

# Exploring the Frontier of Universal Machine Learning Potentials

Part 2: Insights from OMol25 and UMA

Brandon Wood

Research Scientist, FAIR at Meta





## Recent Members



Muhammed  
Shuaibi



Anuroop  
Sriram



Daniel  
Levine



Ray  
Gao



Vahe  
Gharakhanyan



Misko  
Dzamba



Ben  
Miller



Xiang  
Fu



Jehad  
Abed



Lowik  
Chanussot



Kyle  
Michel



Jagriti  
Sahoo



Brandon  
Wood



Ammar  
Rizvi



Luis  
Barroso  
-Luque



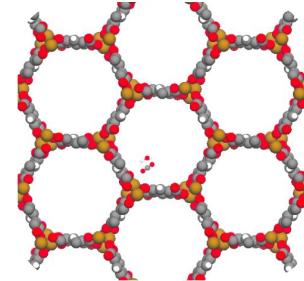
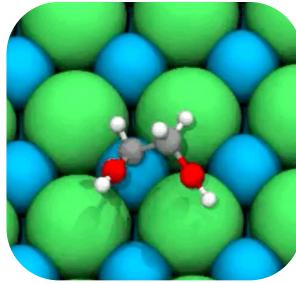
Zack  
Ulissi



Larry  
Zitnick

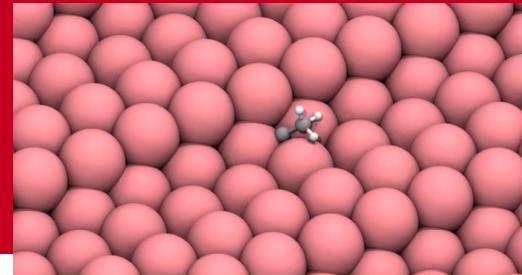
Why does Meta care about chemistry?

Using AI to design and discover materials and **molecules** for applications from climate change to AR glasses

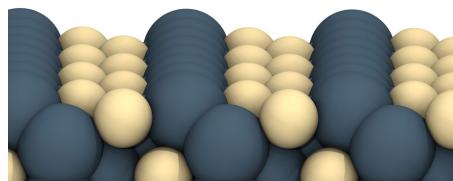


## Open Catalyst Project

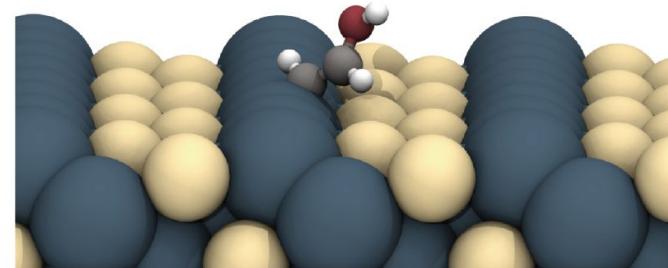
Using AI to model and discover new catalysts to address the energy challenges posed by climate change.



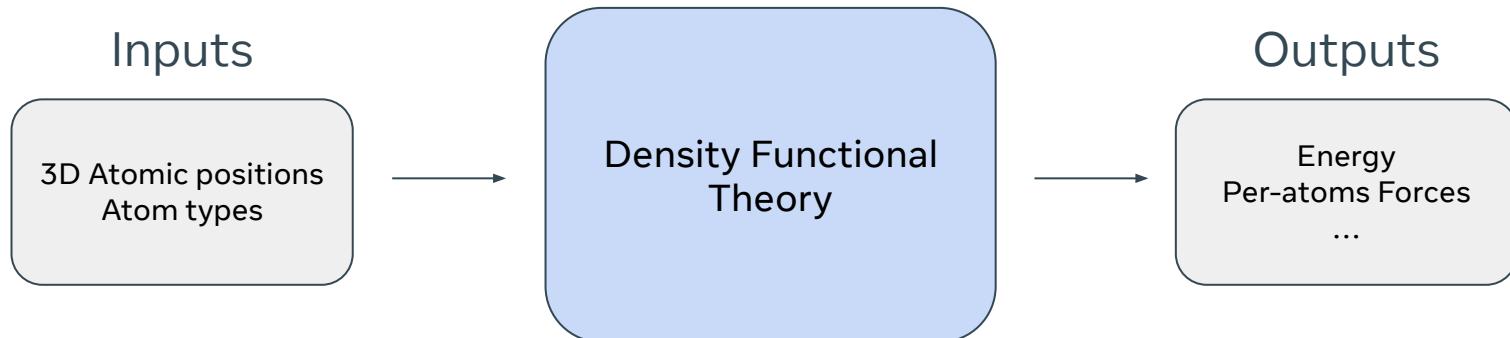
## Adsorbate



## Catalyst Surface



# Augment DFT with ML Potential

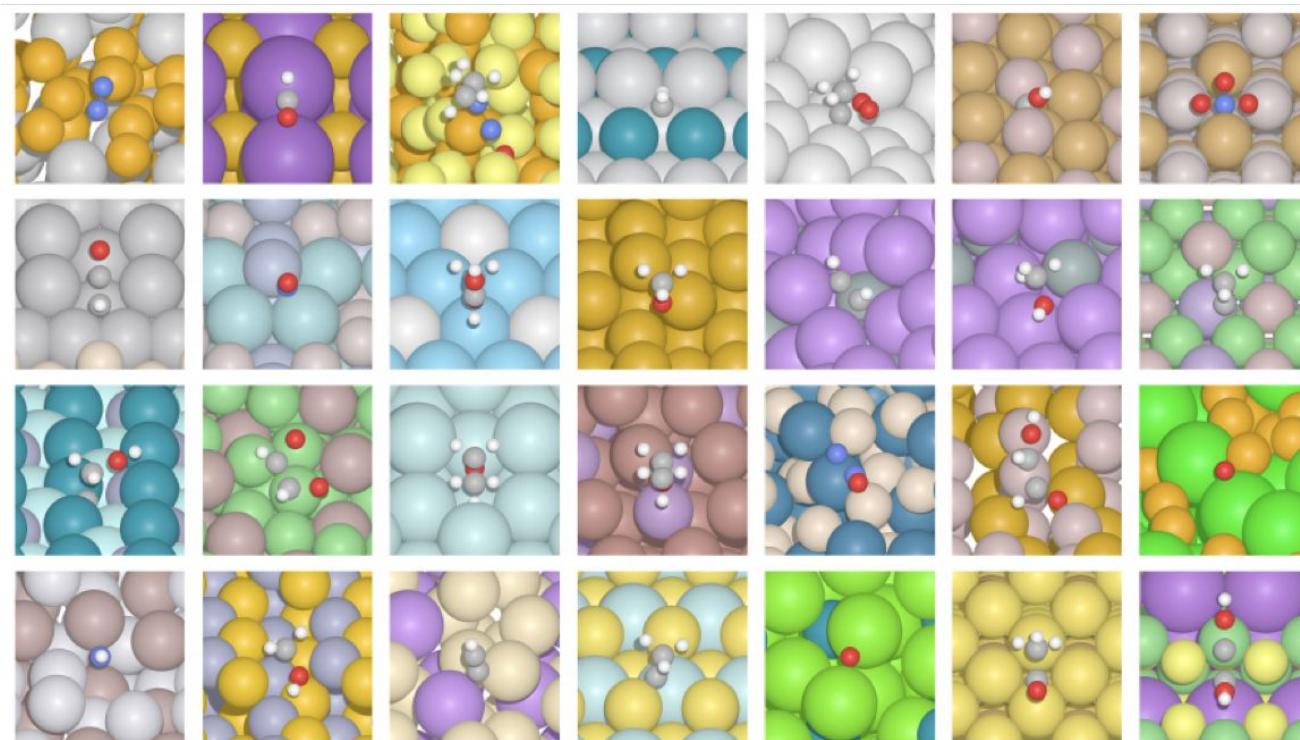


# Augment DFT with ML Potential

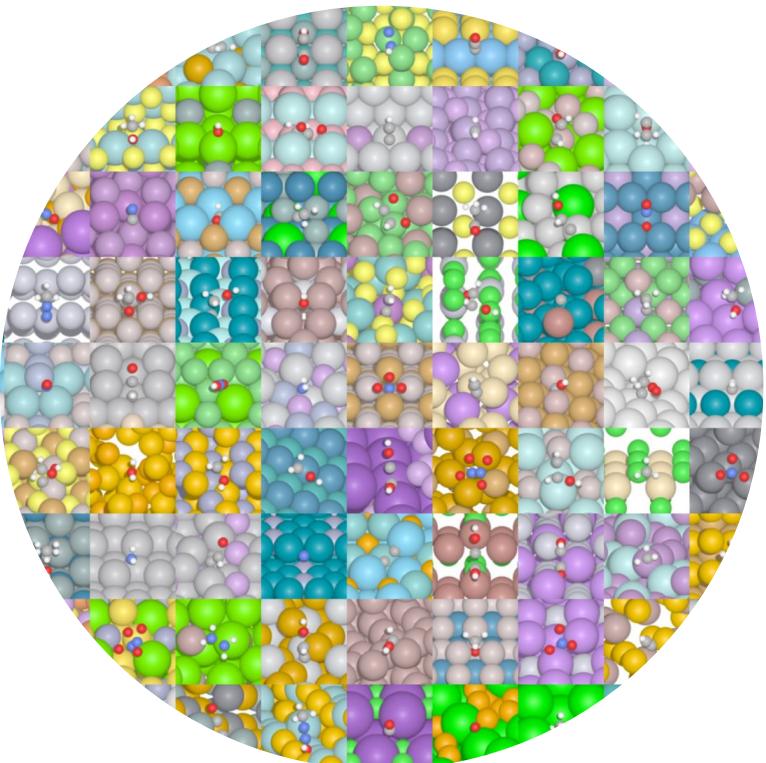


10,000x faster than DFT

# Adsorption energies across a huge design space!

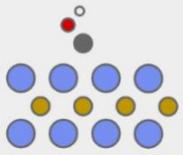


# Open Catalysts 2020 Dataset



- Largest and most diverse catalysis dataset
- 1.3M DFT relaxations ~ 130M training examples
- 200M CPU-hours to compute on 50k servers
- Tasks, baseline models, and community challenge

Catalysis 230M



2020

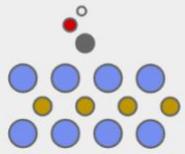
2023

2024

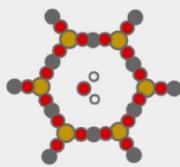
2025

Open Catalyst

Catalysis 230M



ODAC 29M



2020

2023

2024

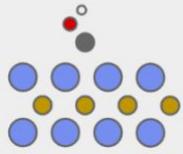
2025



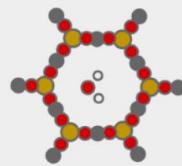
Open Catalyst

Open Direct Air Capture

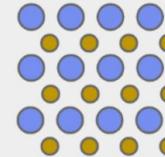
Catalysis 230M



ODAC 29M



Materials 100M



2020

2023

2024

2025

Open Catalyst

Open Direct Air Capture

Open Materials





Luis  
Barroso  
-Luque

# Open Materials 2024 (OMat24)

Open source  
models + data @ 😊

100M+  
non-equilibrium  
structures

Applications:

Renewable energy storage  
& CO<sub>2</sub> reduction



Optics & Electronics

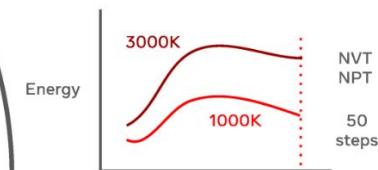


... and much more!

$$p \sim \exp(-e/kT)$$

Boltzmann  
sampling

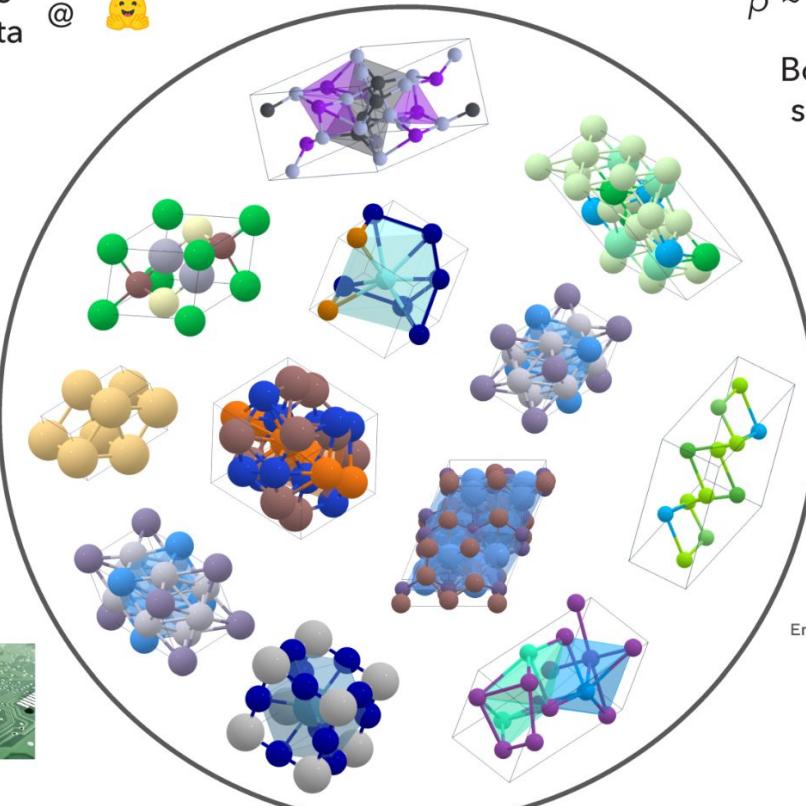
300K  
500K  
1000K

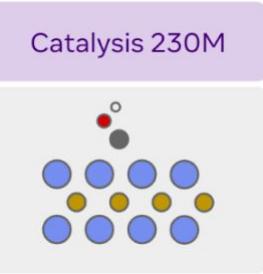


AIMD



Rattled  
relaxation

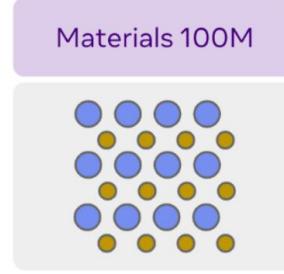




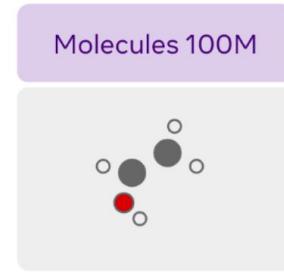
2020



2023



2024



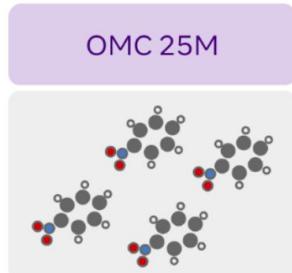
2025

Open Catalyst

Open Direct Air Capture

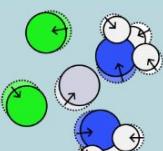
Open Materials

Open Molecules  
Open Molecular Crystals





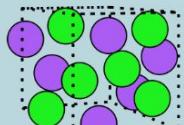
reaction pathways



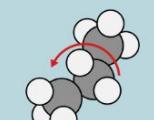
rattling



optimization



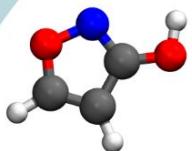
dynamics



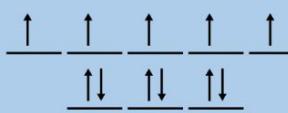
conformers

## Sampling Strategies

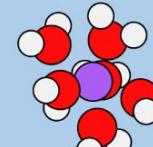
small molecules



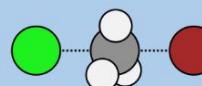
electrolytes



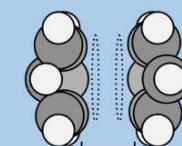
Charge + spin



Solvation



Reactivity



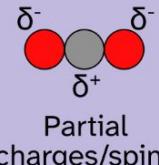
Short-/long-range interactions

## Chemical Complexity

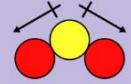
## Properties



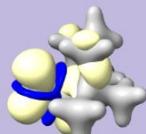
Energetics



Partial charges/spins



Multipoles



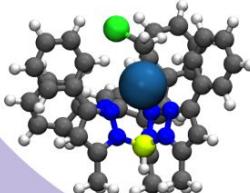
Electron densities



Natural orbitals

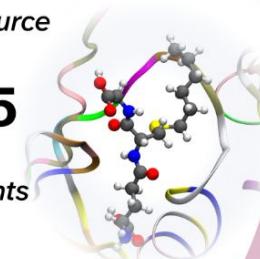
*...and more!*

metal complexes



up to 350 atoms

83 elements

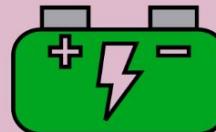


biomolecules

## Applications



Medicine



Batteries



Manufacturing



Climate

# Open Molecules 2025: A collaborative effort



Daniel  
Levine  
(Meta)



Muhammed  
Shuaibi  
(Meta)



Evan  
Spotte-Smith  
(CMU)



Michael  
Taylor  
(LANL)



Muhammad  
Hasyim  
(NYU)



Kyle  
Michel  
(Meta)



Ilyes  
Batatia  
(Cambridge)



Gabor  
Csanyi  
(Cambridge)



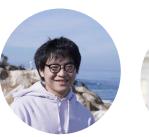
Misko  
Dzamba  
(Meta)



Peter  
Eastman  
(Stanford)



Nathan Frey  
(Prescient /  
Genentech)



Xiang  
Fu  
(Meta)



Vahe  
Gharakhanyan  
(Meta)



Aditi  
Krishnapriyan  
(Berkeley)



Joshua  
Rackers  
(Prescient /  
Genentech)



Sanjeev  
Raja  
(Berkeley)



Ammar  
Rizvi  
(Meta)



Andrew  
Rosen  
(Princeton)



Zack  
Ulissi  
(Meta)



Santiago  
Vargas  
(LBNL)



Larry  
Zitnick  
(Meta)



Sam  
Blau  
(LBNL)



Brandon  
Wood  
(Meta)

# Open source!

Hugging Face

Models Datasets Spaces Community Docs Enterprise Pricing

facebook OMol125 AI like 128 Following AI at Meta 6.59k OMol25

arxiv:2505.08762 License: other

[Model card](#) [Files and versions](#) [Settings](#) [Edit model card](#)

**Gated model** You have been granted access to this model

## The Open Molecules 2025 (OMol25) Dataset, Evaluations, and Models

Sampling Strategies: reaction pathways, rattling, conformers, dynamics.

Chemical Complexity: small molecules, electrolytes, solvation, short-long-range interactions, charge + spin.

Properties: energetics (E, F), partial charges/spins, multipoles, electron densities, natural orbitals, metal complexes, biomolecules.

Applications: medicine, batteries, manufacturing, climate.

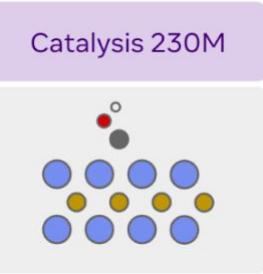
Downloads last month: Downloads are not tracked for this model. [How to track](#)

Inference Providers: This model isn't deployed by any Inference Provider. [Ask for provider support](#)

Collection including facebook/OMol25: FAIR Chemistry Collection. 4 items · Updated May 13 · △ 6

**Dataset**

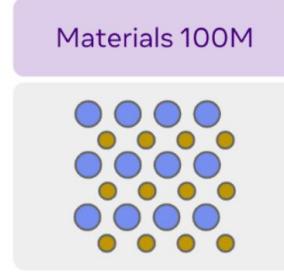
LICENSE: The OMol25 dataset is provided under a CC-BY-4.0 license



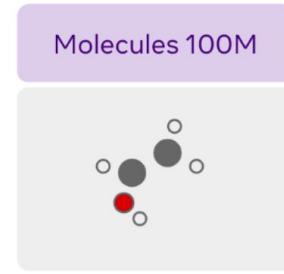
2020



2023



2024



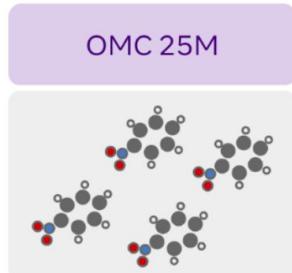
2025

Open Catalyst

Open Direct Air Capture

Open Materials

Open Molecules  
Open Molecular Crystals



# Playbook

- 1) Generate new dataset

# Playbook

- 1) Generate new dataset
- 2) Train models on said dataset

# Playbook

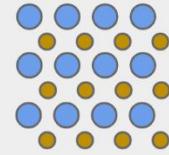
- 1) Generate new dataset
- 2) Train models on said dataset
- 3) If interested in new chemistry that is sufficiently OOD repeat steps 1 and 2

Can we use all the data to train a single  
model that benefits all applications?

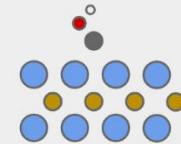
Molecules 100M



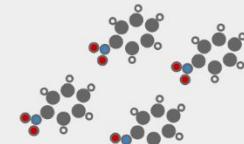
Materials 100M



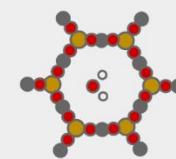
Catalysis 230M



OMC 25M

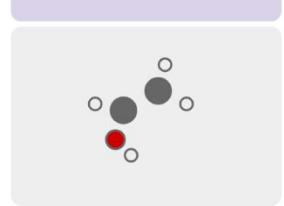


ODAC 29M

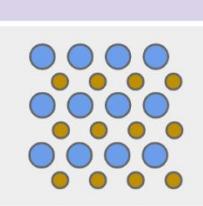


Elements 1-94

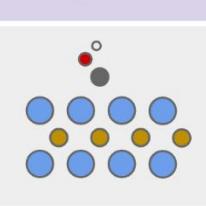
Molecules 100M



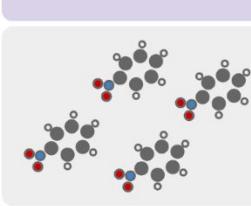
Materials 100M



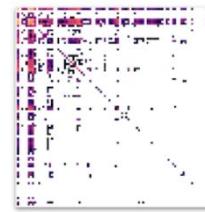
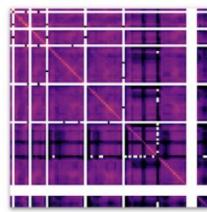
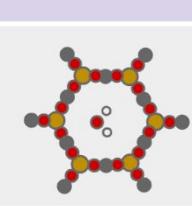
Catalysis 230M



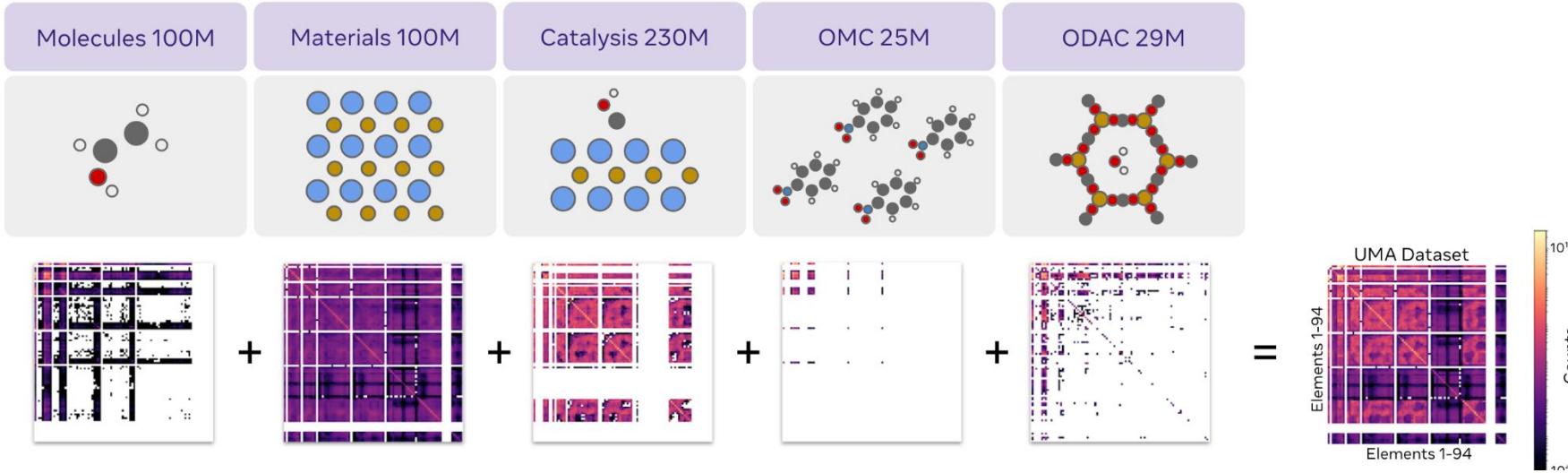
OMC 25M

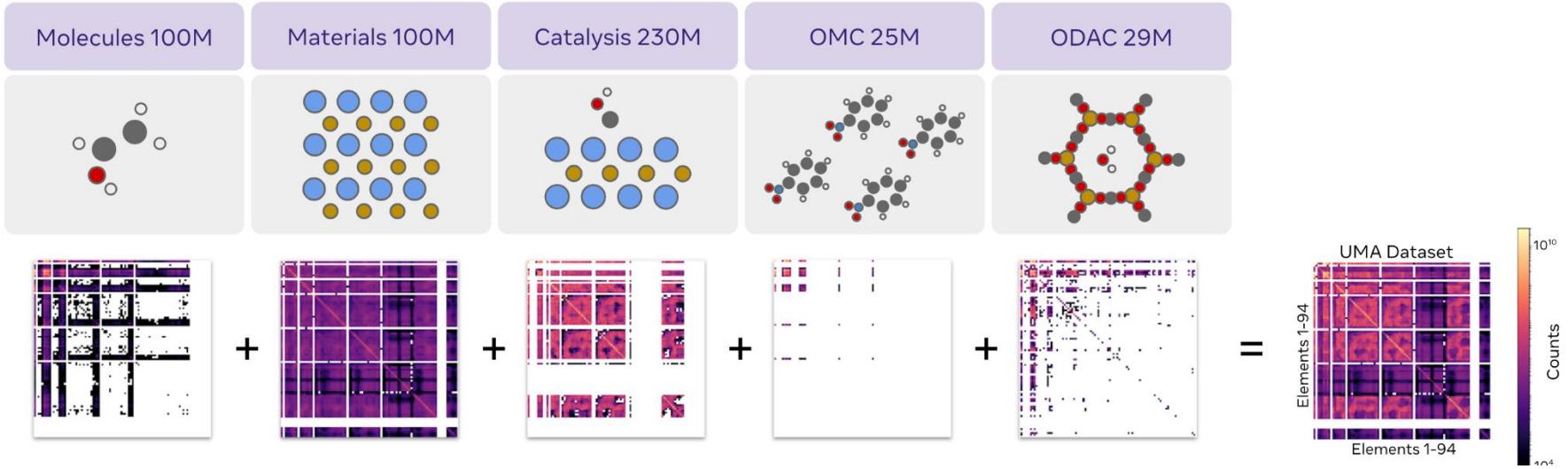


ODAC 29M

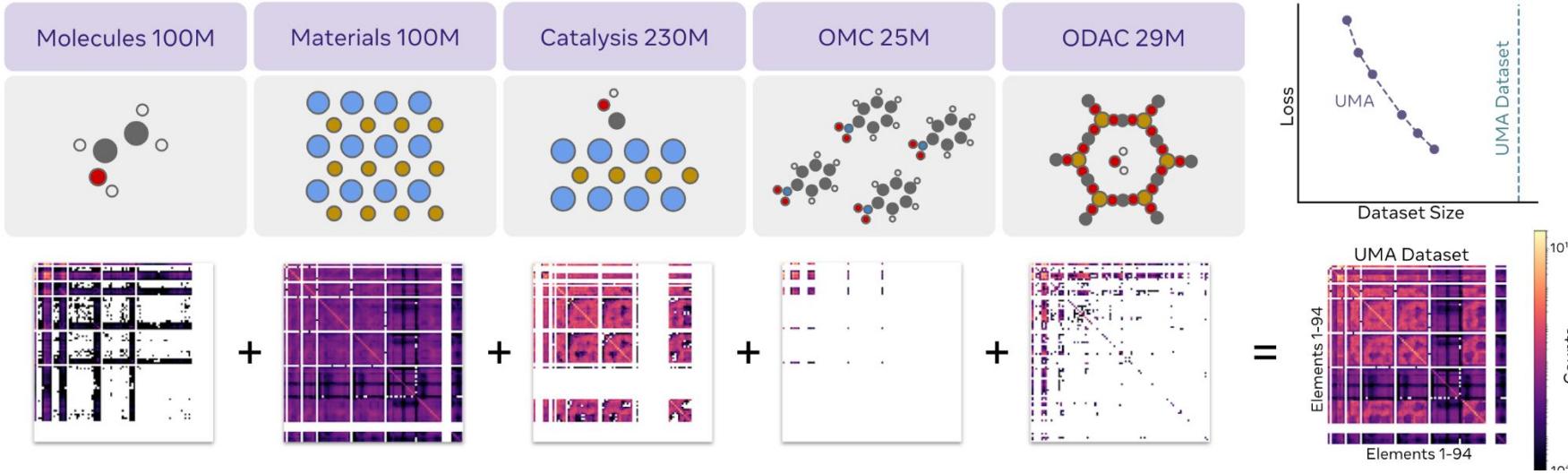


Elements 1-94





30 Billion atoms!



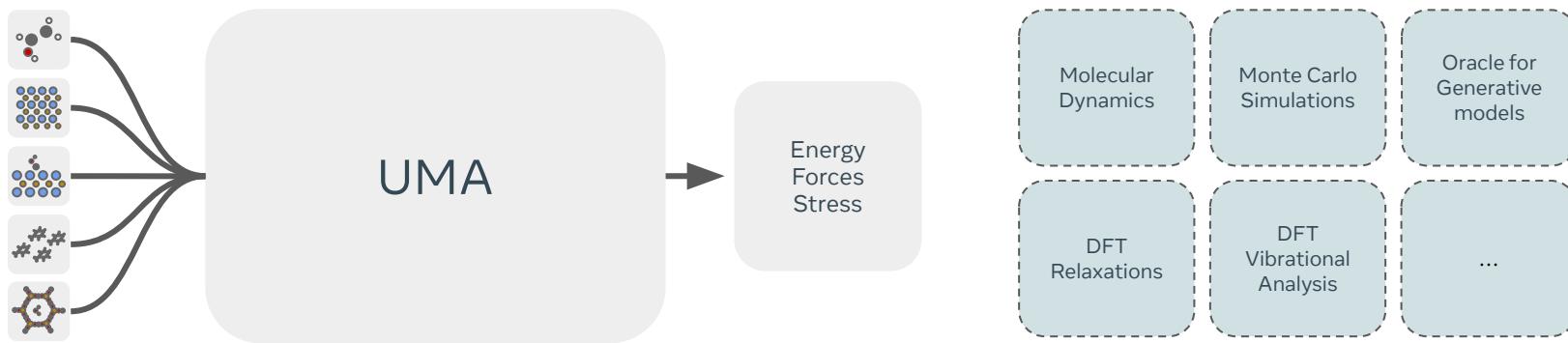
# Universal Model for Atoms (UMA)



Energy  
Forces  
Stress

“A single model that works out-of-the-box for molecules, materials, and more without specialized fine-tuning”

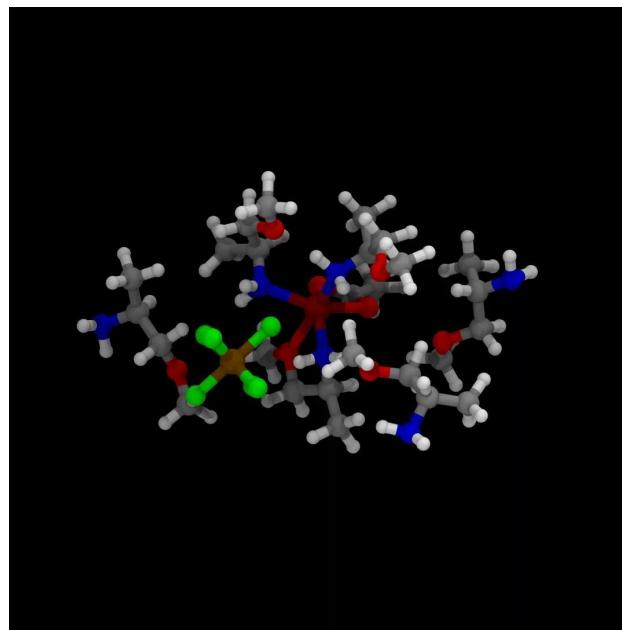
# Universal Model for Atoms (UMA)



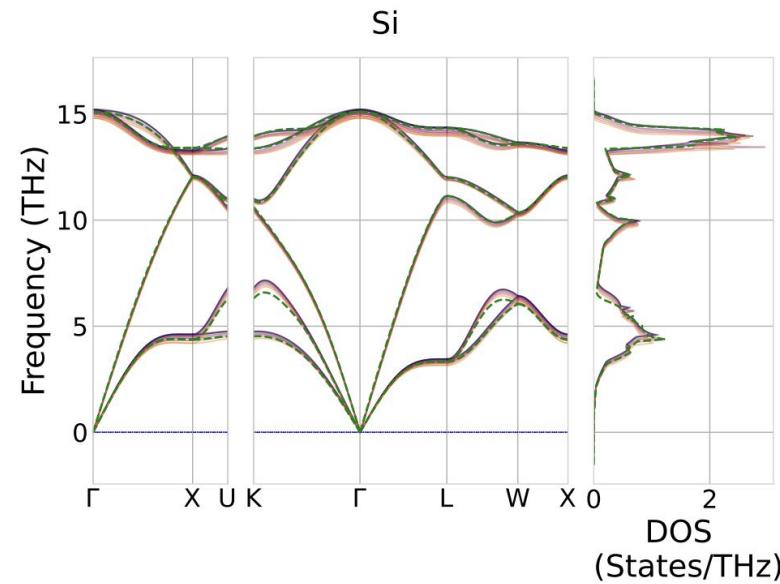
# Designing a model for physical property prediction: eSEN (ICML 2025)



Molecular dynamics

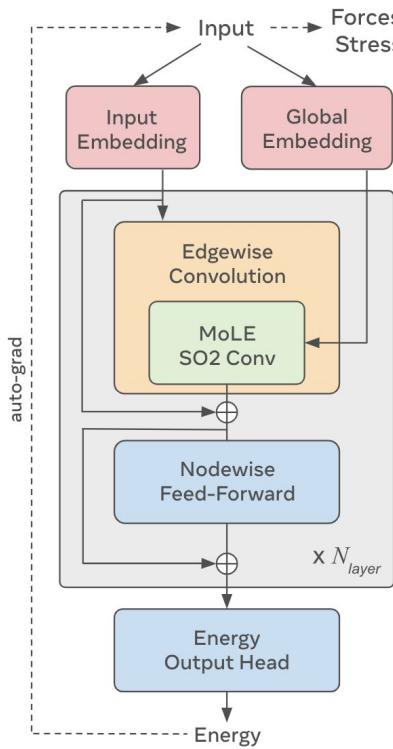


Vibrational analysis

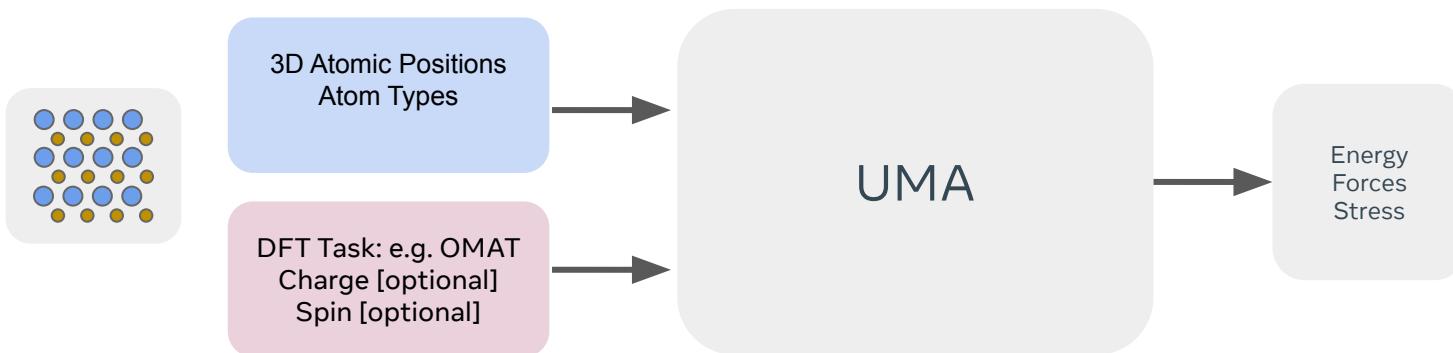


and more!

# UMA Architecture based on eSEN

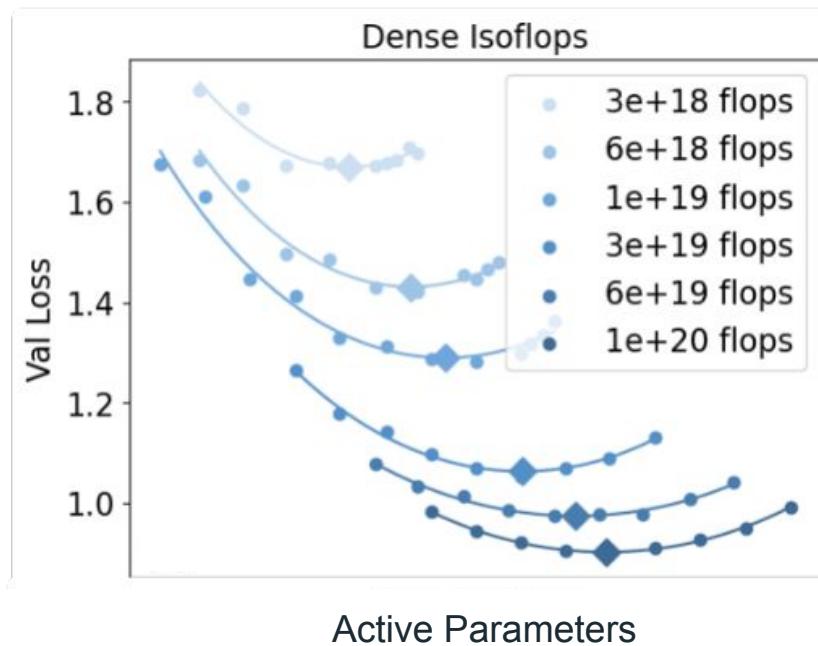


# UMA Inputs/Outputs

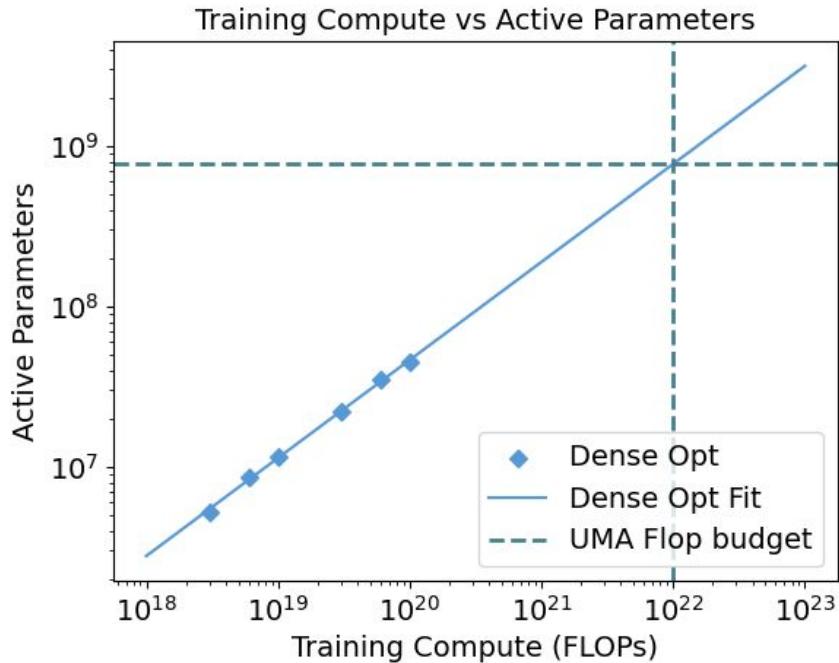


How large of model is needed to fit the data?

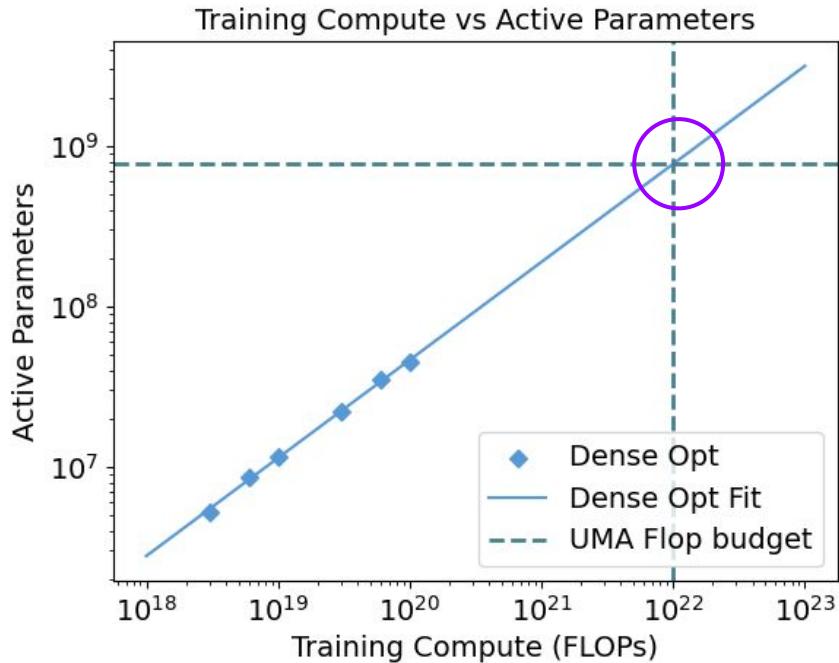
# Scaling laws



# We need large parameter models to fit the data



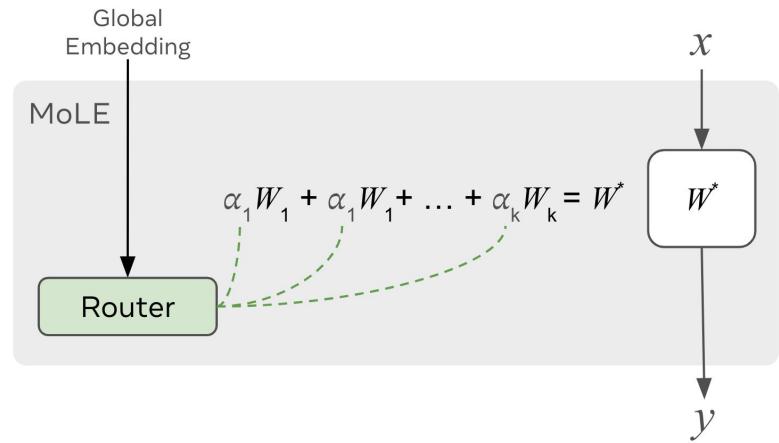
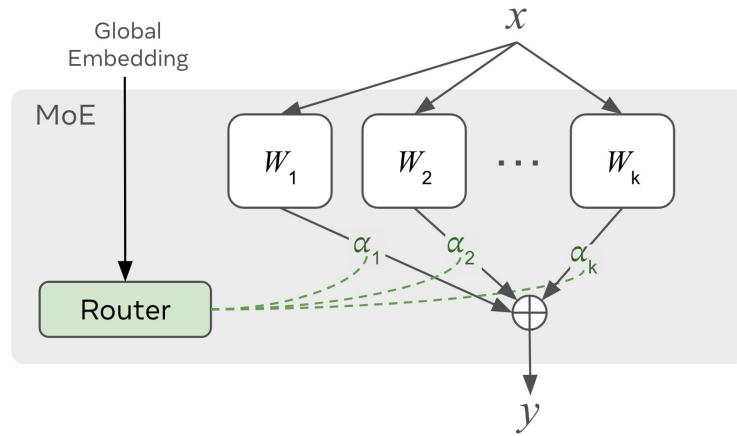
# We need large parameter models to fit the data



Extrapolated compute optimal model requires ~700M params

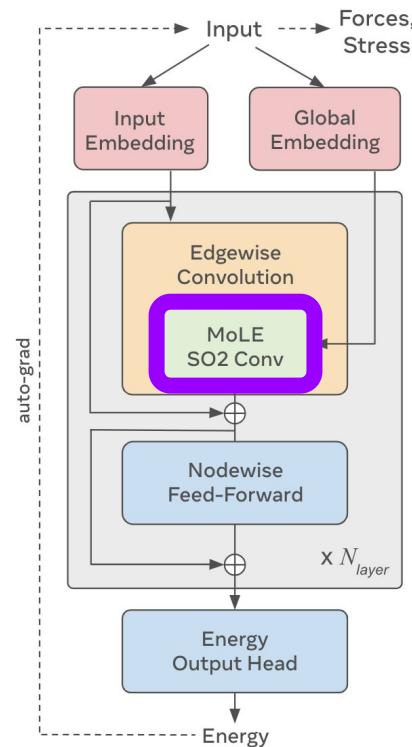
But aren't large models slow?

# Mixture of Linear Experts (MoLE)

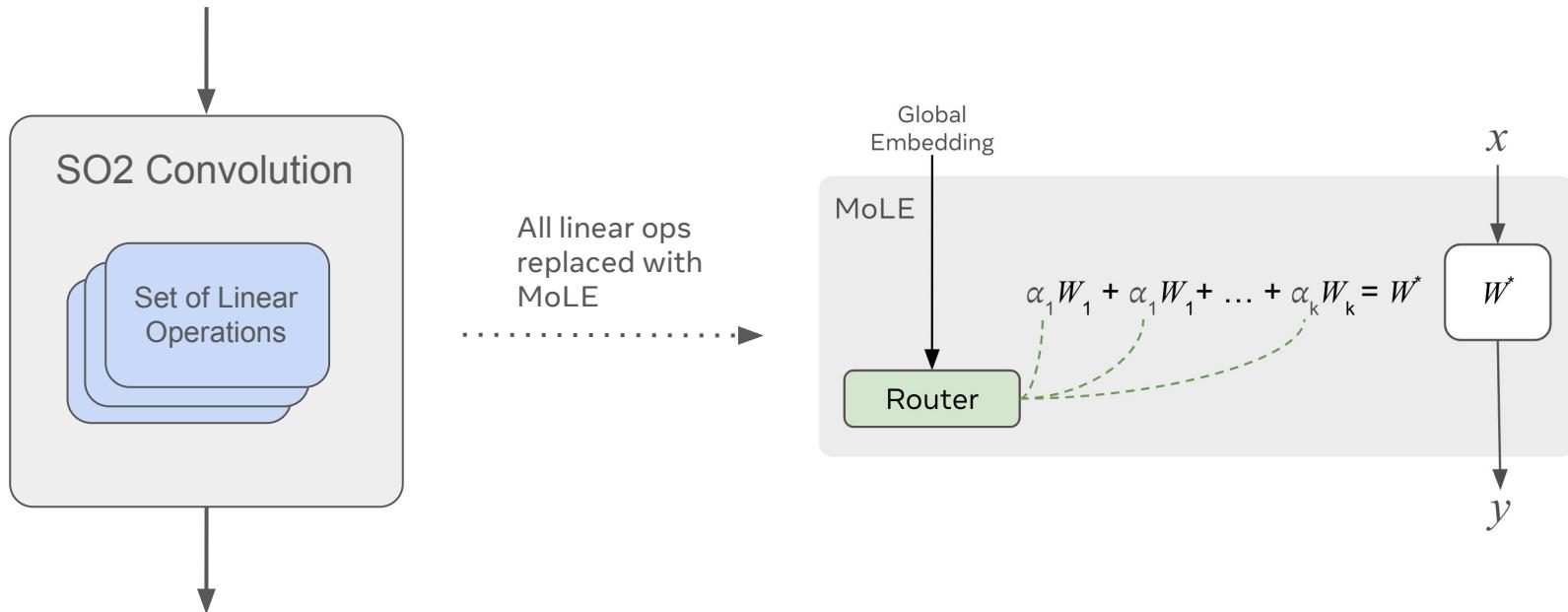


Increase capacity without sacrificing speed

# Mixture of Linear Experts (MoLE)



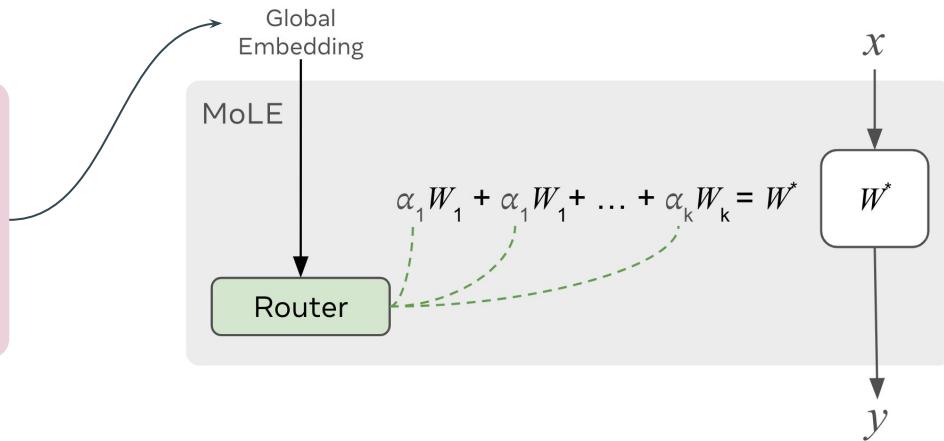
# Mixture of Linear Experts (MoLE)



# Mixture of Linear Experts (MoLE)

Global embedding:

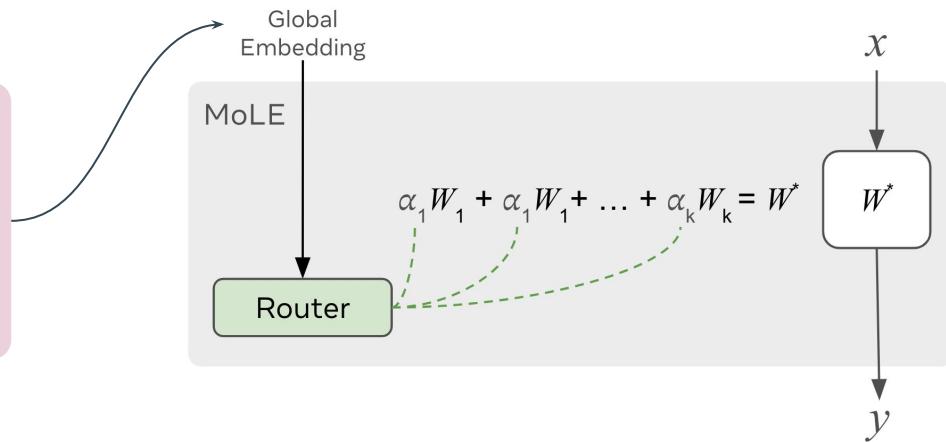
- Atomic composition
- DFT task
- Charge
- Spin



# Mixture of Linear Experts (MoLE)

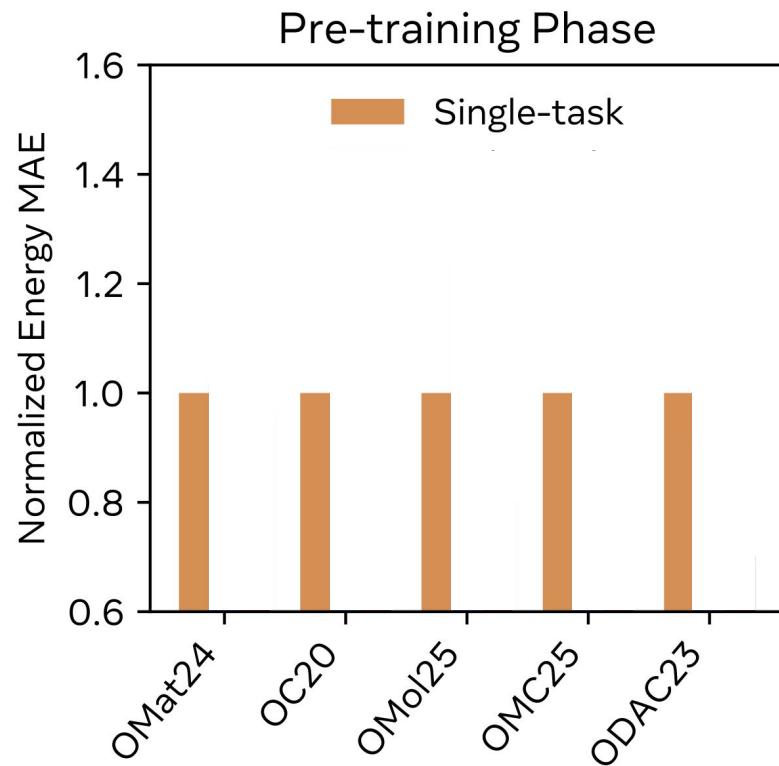
Global embedding:

- Atomic composition
- DFT task
- Charge
- Spin

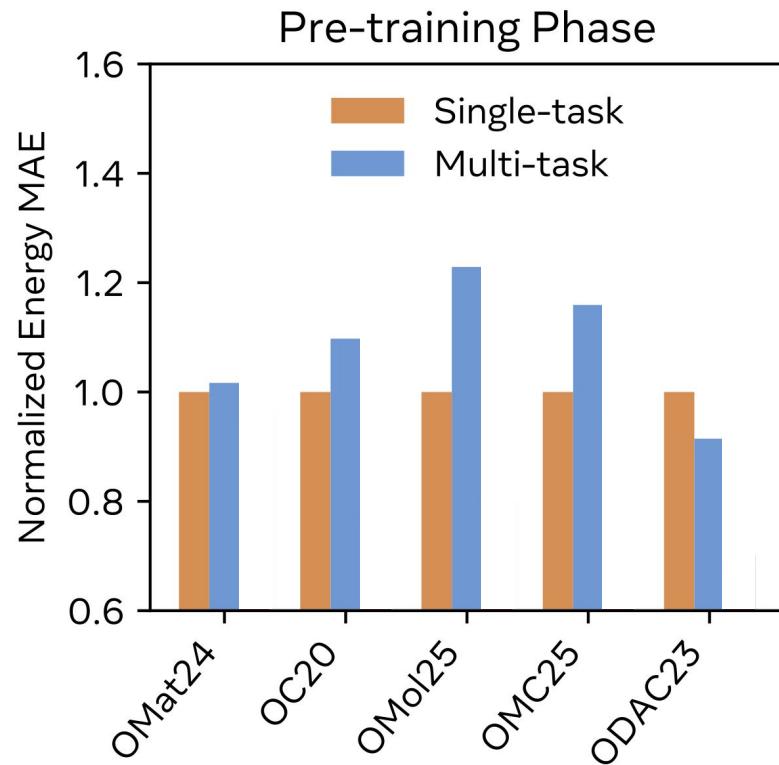


Pre-merging experts weights is possible for single systems where global embedding is constant!

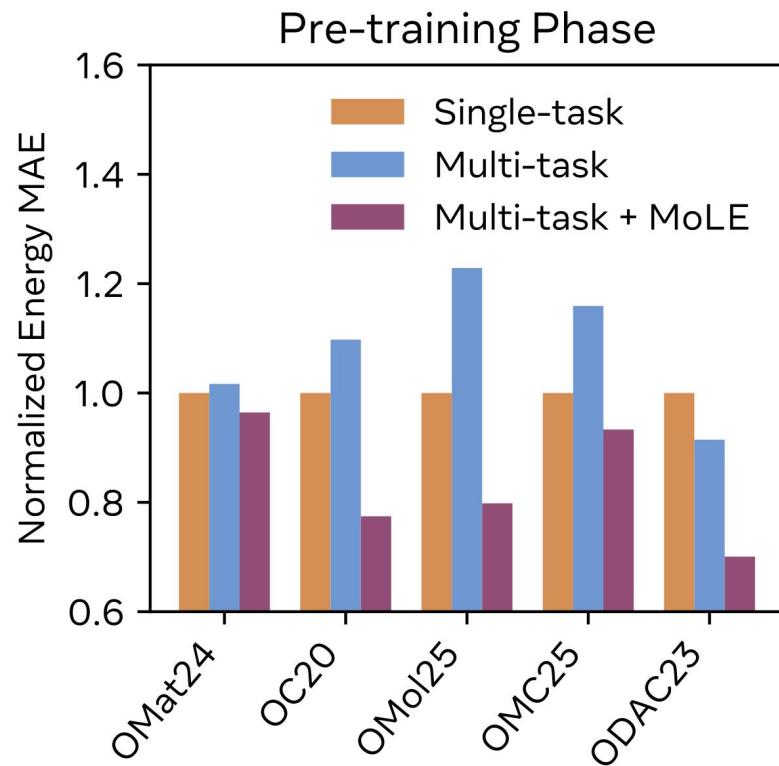
# MoLE in small parameter regime



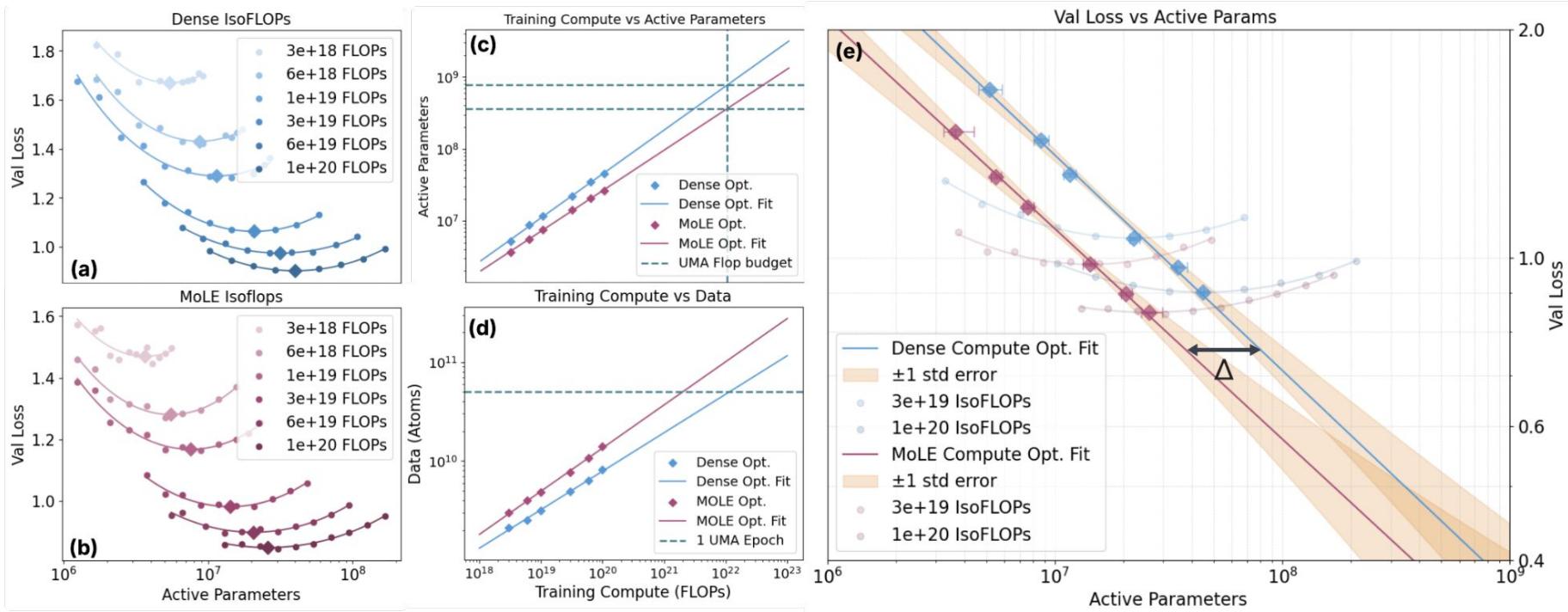
# MoLE in small parameter regime



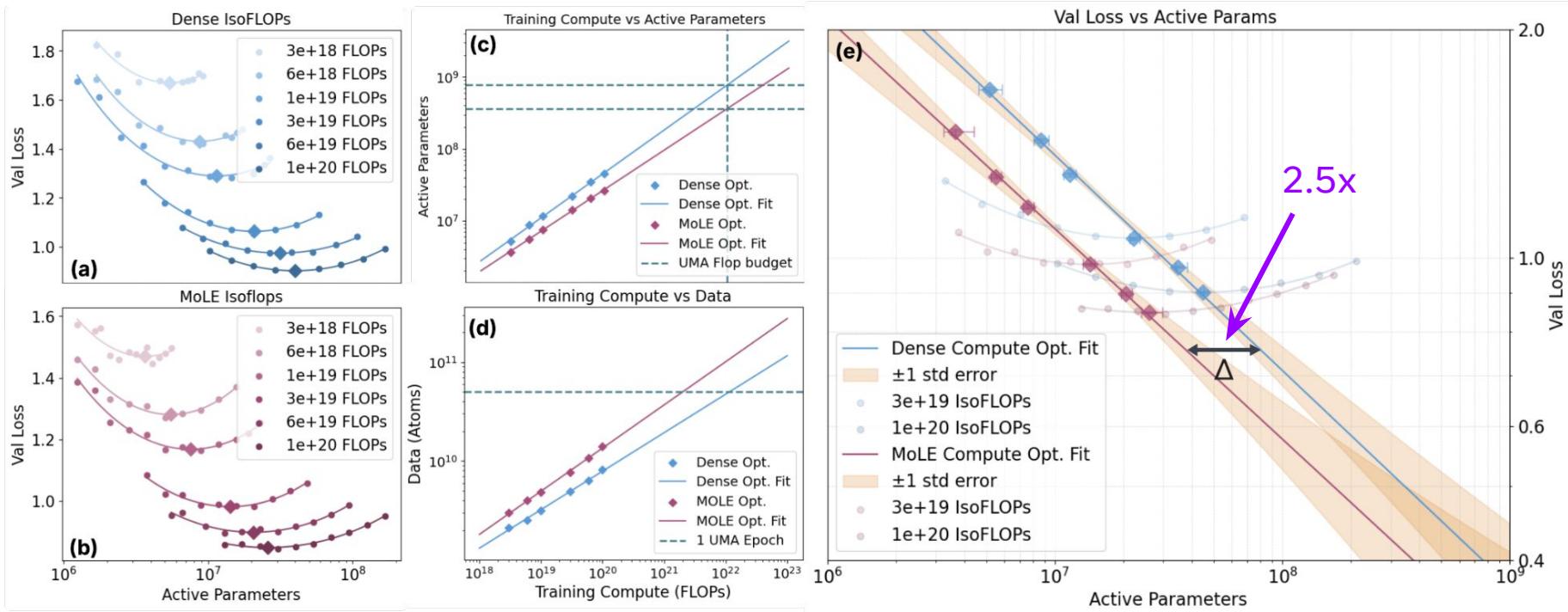
# MoLE in small parameter regime



# Scaling laws



# Scaling laws



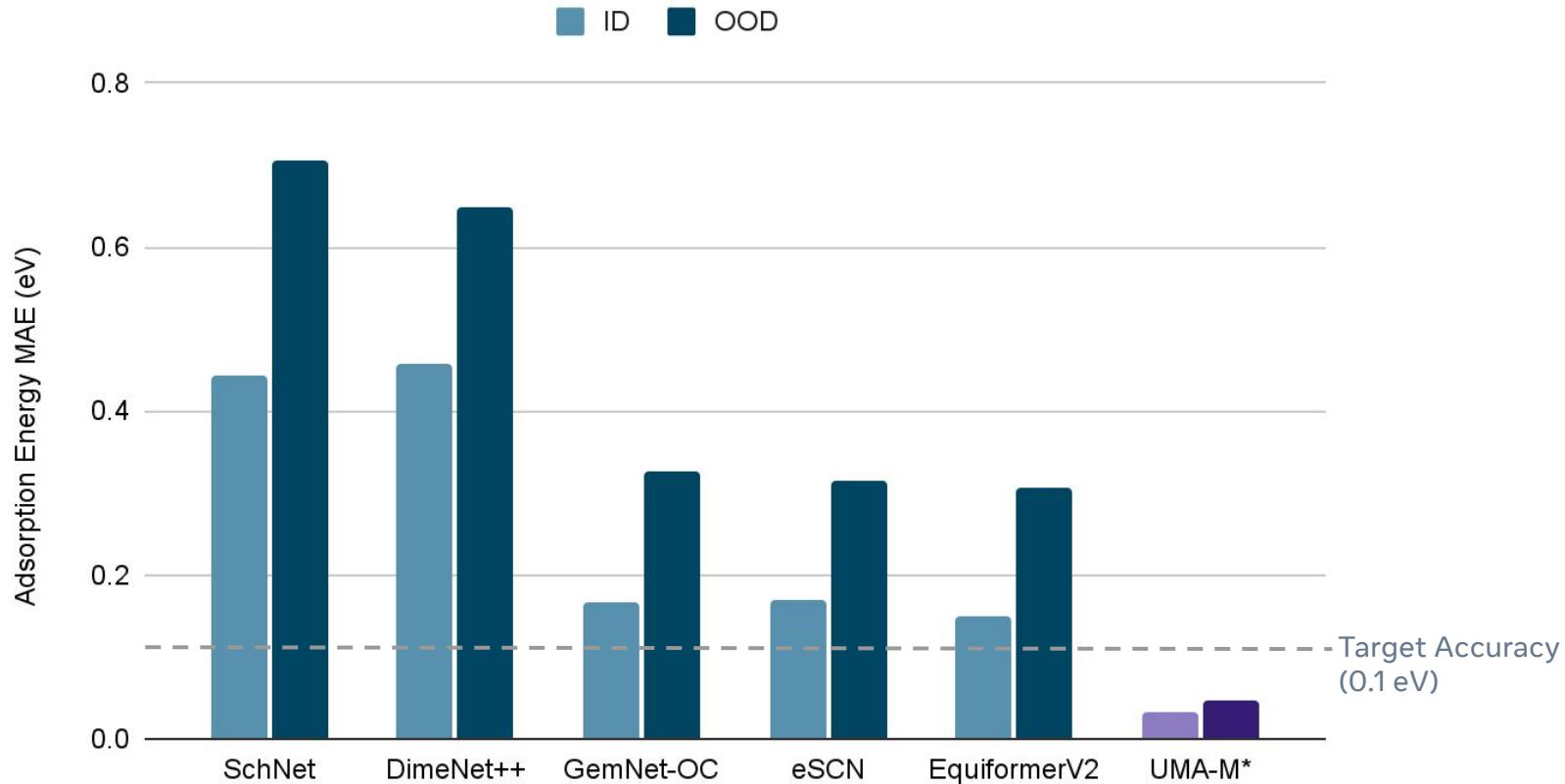
# UMA family of models

Model	Total Parameters	Active Parameters	Inferences per second for 1k Atoms	Max Atoms per 80GB GPU	Conservative
UMA-S	150M	6M	16	100k+	✓
UMA-M	1.4B	50M	3	10k+	✓
UMA-L	700M	700M	1.6	1k+	✗

Inference speed and max atoms measured on Nvidia H100 with a periodic system that has  $\approx 50$  neighbors per atom within 6Å, see Appendix D

So how does a single model perform?

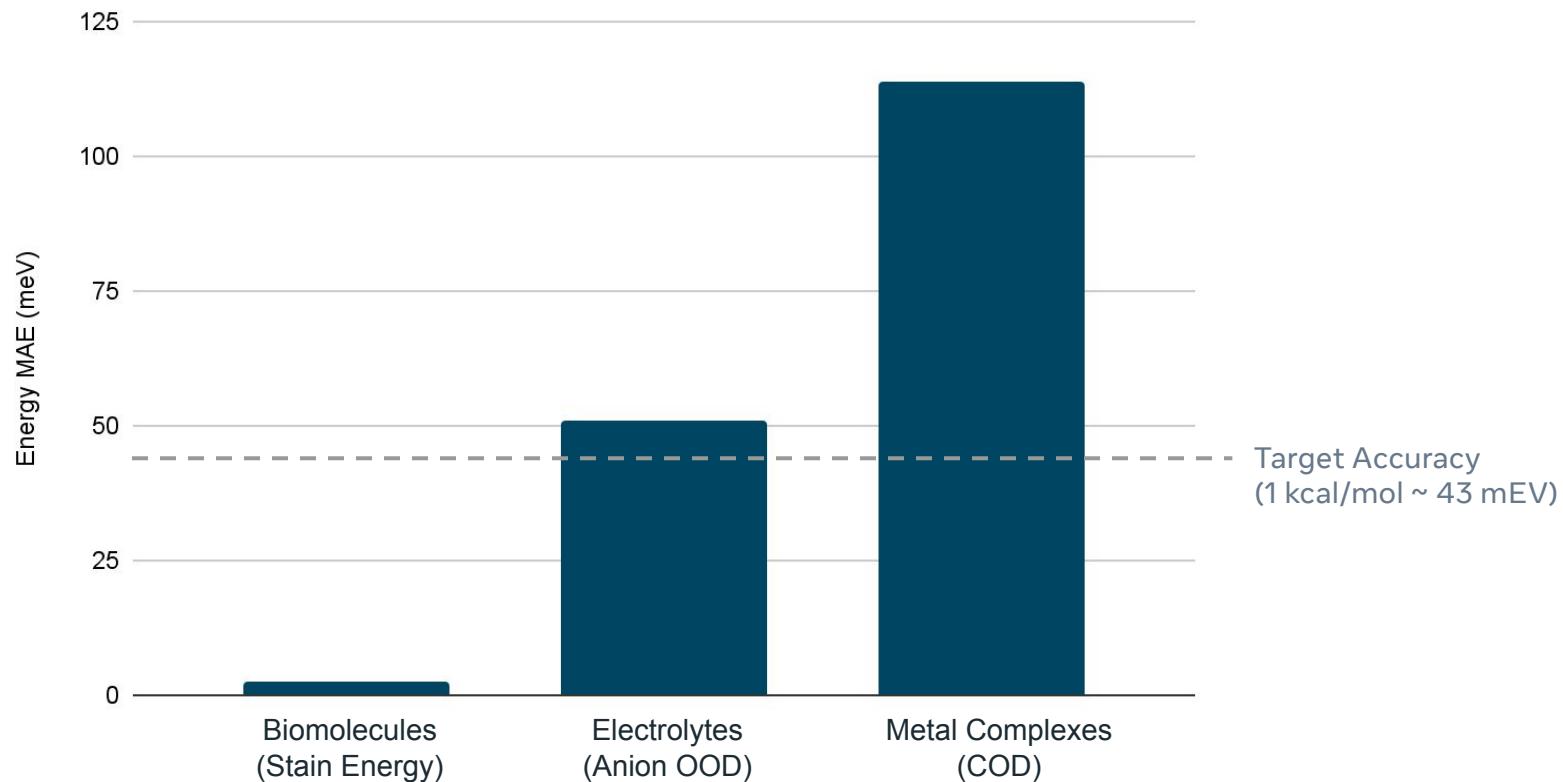
# Catalysis: OC20 S2EF



# Materials: Matbench Discovery

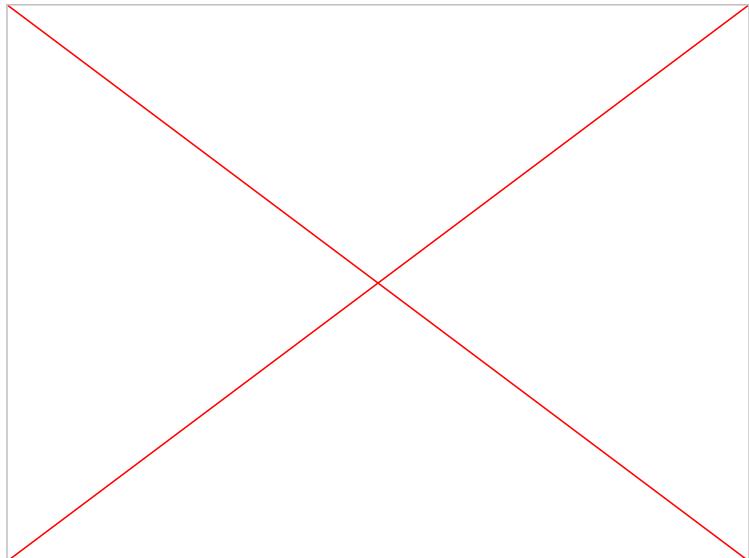
	F1	RMSD	K <sub>SRME</sub>
UMA-M	0.930	0.061	0.195
eSEN-30M-OAM	0.925	0.061	0.170
ORB v3	0.905	0.075	0.210
SevenNet-MF-ompa	0.901	0.064	0.317
MACE-MPA-0	0.852	0.073	0.412
MatterSim v1 5M	0.862	0.073	0.574

# Molecules: OMol25 benchmarks



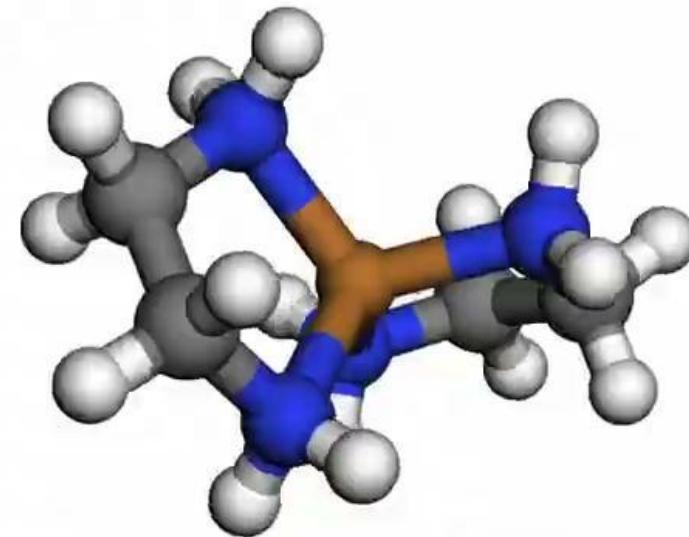
# Fun results!

Cu1+



Tetrahedral

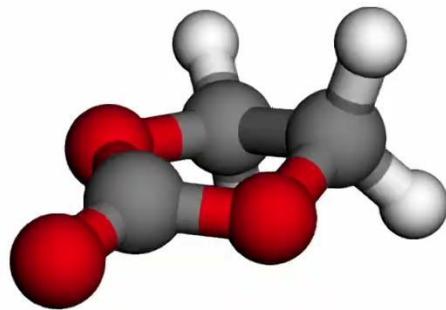
Cu2+



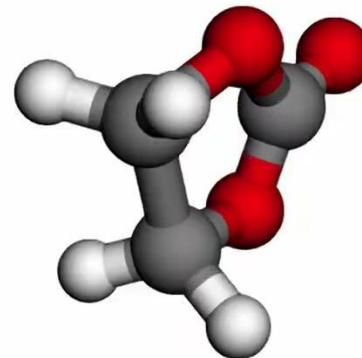
Square planar

# Fun results!

Neutral ethylene carbonate



Radical anion EC



---

Stable

---

Ring bond breaks

# Takeaways

- **Data is key** and with more data we can build more capable models. A wide data distribution encourages generalization and prevents overfitting

# Takeaways

- **Data is key** and with more data we can build more capable models. A wide data distribution encourages generalization and prevents overfitting
  - We are still data bound

# Takeaways

- **Data is key** and with more data we can build more capable models. A wide data distribution encourages generalization and prevents overfitting
- It is possible to train a single model that achieves strong performance across different domains and benchmarks without specialized fine-tuning

# Limitations/weaknesses

- Long-range interactions i.e. using a 6A cutoff
- Charge/spin
- Outliers
- Benchmarks vs models in the wild
- Inference speed

# Try UMA for yourself!

Educational Demo — <https://facebook-fairchem-uma-demo.hf.space>

The screenshot displays the "Meta's Universal Model for Atoms (UMA) Demo" interface. On the left, a sidebar titled "Learn more about UMA" contains sections like "What is UMA?", "Should I trust UMA?", "Why does this matter?", "How fast are these simulations?", "Model Disclaimers", and "Open source packages in this demo". Below this is a "Debugging" section with "Simulation took >5min" and "Redirect error on login".

The central part of the interface features a diagram of the UMA architecture. It shows an "Input Task" (OMM, OMC, OMm, ODCG, OCG) leading to a "Task Embedding" block, which then feeds into a "Composition" block. This is followed by a "Router" block and an "Expert" block (labeled "Expert", "Expert", "..."). The "Expert" block leads to a "Merged Mixture of Linear Experts UMA Model", which outputs "Energy", "Forces", and "Stress". Below the diagram, a text block explains the UMA as a large mixture-of-linear-experts graph network model trained on billions of atoms across five open-science simulation datasets.

At the bottom left, there is a "Simulation inputs" section where users can upload an ASE-compatible structure (e.g., metal\_cpx.pdb). A validation errors section shows a "Validation Errors" button. A "Sign in with Hugging Face" button is also present.

On the right, the "UMA Simulation Results" section shows a "Visualization" tab with a 3D ball-and-stick model of a transition metal complex. The visualization includes a zoom and rotate tool. Below the visualization, a text box asks, "What should I look for in this simulation?". A "Log" tab shows a "Simulation Trajectory (ASE traj file)" named tmpwjjdc6jij.traj with a size of 563.6 KB.

# Try UMA for yourself!

Code with ASE calculator — <https://github.com/facebookresearch/fairchem>



tests passing pypi v2.1.0 python 3.10+

Open in GitHub Codespaces

fairchem is the FAIR Chemistry's centralized repository of all its data, models, demos, and application efforts for materials science and quantum chemistry.

FAIRChem version 2 is a breaking change from version 1 and is not compatible with our previous pretrained models and code. If you want to use an older model or code from version 1 you will need to install [version 1](#), as detailed [here](#).

Some of the docs and new features in FAIRChem version 2 are still being updated so you may see some changes over the next few weeks. Check back here for the latest instructions. Thank you for your patience!

# Questions?

## OMol25

Paper: <https://arxiv.org/abs/2505.08762>

Dataset: <https://huggingface.co/facebook/OMol25>

## UMA

Paper: <https://arxiv.org/abs/2506.23971>

Models: <https://huggingface.co/facebook/UMA>

Code: <https://github.com/facebookresearch/fairchem>

Contact: bmwood@meta.com

