



# Hands-on 11 : MLP04 - Screening

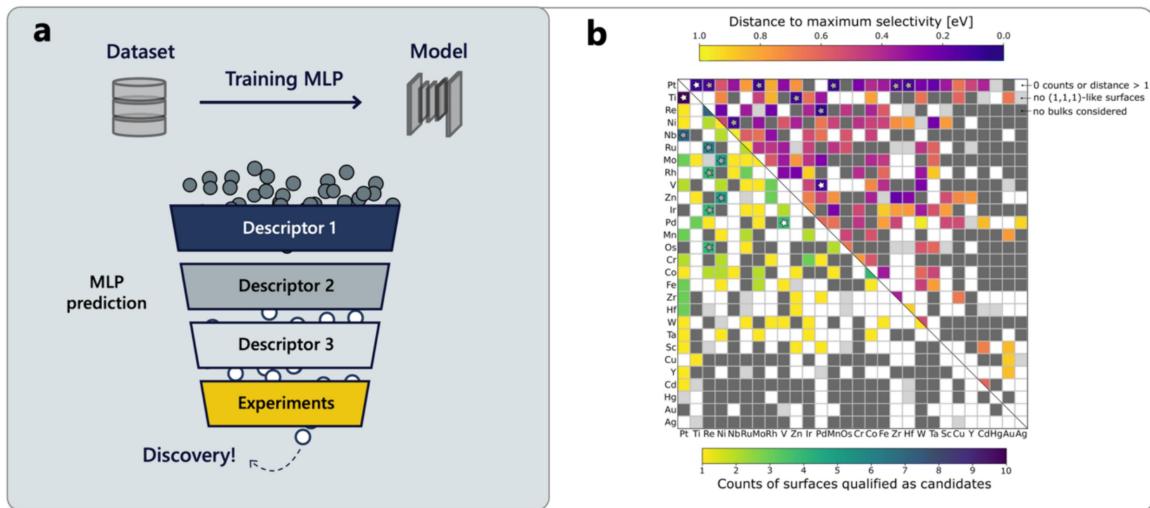
## Notice

1. From next class: Student presentation.
2. will be Zoom recorded,
3. At least one question during the 5 days of presentations needed for participation score

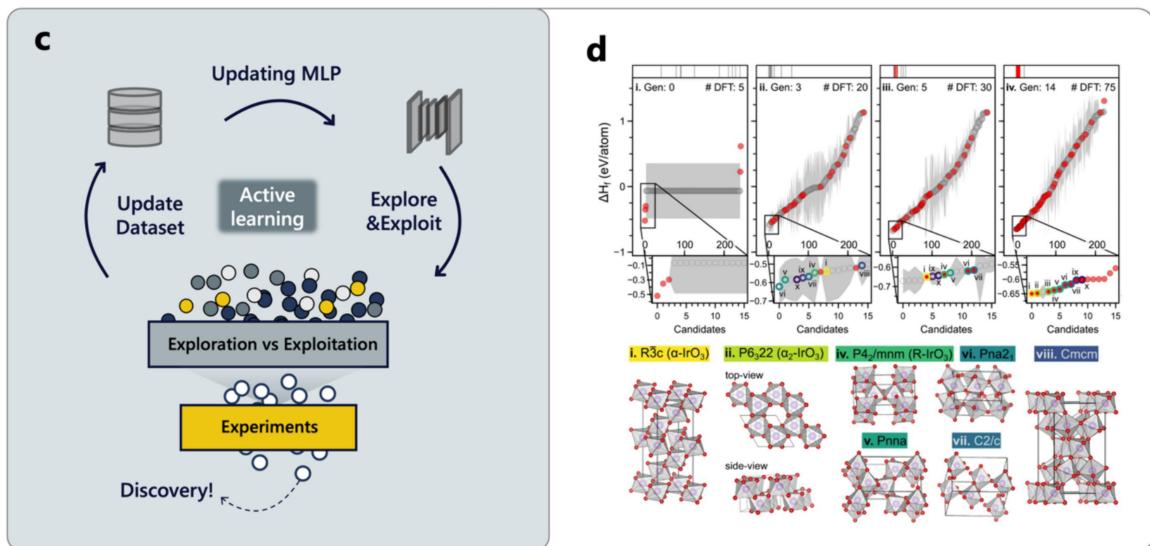
Date	발표1	발표2	발표3	발표4
2024-11-28 (Thu)	이유진/김윤경/한세희	이찬형/조태연/김영민	정종윤/박원규/송선우	최겸/강우종/남건욱
2024-12-03 (Tue)	이채원/이승우/박현태	박서연/김기범(20543)/이성빈	정은영/김민우/정제연	전해관/박유택/전현수
2024-12-05 (Thu)	홍영택/문진욱/김광욱	황수성/홍승효/김관영	이호영/김영재/이승환	조현성/최새롬/오정호
2024-12-10 (Tue)	전혁준/이세웅/성기현	허원준/이훈로/김민욱	서화경/김미연/정하영	한호식/전우찬/문형석
2024-12-12 (Thu)	김기범(24529)/김명준/유현지	김호재/장건익/구진숙	DROUX ANOUK/WIJEWARDENA	

## ▼ High throughput screening

## Funnel-type Search Space Screening

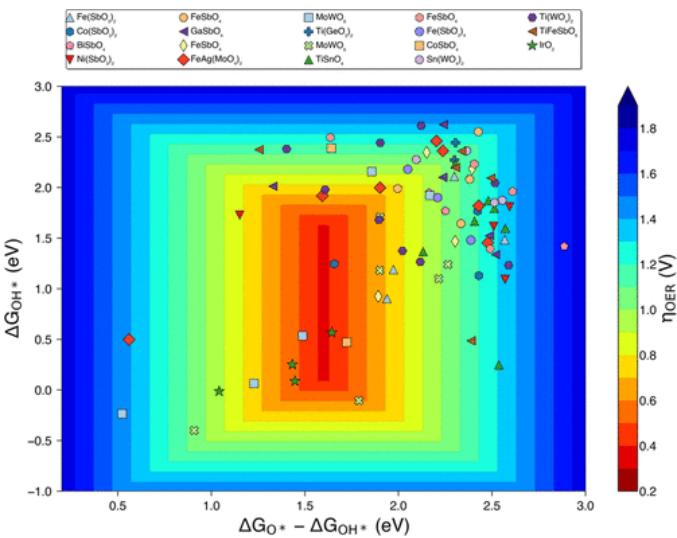
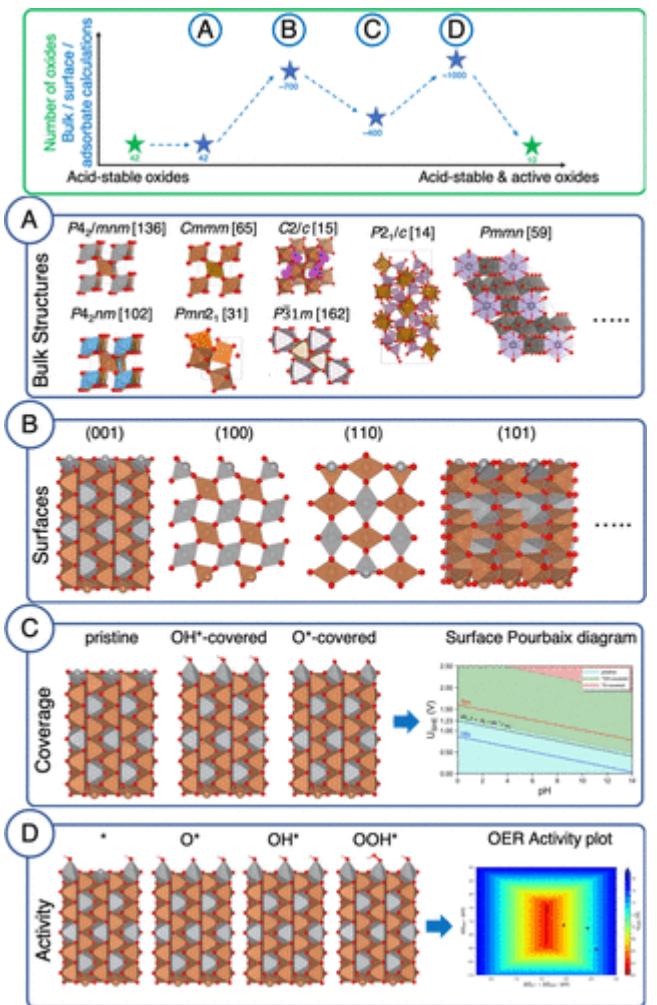


## Active Learning Exploration of Search Space



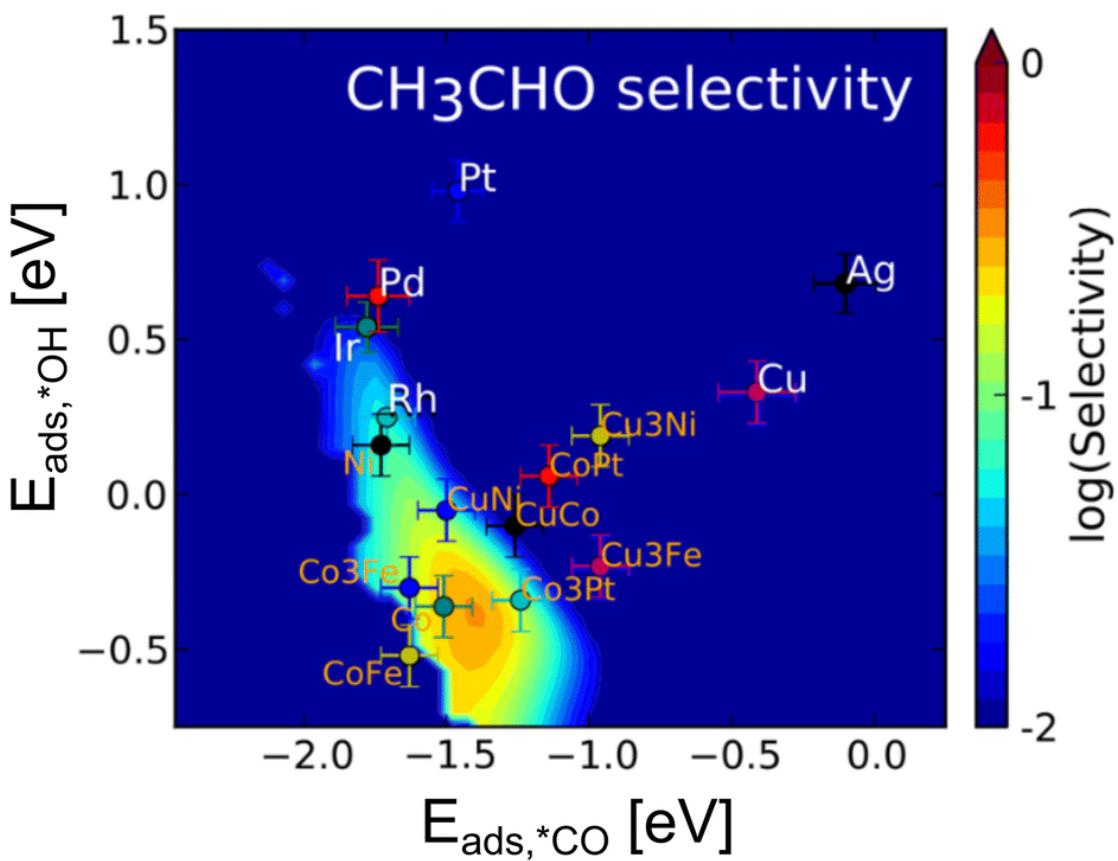
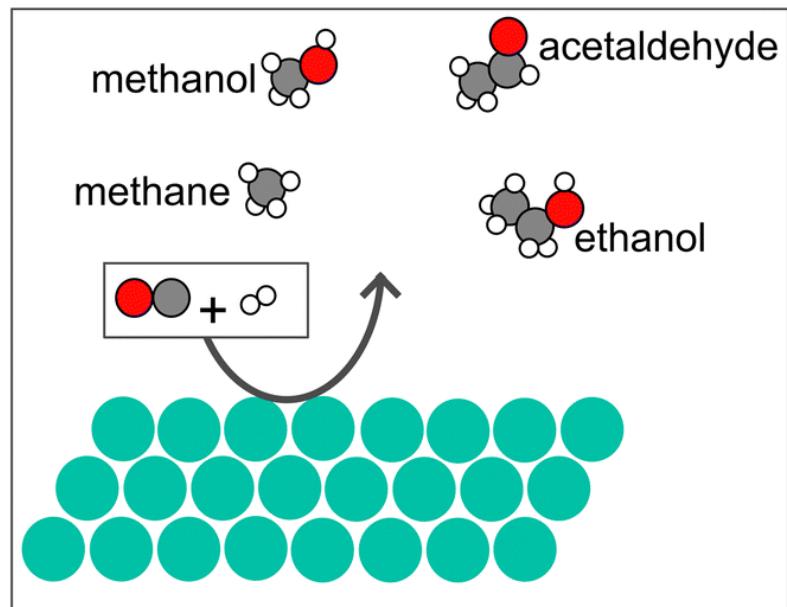
S. Choung, W. Park, J. Moon and J.W.Han Chemical Engineering Journal  
494, 2024, 152757.

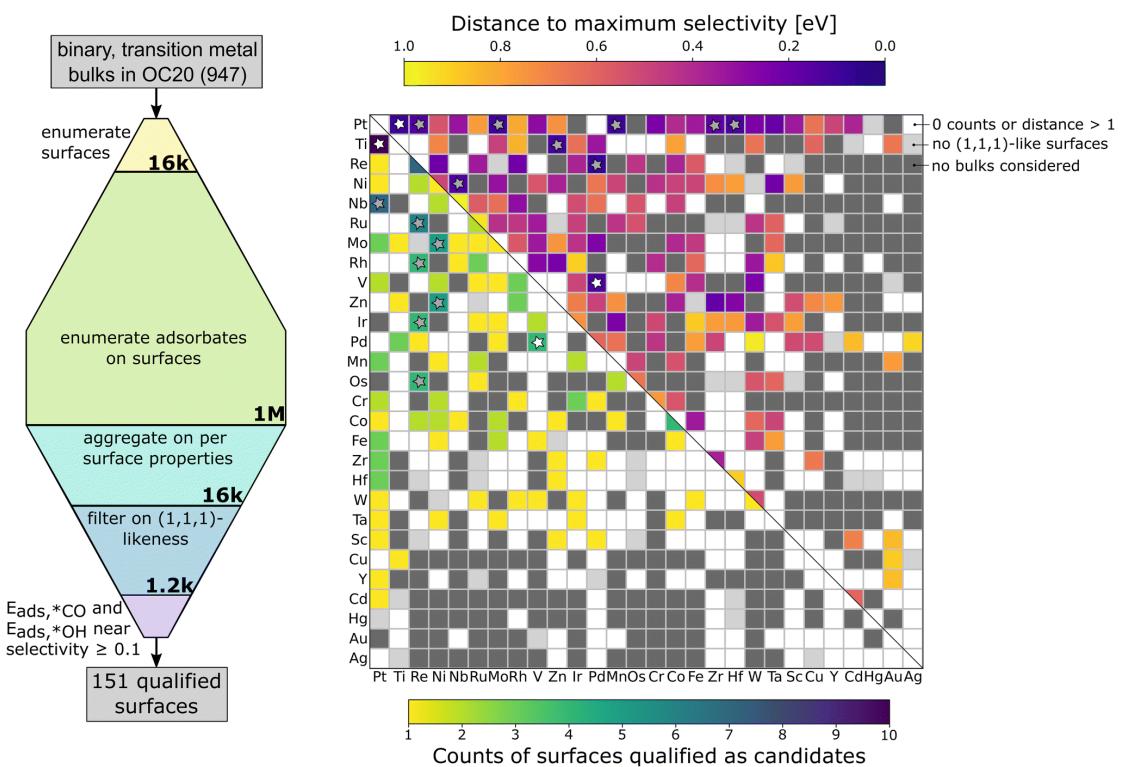
## ▼ Acid stable oxide



ACS Energy Lett. 2020, 5, 12, 3778–3787

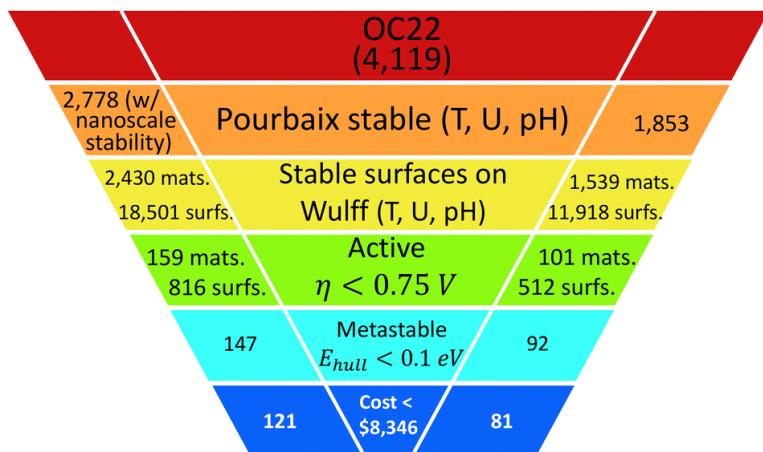
▼ Bimetallic using OC20 pretrained model

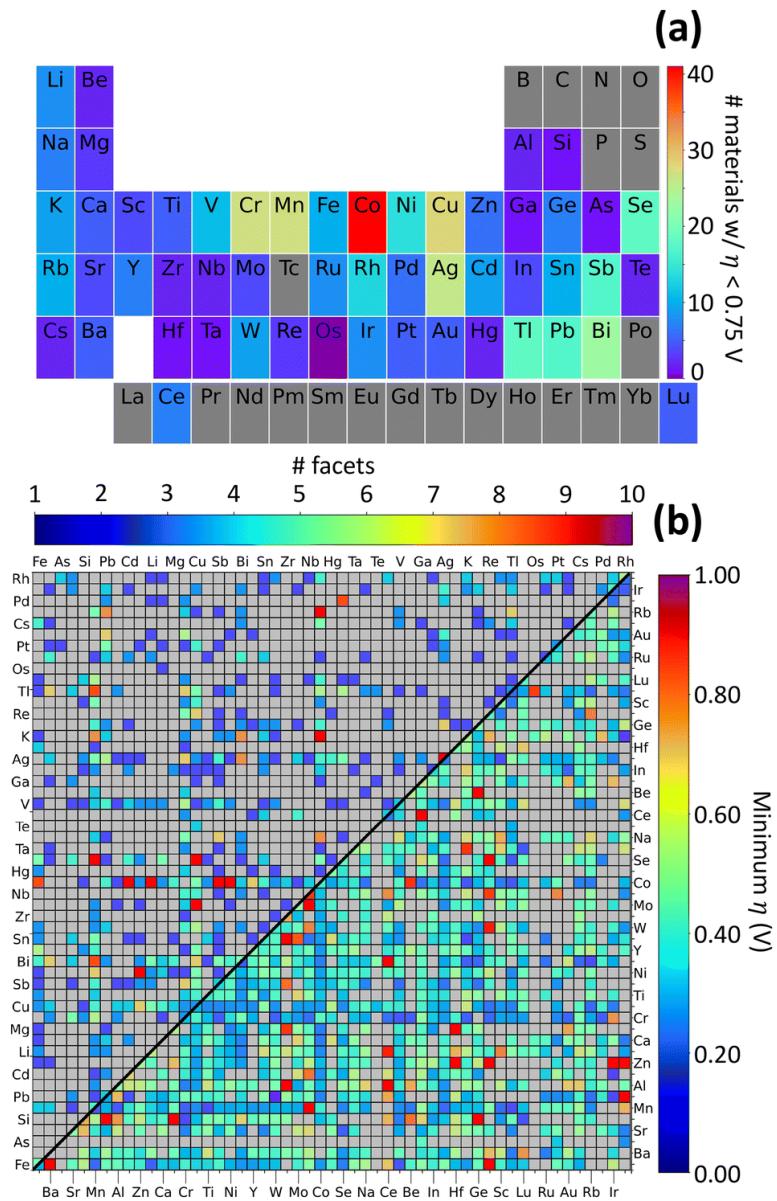




B. Wander et al. Catal. Sci. Technol., 2022, 12, 6256-6267

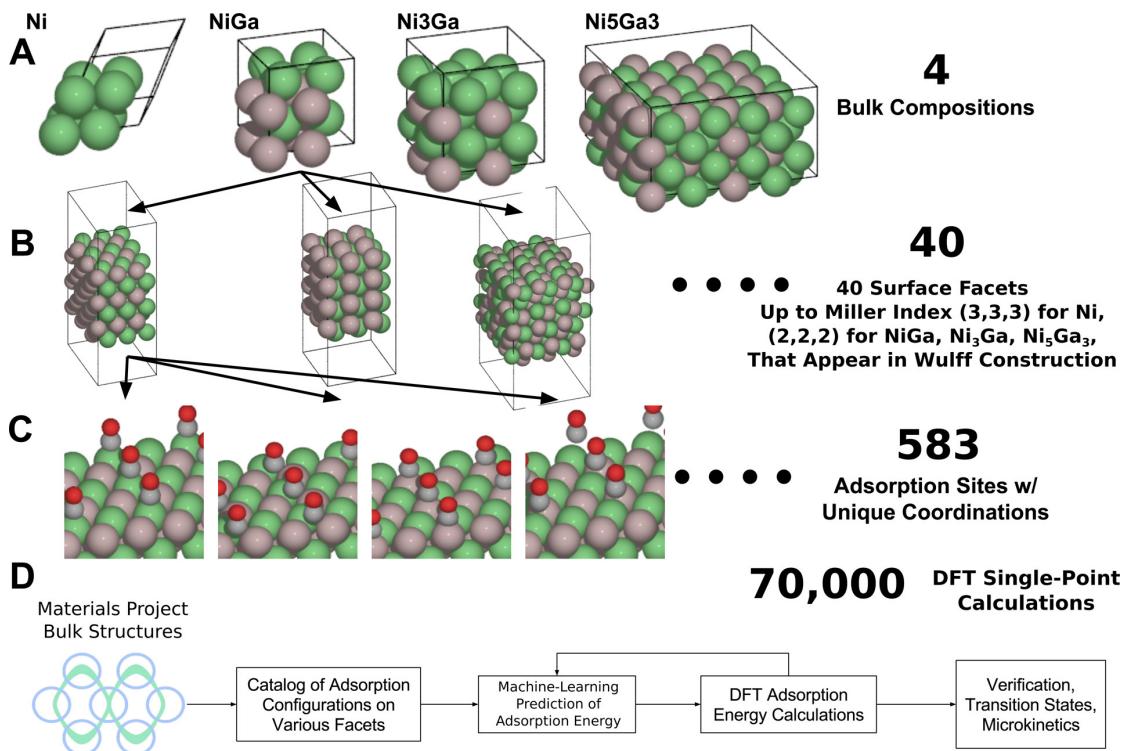
## ▼ OER catalyst using OC22 pretrained model





R. Tran et al. *Nanoscale*, 2024, 16, 17090-17101

## ▼ High throughput screening is not trivial



Ulissi et al. *ACS Catal.* 2017, 7, 10, 6600-6608.

## ▼ Handson

### 0. pre-trained model choice

using Catalysis-hub dataset from this publication

Journal of Chemical Theory and Computation > Vol 20/Issue 16 > Article  
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CONDENSED MATTER, INTERFACES, AND MATERIALS | August 8, 2024

**Density Functional Tight-Binding Models for Band Structures of Transition-Metal Alloys and Surfaces across the *d*-Block**

Filippo Balzaretti, and Johannes Voss\*

[Open PDF](#) [Supporting Information \(1\)](#) [Find It @ SNU](#)

Cite Share Jump to Expand

"Density Functional Tight-Binding Models for Band Structures of Transition-Metal Alloys and Surfaces across the <i>d</i>-<i>f</i>-Block". [Balzaretti, Filippo; Voss, Johannes](#). *Journal of Chemical Theory and Computation*. (2024) #BalzarettiDensity2024.

TABLE GRAPHQL QUERY FETCH CSV ASE ATOMS DOI: 10.1021/ACS.JCTC.4C00345.

- (1/69)  $0.5\text{H}_2(\text{g}) + * \rightarrow \text{H}^*$ 
  - Composition: Ag16
  - Reaction Energy: 0.36 eV
  - DFT Code/Functional: VASP-5.4.4 /GGA-RPBE
  - Facet: 111
  - Sites: {"Hstar": "fcc"}

[STRUCTURES >](#)
- (2/69)  $\text{H}_2\text{O}(\text{g}) - \text{H}_2(\text{g}) + * \rightarrow \text{O}^*$ 
  - Composition: Ag16
  - Reaction Energy: 2.26 eV
  - DFT Code/Functional: VASP-5.4.4 /GGA-RPBE
  - Facet: 111
  - Sites: {"Ostar": "fcc"}

[STRUCTURES >](#)
- (3/69)  $0.5\text{N}_2(\text{g}) + * \rightarrow \text{N}^*$ 
  - Composition: Ag16
  - Reaction Energy: 3.23 eV
  - DFT Code/Functional: VASP-5.4.4 /GGA-RPBE
  - Facet: 111
  - Sites: {"Nstar": "fcc"}

[STRUCTURES >](#)

- CHGNet

Adsorbate_name	Normal rate (%)	MAE_total (eV)	MAE_normal (eV)	MAE_outlier (eV)	Num_total	Num_normal	Num_outlier
H	<b>91.30</b>	0.253	<b>0.264</b>	0.131	23	21	2
N	<b>95.65</b>	0.471	<b>0.492</b>	0.001	23	22	1
O	<b>100.00</b>	0.996	<b>0.996</b>	0.000	23	23	0

- MACE

Adsorbate_name	Normal rate (%)	MAE_total (eV)	MAE_normal (eV)	MAE_outlier (eV)	Num_total	Num_normal	Num_outlier
H	<b>100.00</b>	0.157	<b>0.157</b>	0.000	23	23	0
N	<b>100.00</b>	0.434	<b>0.434</b>	0.000	23	23	0
O	<b>86.96</b>	2.039	<b>2.013</b>	2.217	23	20	3

<https://www.catalysis-hub.org/publications/BalzarettiDensity2024>

## 1. Bulk structure from Materials Project

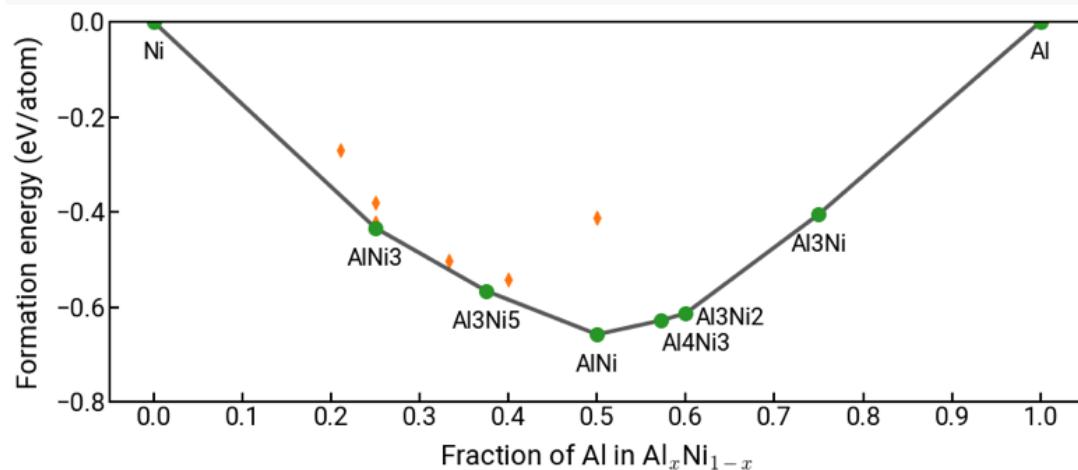
API Key Please fill in API

```
API_KEY = "#####" # Provide your API Key here
```

<https://next-gen.materialsproject.org/api>

We are going to get 'Cubic' bimetallic alloy with energy over hull <0.2 eV

Energy over hull



[https://enze-chen.github.io/mi-book-2021/week\\_1/02/materials\\_project\\_blank.html](https://enze-chen.github.io/mi-book-2021/week_1/02/materials_project_blank.html)

## 2. Slab generation and adsorption site search

## 3. Hydrogen evolution reaction volcano plot

- Assignment

Please refer to the following code:

[https://github.com/s-choung/Simulation\\_tutorials/blob/main/handson11.ipynb](https://github.com/s-choung/Simulation_tutorials/blob/main/handson11.ipynb)

Rerun the part

`random_combinations = random.sample(metal_combinations, 100)` and attach a picture of the best catalyst and its corresponding adsorption configuration in your case.