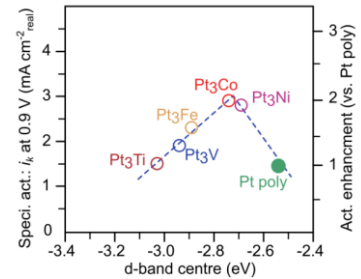
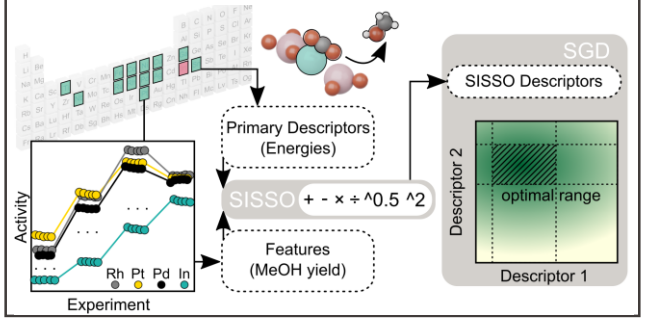
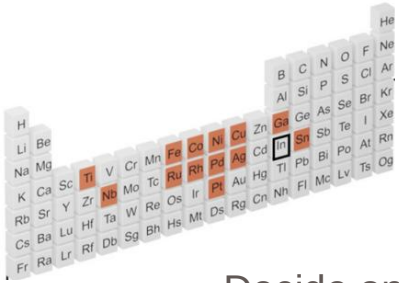


Multiple slab calculations required



Stamenkovic et al. Nature Materials, 2007, 6, 241–247; Khatamirad, Fako et al. Catal. Sci. Technol., 2023,13, 2656-2661

What if we oversimplify a Real Catalysts?

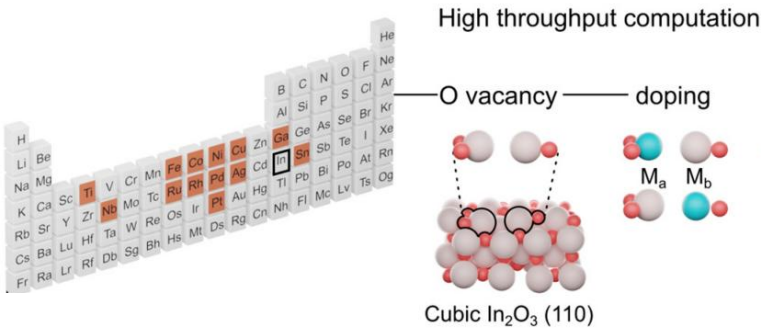


Decide on what is the **base material** and **search domain**

CO_2 reduction on promoted In_2O_3

- Khatamirad, Fako et. al. Catal. Sci. Technol., 2023, 13, 2656–2661

What if we oversimplify a Real Catalysts?



Find a **model structure** capable of
expressing the **effects across the design space**

CO_2 reduction on promoted In_2O_3

- Khatamirad, Fako et. al. Catal. Sci. Technol., 2023, 13, 2656–2661

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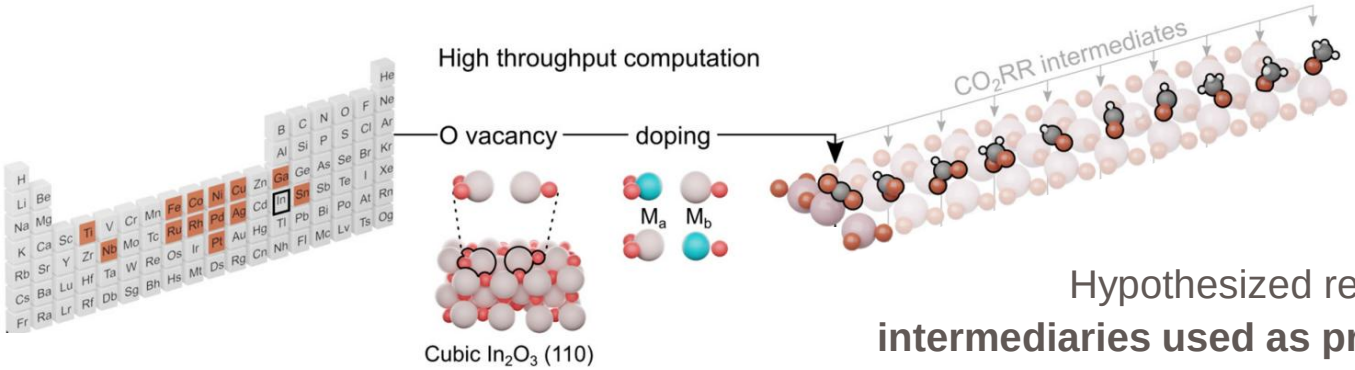

Hypothesized reaction **intermediaries used as probes**.
They need to be placed at the **active site** in a consistent and strategic way.

CO_2 reduction on promoted In_2O_3

Khatamirad, Fako et. al. Catal. Sci. Technol., 2023, 13, 2656–2661

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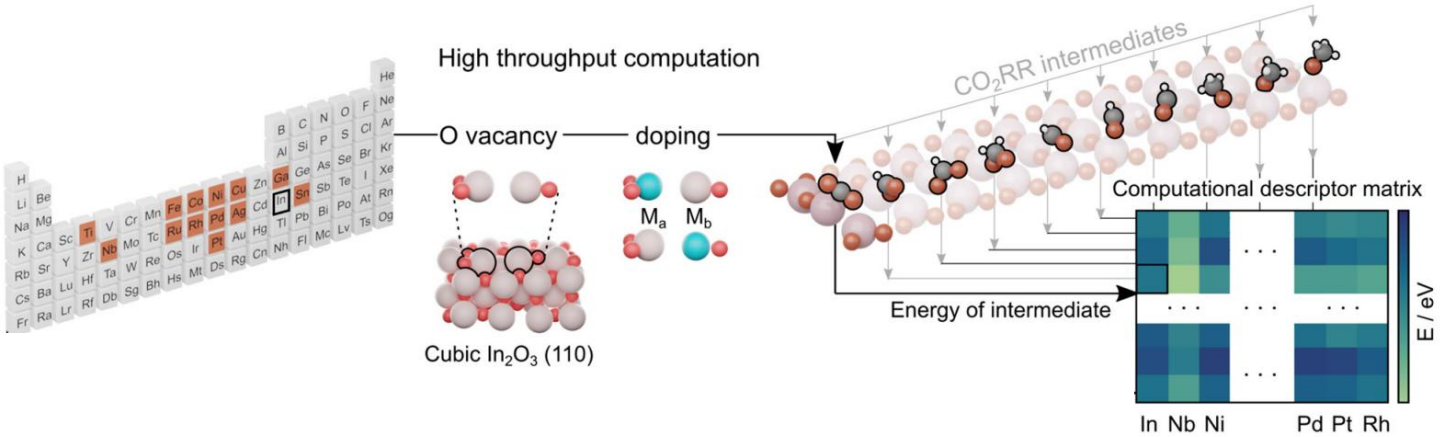

Density Functional Theory driven simulations to find the local minima.
These energies express the effect of the promoter on the base structure.
Prohibitively expensive for high-throughput screening!

CO_2 reduction on promoted In_2O_3

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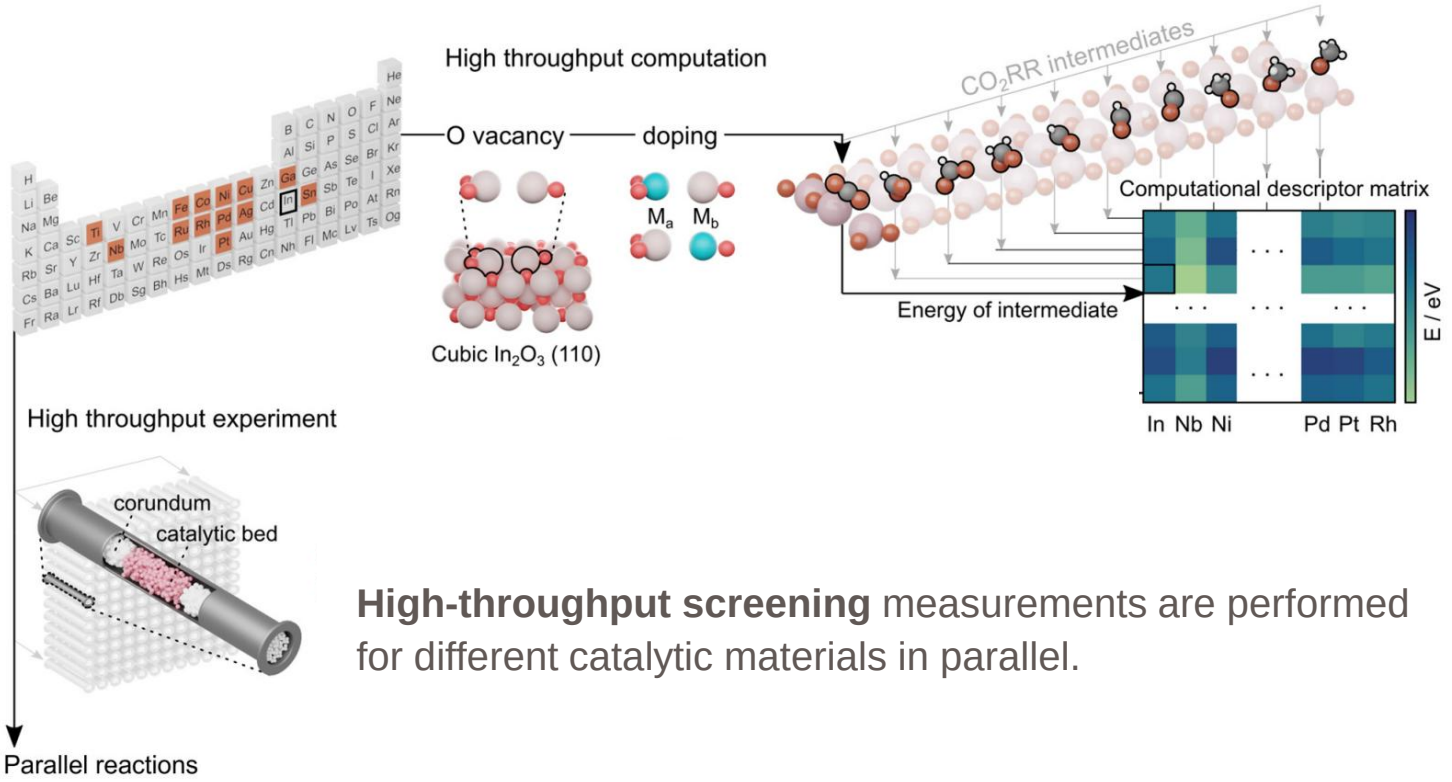

High-throughput screening measurements are performed for different catalytic materials in parallel.

CO_2 reduction on promoted In_2O_3

Khatamirad, Fako et. al. Catal. Sci. Technol., 2023, 13, 2656–2661

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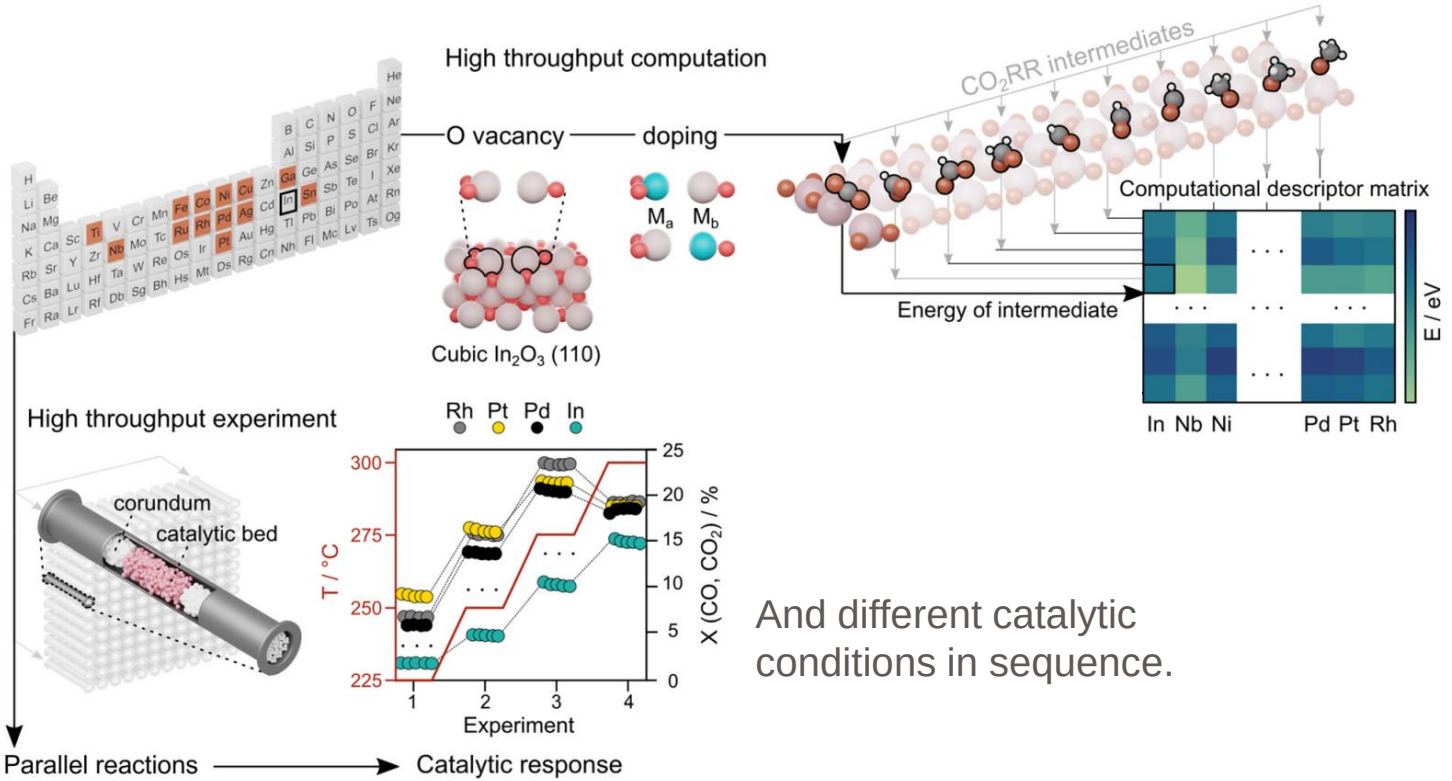

And different catalytic conditions in sequence.

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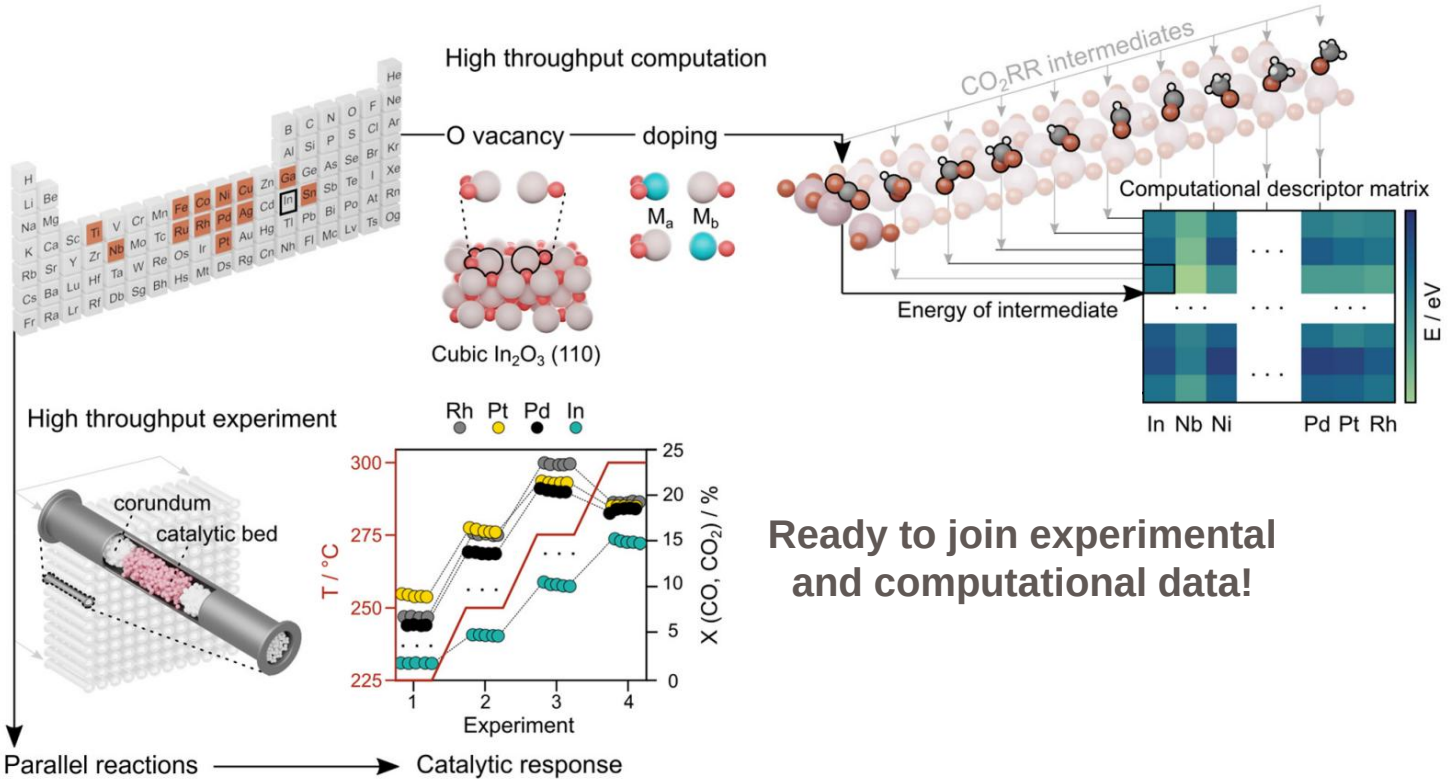

Ready to join experimental and computational data!

CO_2 reduction on promoted In_2O_3

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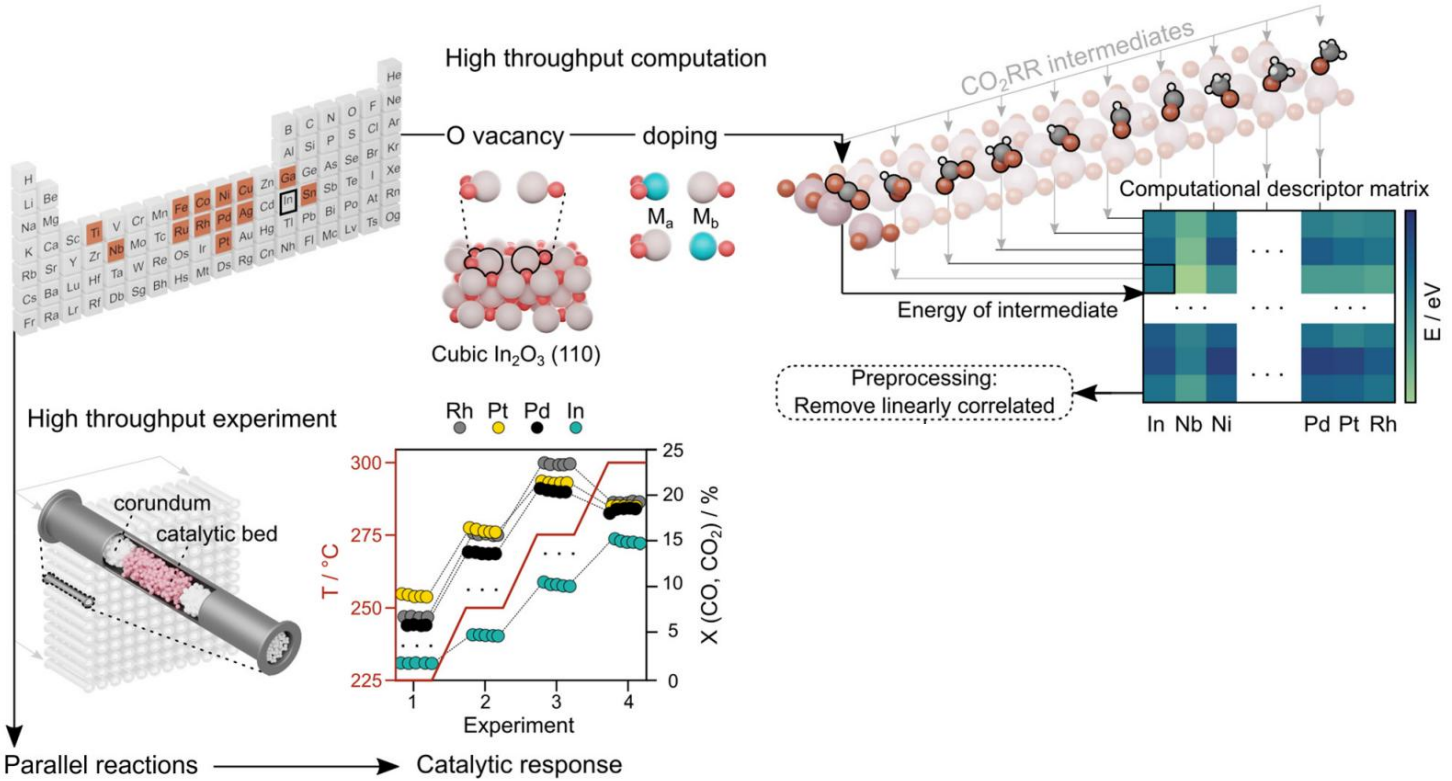

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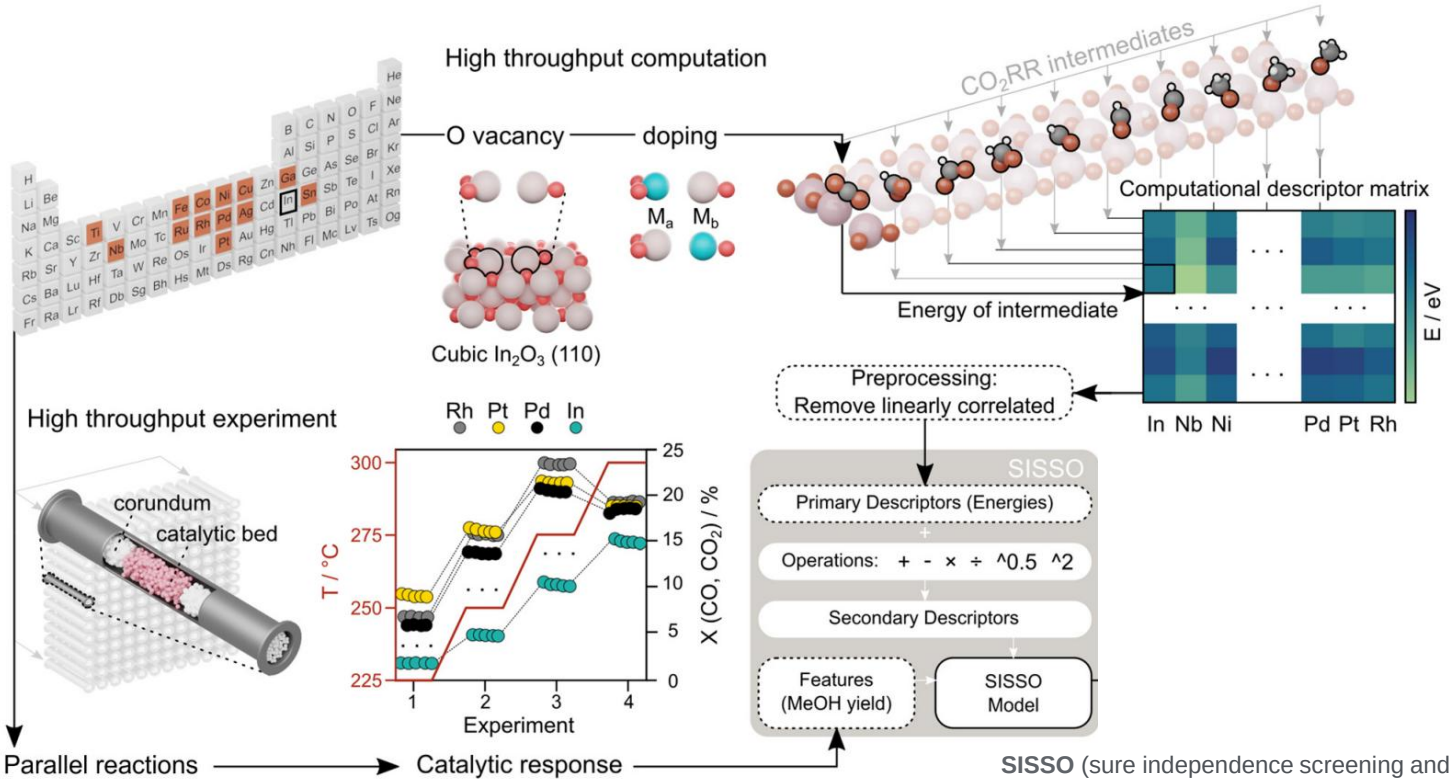

SISSO (sure independence screening and sparsifying operator)

CO_2 reduction on promoted In_2O_3

Khatamirad, Fako et. al. Catal. Sci. Technol., 2023, 13, 2656–2661

Edvin Fako

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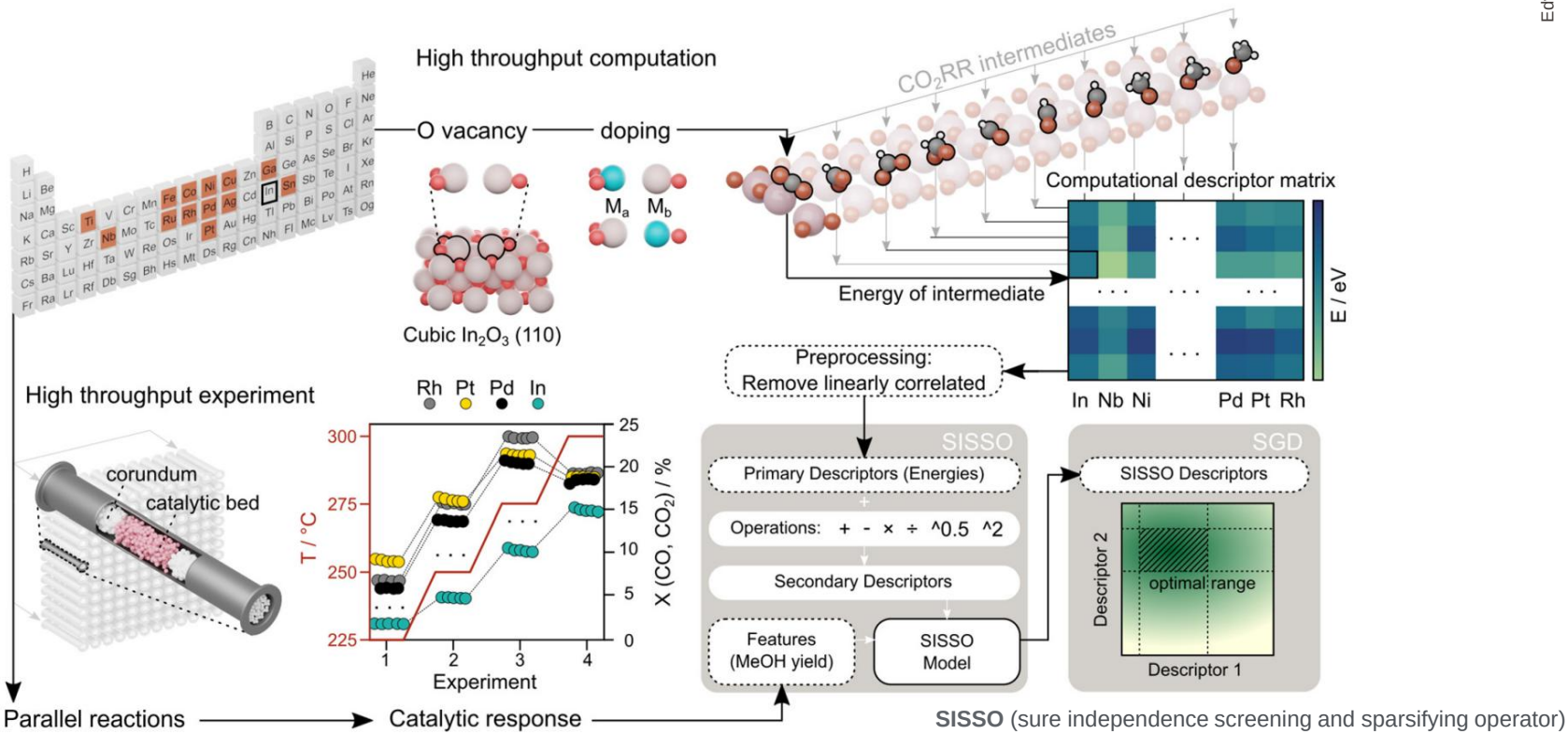

SISSO (sure independence screening and sparsifying operator)

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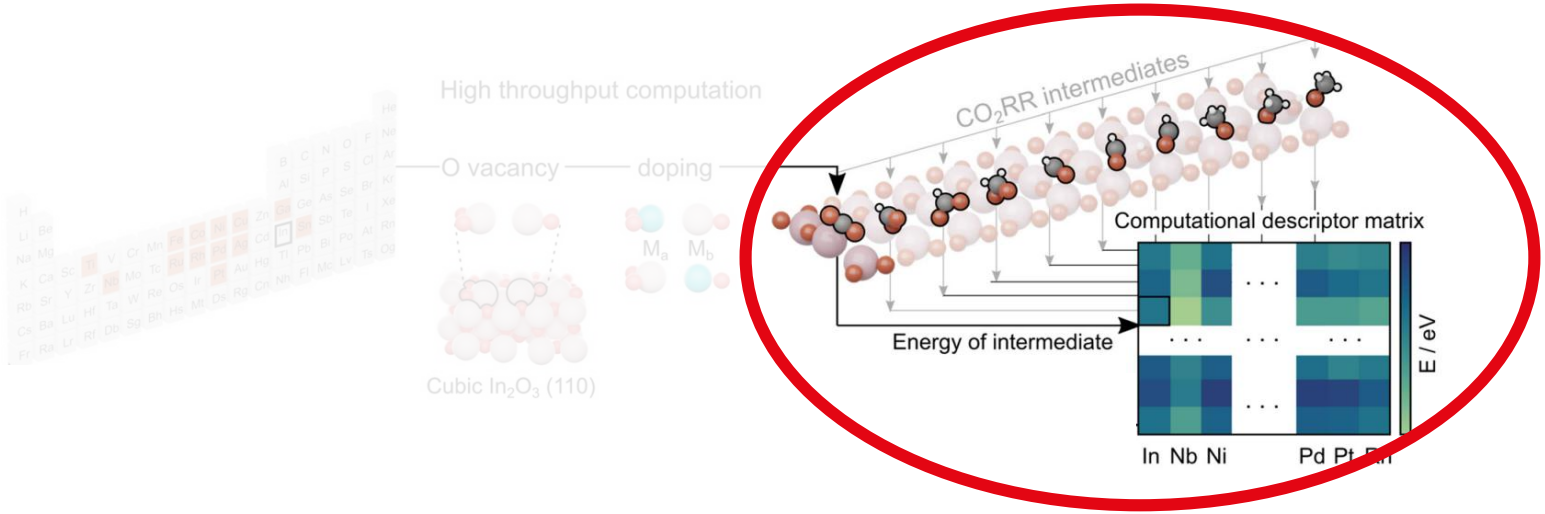
Khatamirad, Fako et. al. Catal. Sci. Technol., 2023, 13, 2656–2661

Limitations of this approach



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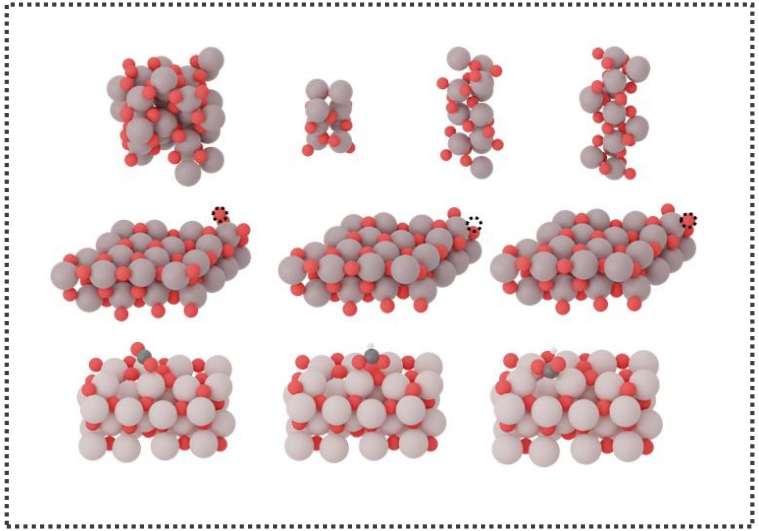
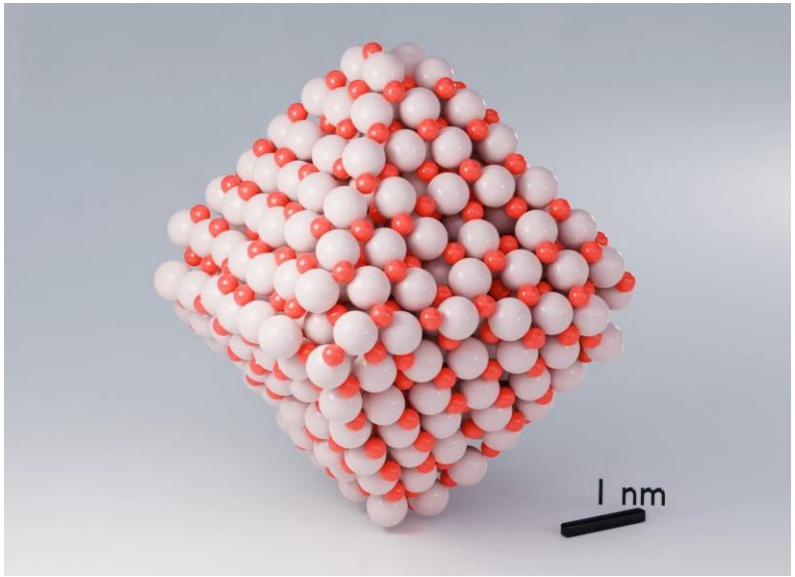
Edvin Fako

Machine Learning at Atomic Scale: Interatomic Potentials





- ML model is 10^3-10^6x faster than reference QM
- Improving at each iteration and converges ~ 5-10 iterations
- ML training takes ~10-24 hours

In_2O_3 particle SOAP-GAP FF

Schaaf L., Fako E., et al., npj Computational Materials (2023) 9:180

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Descriptor versus dynamic approaches

- Approaches of tackling complexity in heterogenous catalysis

Descriptor based approaches: Activity of material described by an array of computationally available properties

d-band model

Bulk O vacancy

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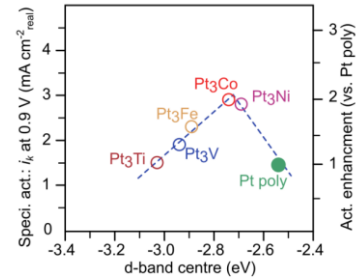

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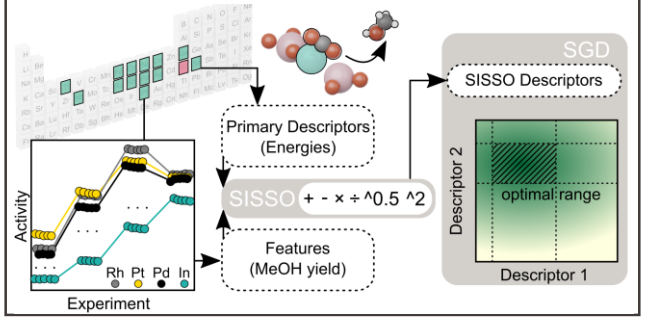

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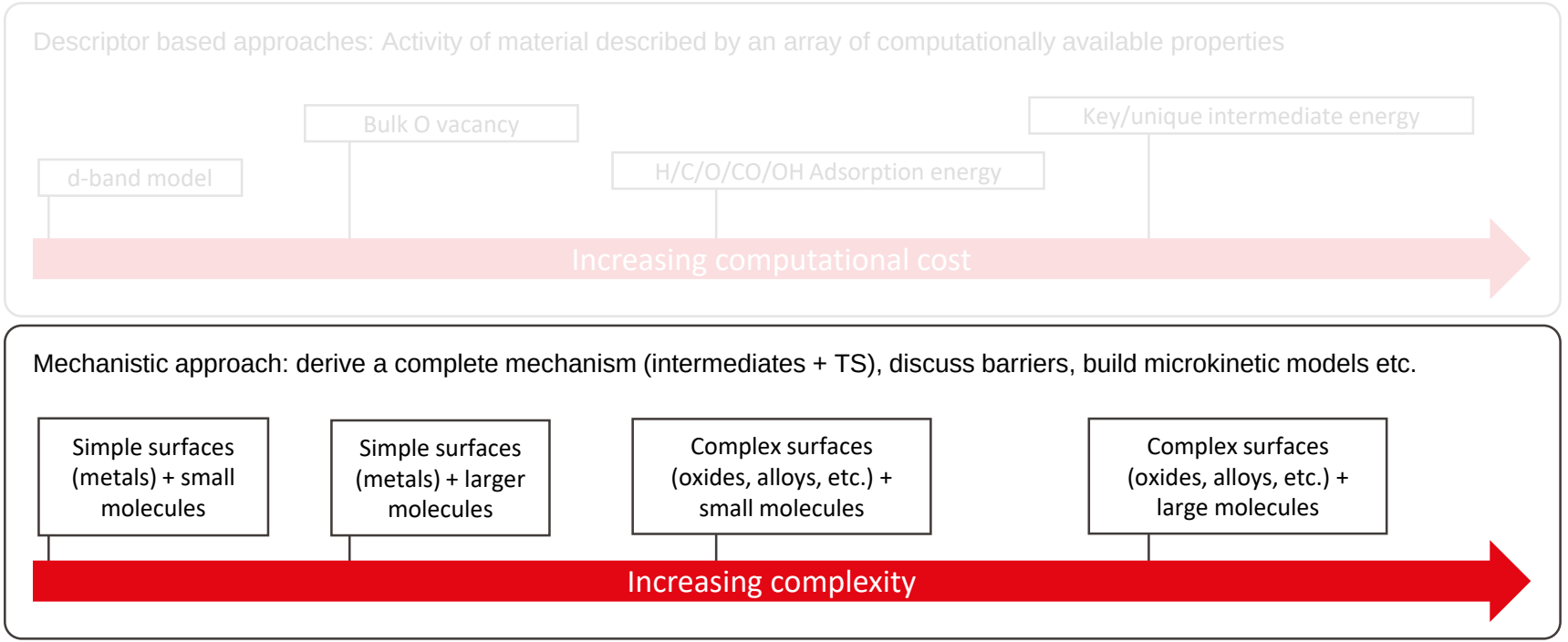
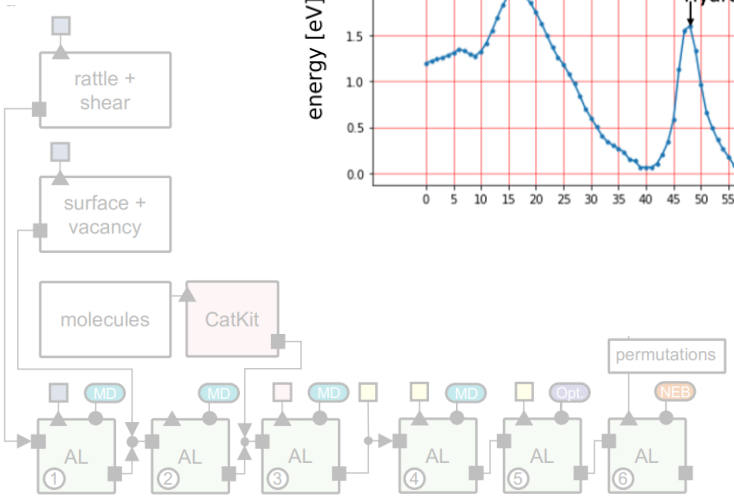
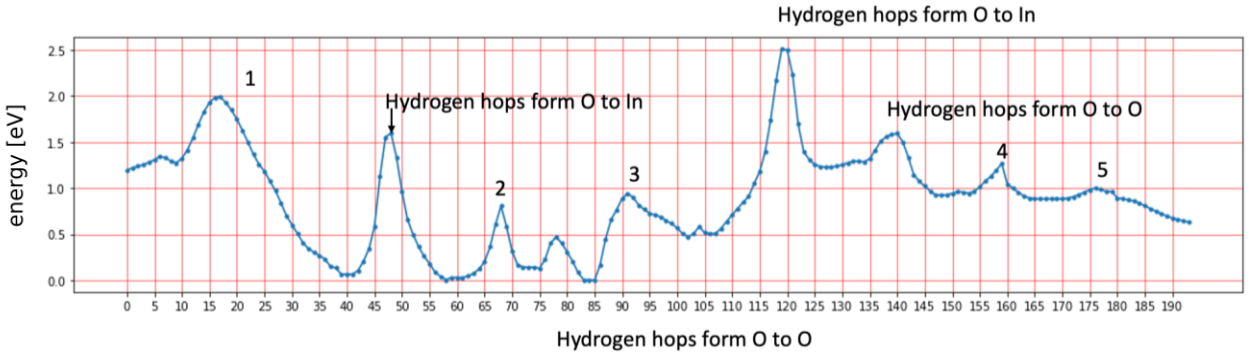
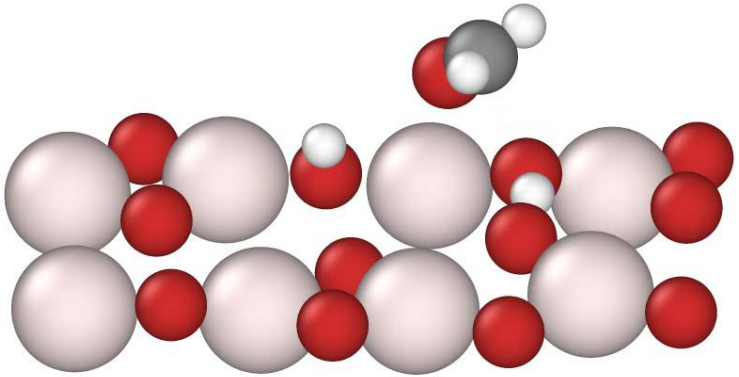


1 NEB = 1 Path

- Place ALL reactants on the surface, run a single NEB along the full reaction path:



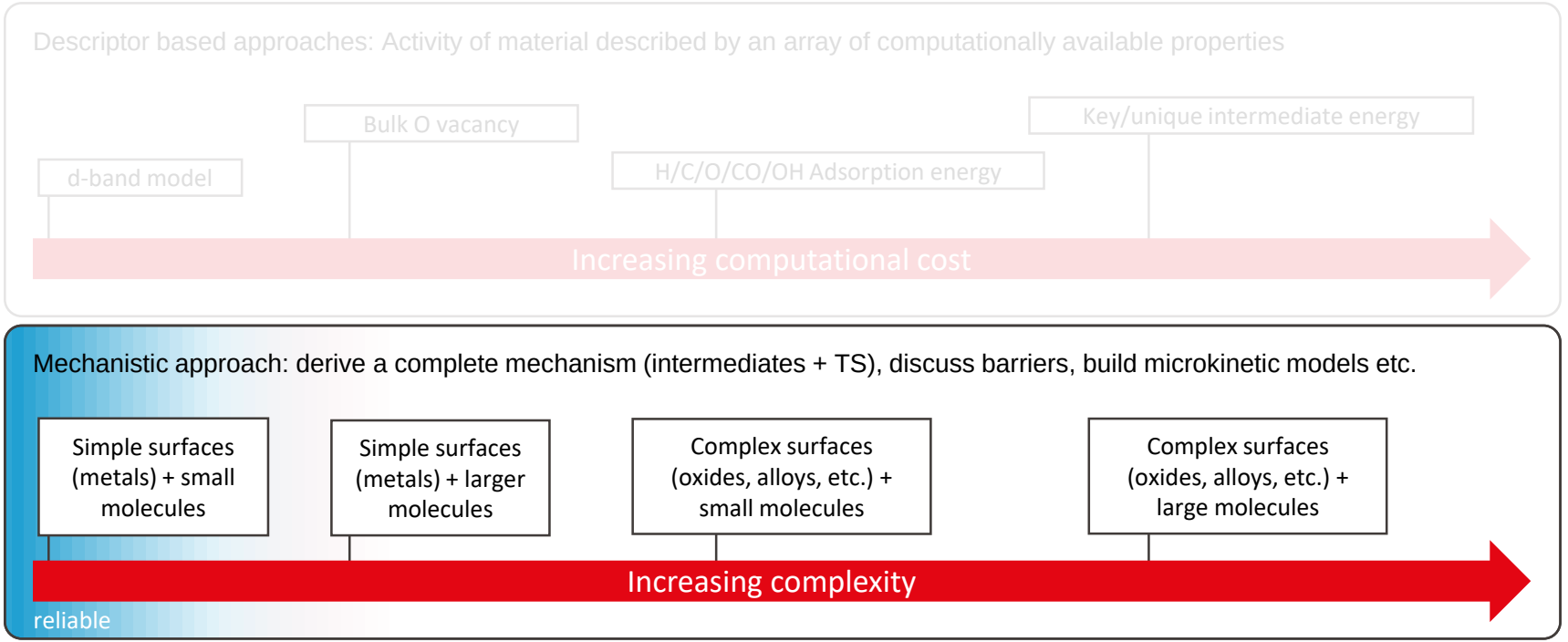




- Schaaf L., Fako E., et al., npj Computational Materials (2023) 9:180

Descriptor versus dynamic approaches

- Approaches of tackling complexity in heterogenous catalysis



Descriptor versus dynamic approaches

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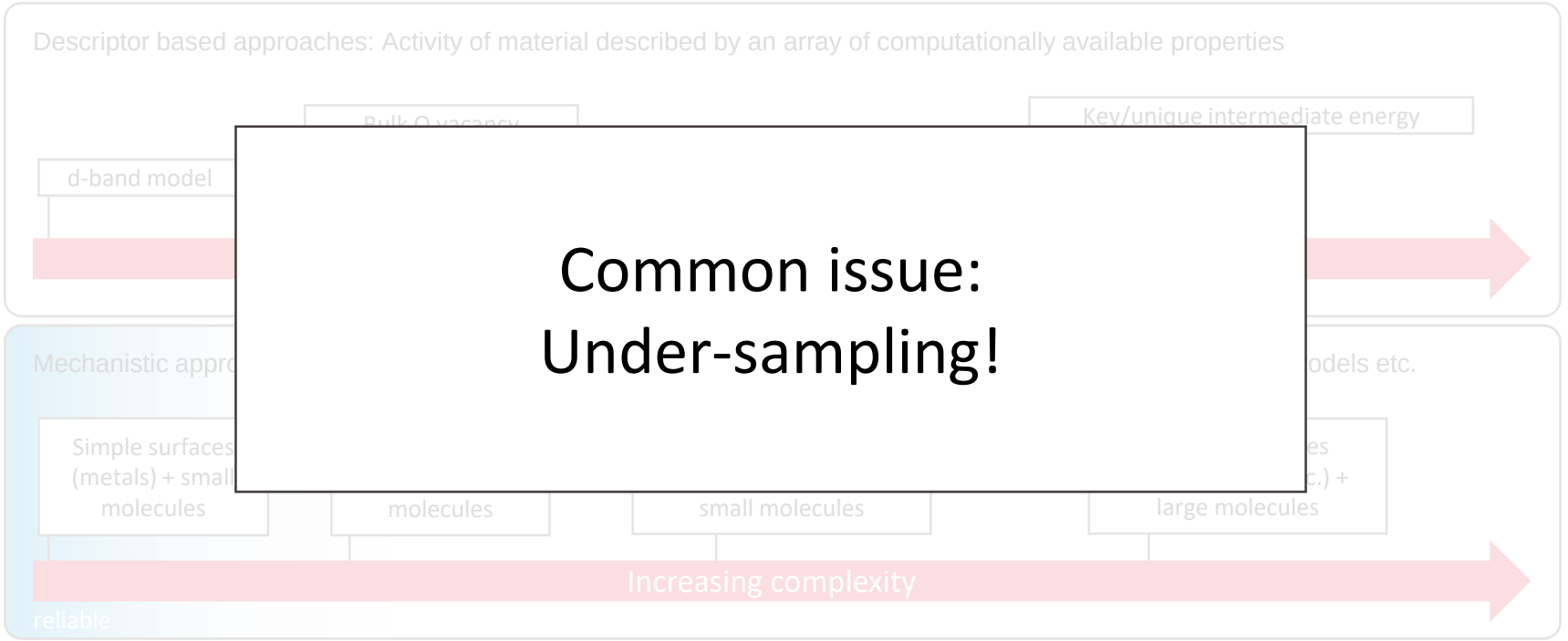
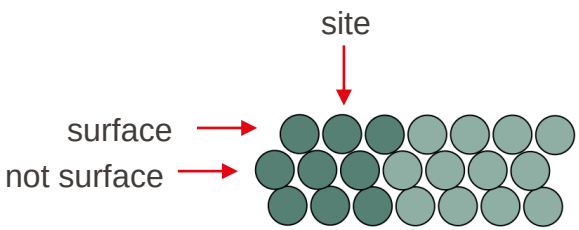
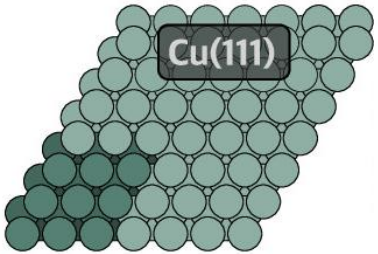


How to understand structures of materials?

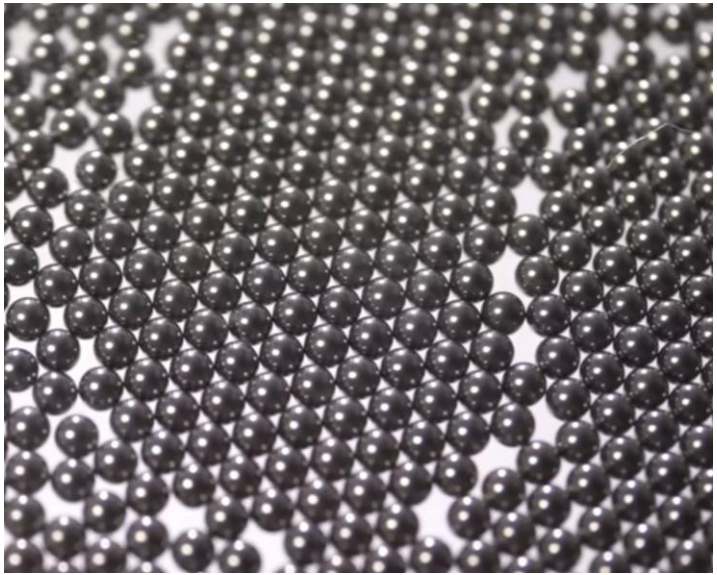
Metal atoms can make multiple covalent bonds, as a result they pack like rigid spheres!



side view



top view



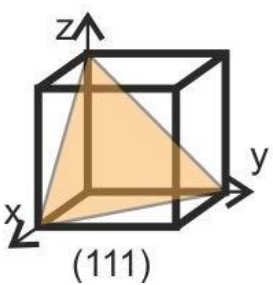
YT Steve Mould: 3000 ball bearings

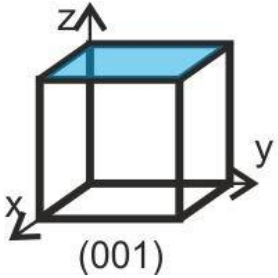
[1] *J. Phys. Chem. C* 2023, 127, 50, 24168-24182; https://www.youtube.com/stevemould

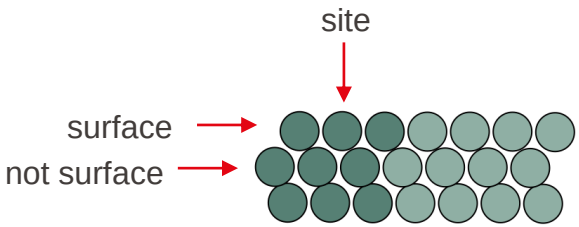
How to understand structures of materials?

The densest packing is the (111)-like, that makes it most stable.

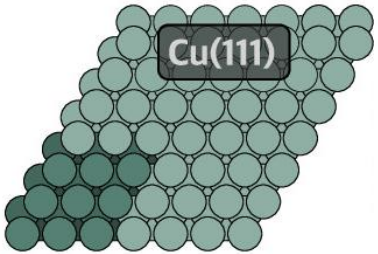
As a result, all other facets can be understood as “steps” of this facet.



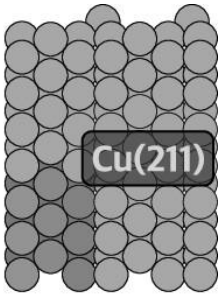


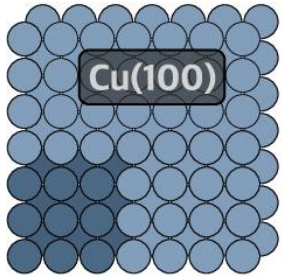


side view



top view





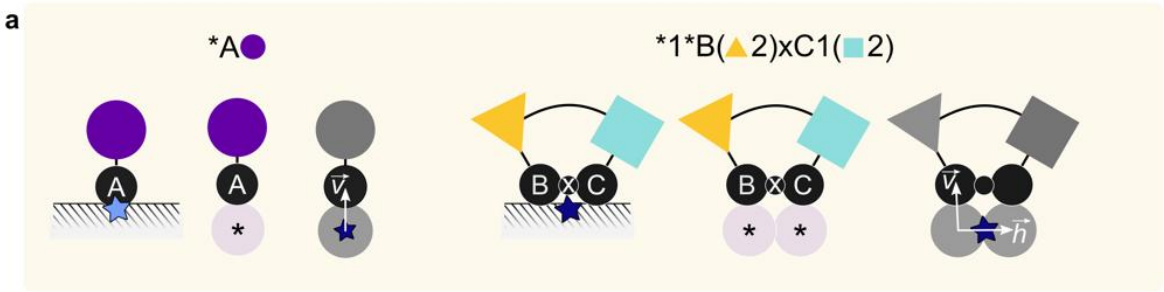
[1] *J. Phys. Chem. C* 2023, 127, 50, 24168-24182; https://www.youtube.com/stevemould

How to sample fragments on a surfaces?

Edvin Fako

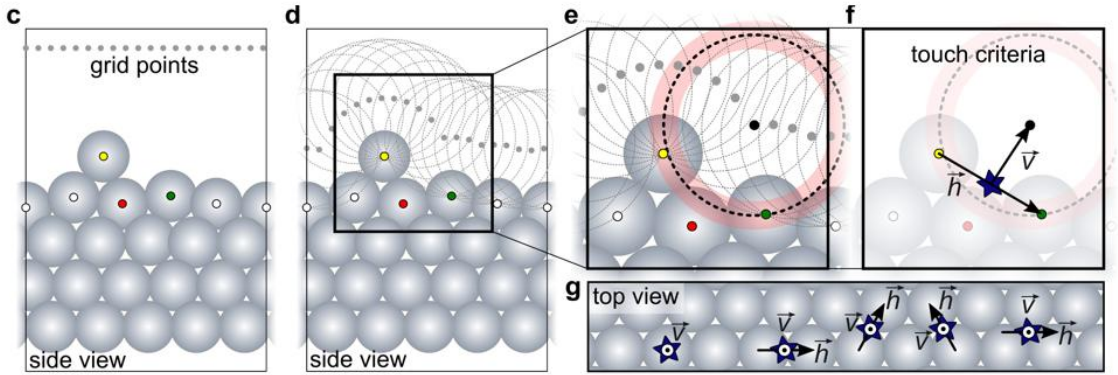
Use *SMILES to sample:

- All species
- All binding motifs



Find all sites on any surface:

- What atoms can be “touched”
- Which of those are “sites”

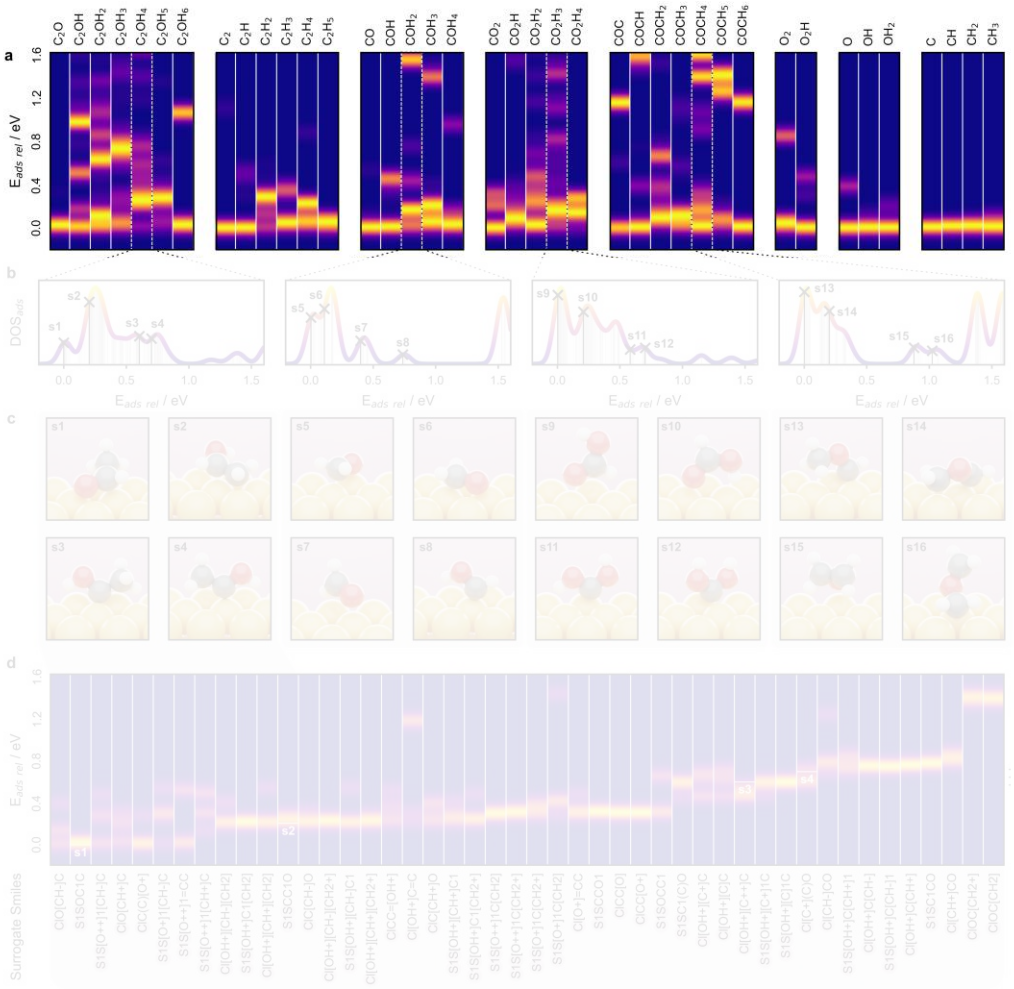


10.26434/chemrxiv-2025-79nj4

Edvin Fako

AutoAdsorbate

- Enumerate:
  - All sites
  - All species
  - All binding motifs
- DOS_{ads} as property of the surface
- Rich information about the chemical properties of the system



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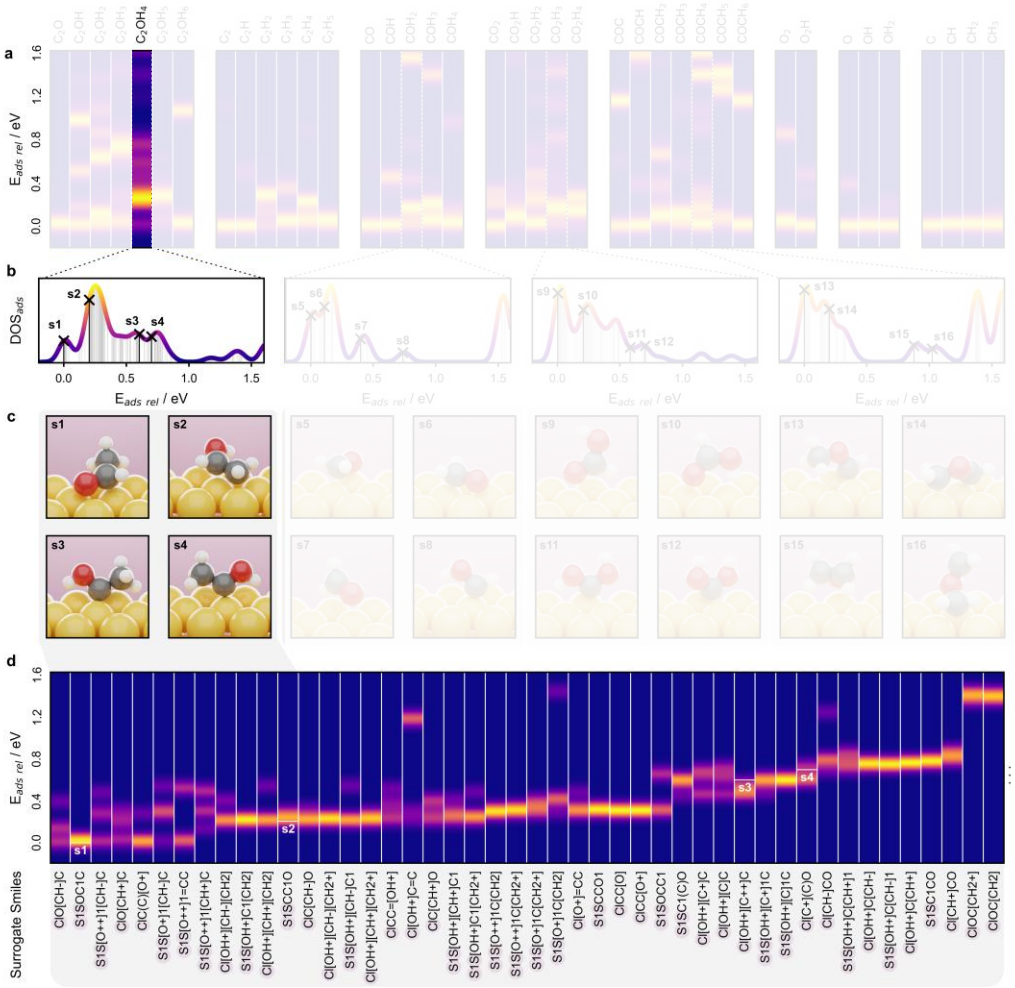

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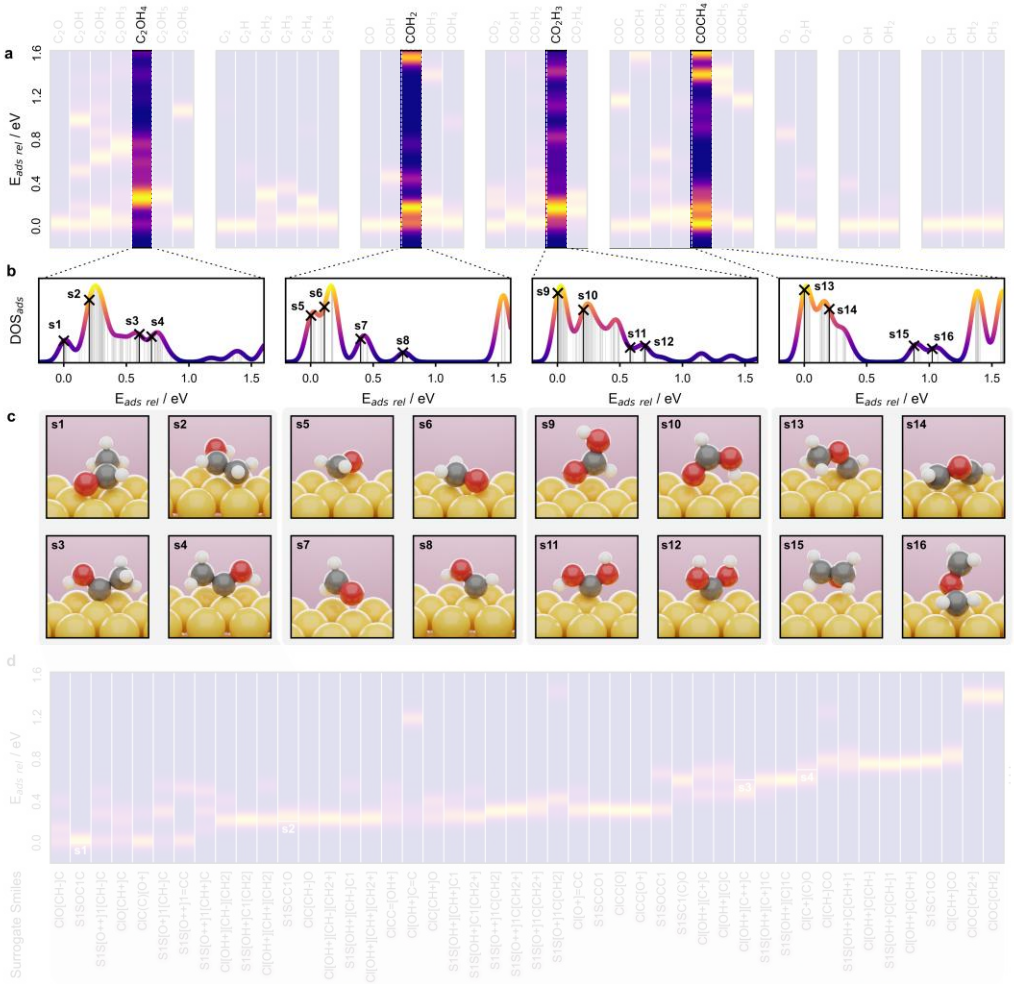

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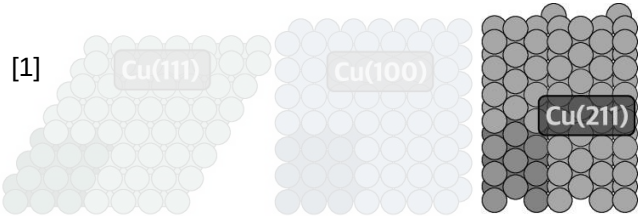
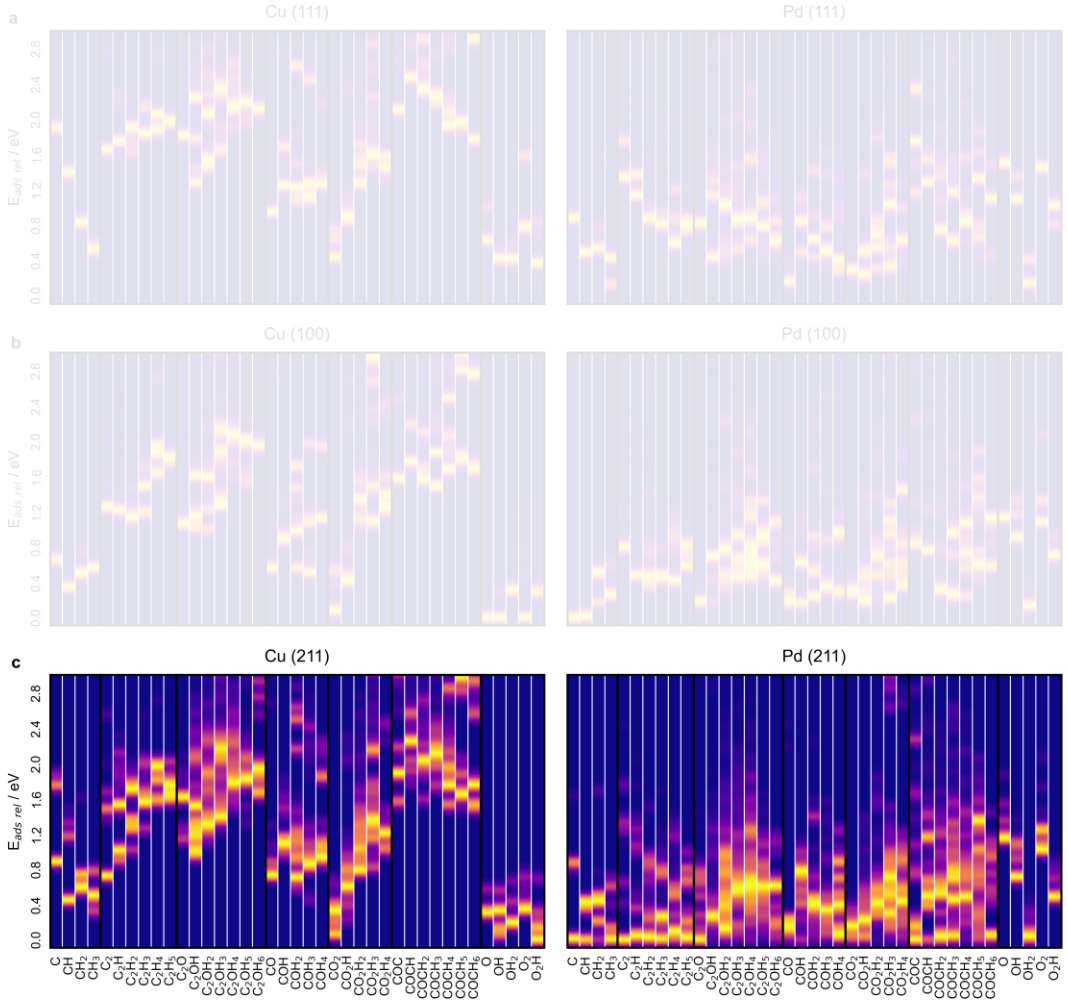
Edvin Fako

AutoAdsorbate

- Compare holistic picture of energetics
  - Computer Vision
- AdsMT – like approach:
  - Predict the DOS_{ads}

[1]





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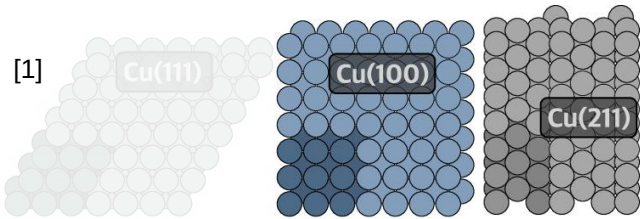

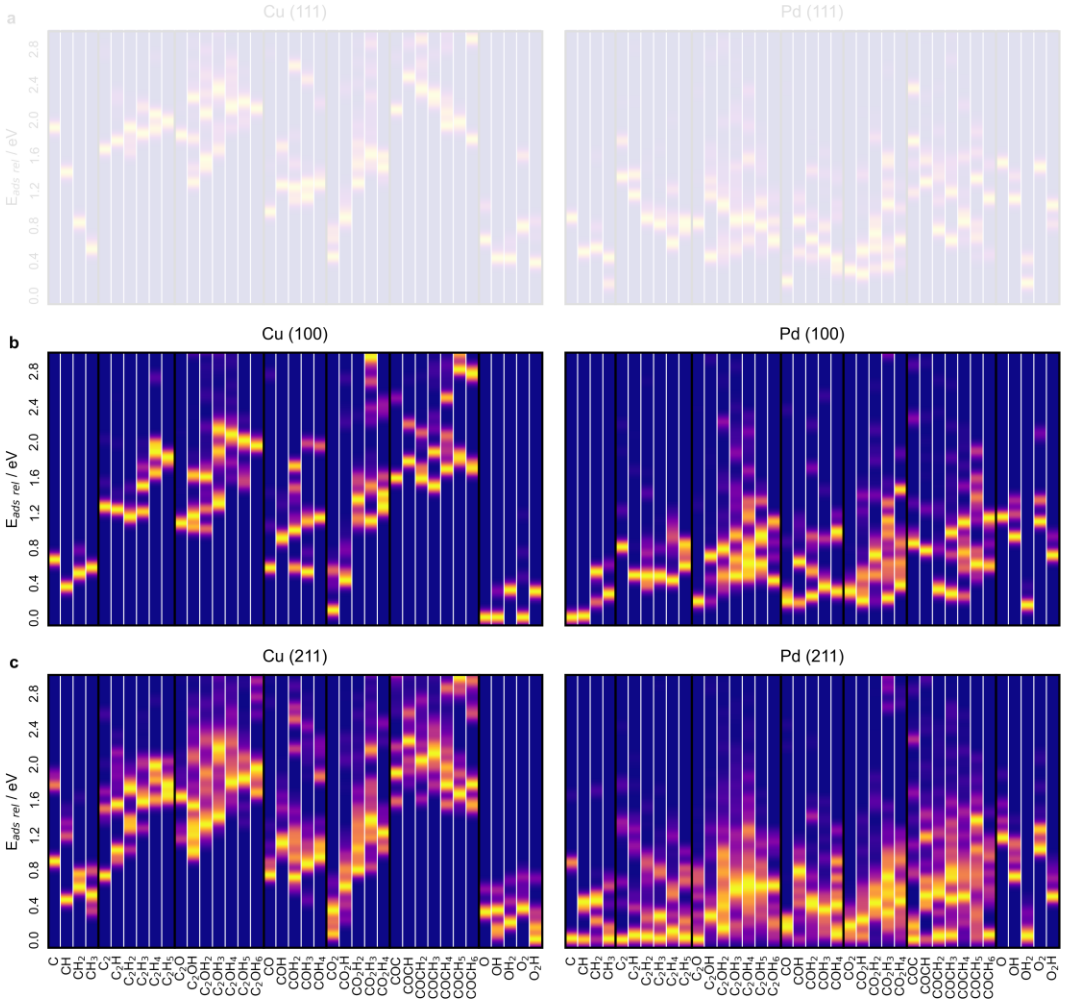

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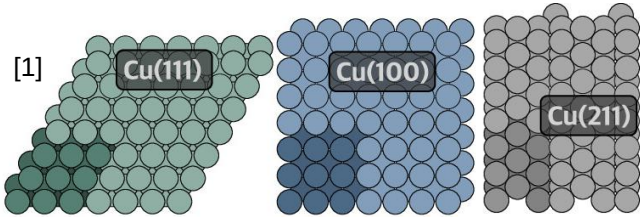

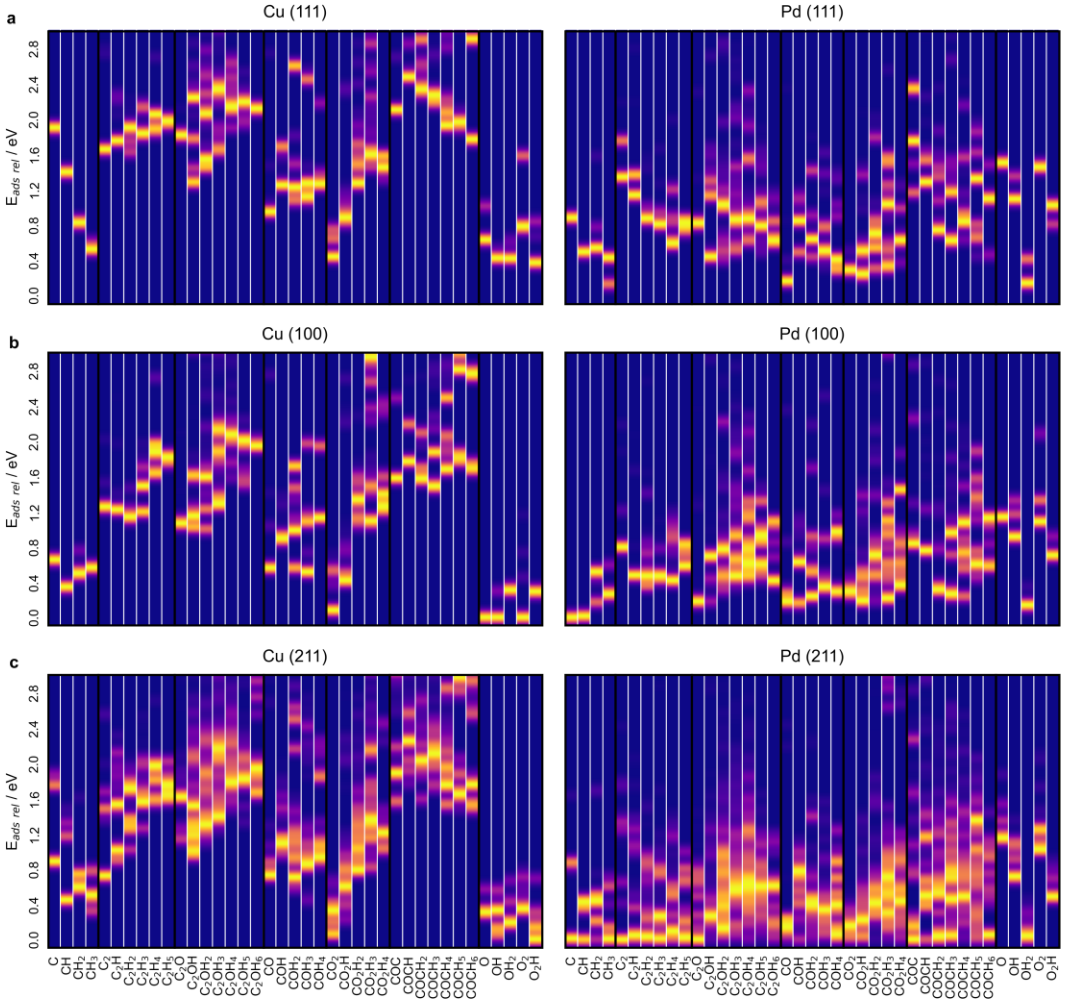

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Outlook

- A sustainable future depends on Heterogeneous Catalysis
- ML can provide a path forward
- We need better data
- MLIP are mature enough to take on the task
- Structure generation is open source

= All the power is in your hands!

Edvin Fako

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Deep descriptor ML
(e.g. comp. vis.)

Dynamic
Gen AI rewards?

Dynamic
LM rewards?

Agents for simulation?

MLIP improvements?

Bayesian
atomistic optimization?

Edvin Fako

Thank you for your attention!