



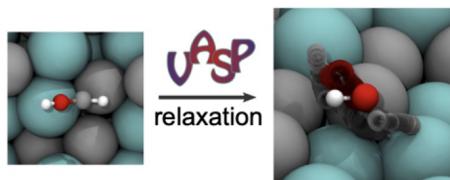
Hands-on 10 : MLP03 - Benchmarking

▼ Recap

Time scale limitation of DFT

Challenges of Theoretical Modeling

Huge computational cost of DFT calculations



- ✓ The DFT computation scales $O(n^3)$ with the number of electrons in the system.
- ✓ The DFT computations of 100 atoms approximately take ~1 hour per relaxation on 12 core CPUs.
→ few hours~ day for get energy of one DFT structure

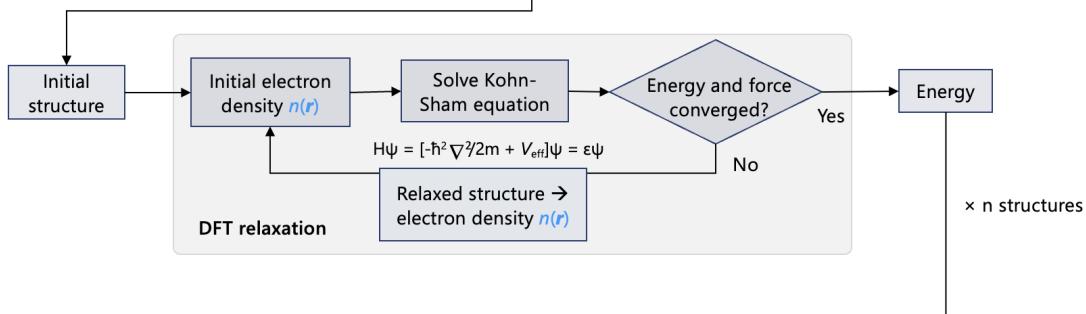
Ulissi et al. ACS Catal., 11, 10, 6059 (2021).

Researcher



"I want the most stable Ru SAC structures on TiO₂ surface."

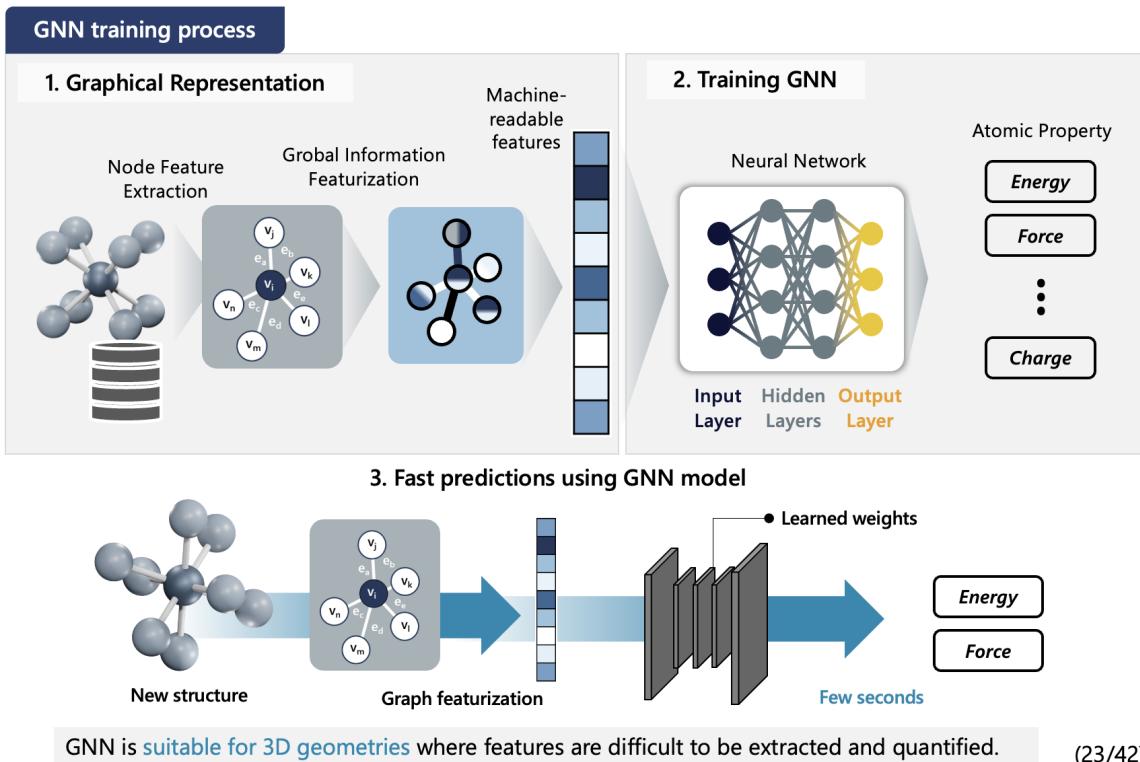
"Heuristically" determined initial structures of Ru/TiO₂



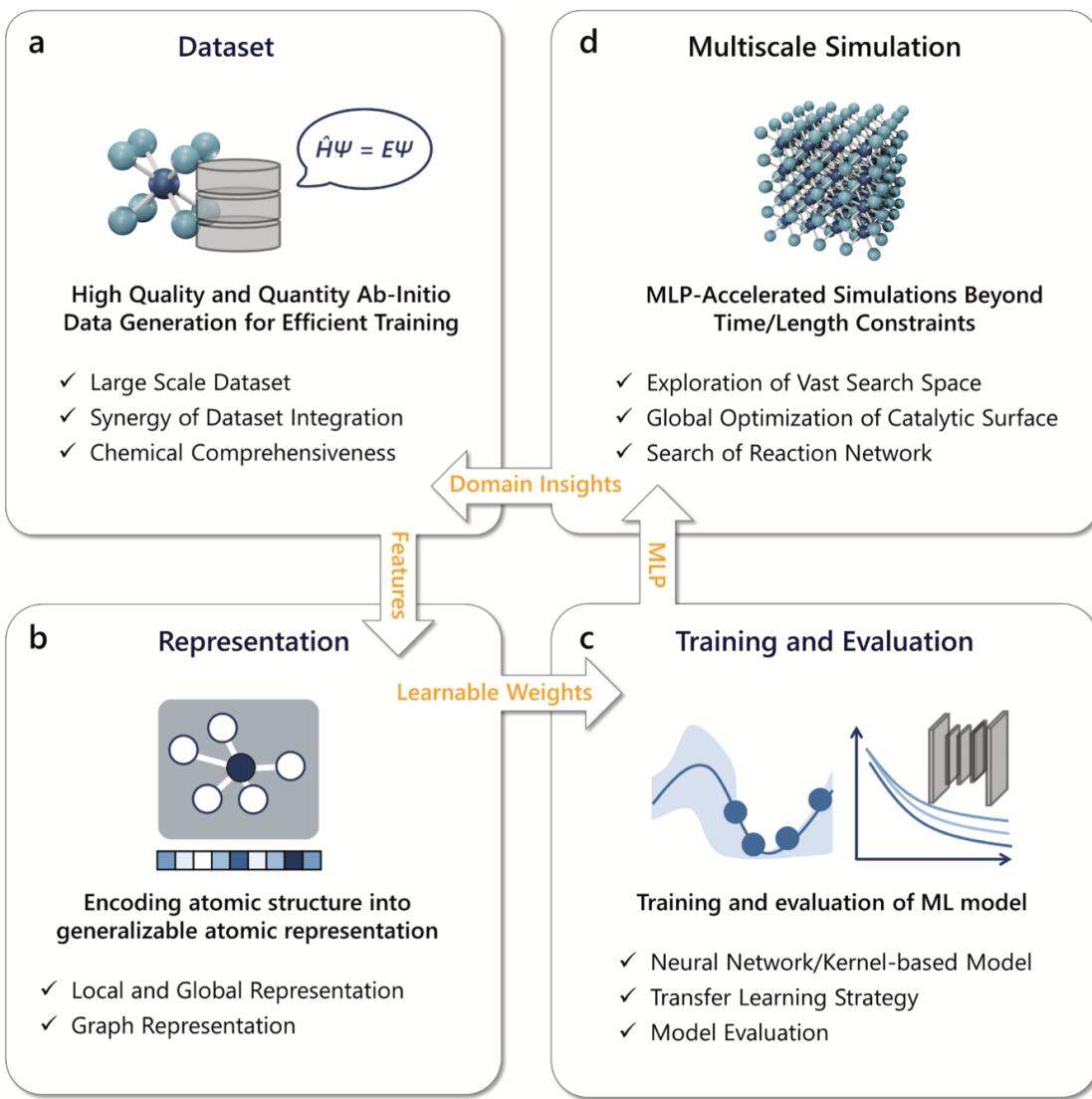
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Machine learning Potential (MLP) using graph neural network

Graph Neural Network (GNN)



<https://www.sciencedirect.com/science/article/pii/S138589472404244X#da005>



<https://www.sciencedirect.com/science/article/pii/S138589472404244X#da005>

Advent of Large dataset

Ab initio datasets of inorganic materials in computational catalysis.

Dataset	Property	Dataset size	Level of theory	Chemical Composition	Accessibility and contribution
Materials Project [34]	Atomic structure, band structure, magnetic properties, and others	1.5×10^5	PBE, HSE06, and $r^2\text{SCAN}$	Inorganic Crystals and molecules	Open source, open contribution,
QMD [35]	Atomic structure, and band structure band gap	1×10^6	PBE	Inorganic Crystals	Open source
NOMAD [36]	Atomic structure, and band structure	3×10^6	PBE, HSE06, HLE17, and others	Inorganic Crystals	Open source, open contribution
AFLOW [37]	Atomic structure, band structure, magnetic properties and phonon spectra	3.5×10^6	PBE	Inorganic Crystals	Open source
OC20 [12]	Atomic structure, Bader charge, total energy, and force,	2.5×10^8	RPBE	molecular adsorptions on inorganic crystal slabs	Open source, community challenges
OC22 [13]	Atomic structure, total energy, and force	1×10^7	PBE	molecular adsorptions on metal oxide slabs	Open source, community challenges
OpenDAC [38]	Atomic structure, total energy and force	3.8×10^7	PBE-D3	CO_2 and H_2O adsorptions on MOFs	Open source, community challenges
Catalysis-Hub [39]	Atomic structure, total energy, and reaction energy	1.3×10^5	PBE, RPBE, PW91 and others	Molecular adsorptions on inorganic crystals	Open source, open contribution,
PFP [40]	Atomic structure, and total energy	9×10^6	PBE and PBE + U	Molecules, transition metal slabs, clusters	Partially open
GNoMe [29]	Atomic structure, total energy, and decomposition energy	3.8×10^5	PBE and $r^2\text{SCAN}$	Inorganic Crystal	Partially open

▼ ‘Universal’ MLP

How researchers are making universal potential?

- Huge scale of database
- Rich informations in representation
- Computational efficiency in application
- Easy to use in ASE, LAMMPS and other packages

Joint Multi-domain Pre-training (JMP)

pre-training strategy that leverages ~120M atomic systems from various datasets (OC20, OC22, ANI-1x, Transition-1x)

state-of-the-art on 34 out of 40 tasks

Published as a conference paper at ICLR 2024

FROM MOLECULES TO MATERIALS: PRE-TRAINING LARGE GENERALIZABLE MODELS FOR ATOMIC PROPERTY PREDICTION

Nima Shoghi^{*1} Adeesh Kolluru² John R. Kitchin²
Zachary W. Ulissi¹ C. Lawrence Zitnick¹ Brandon M. Wood¹

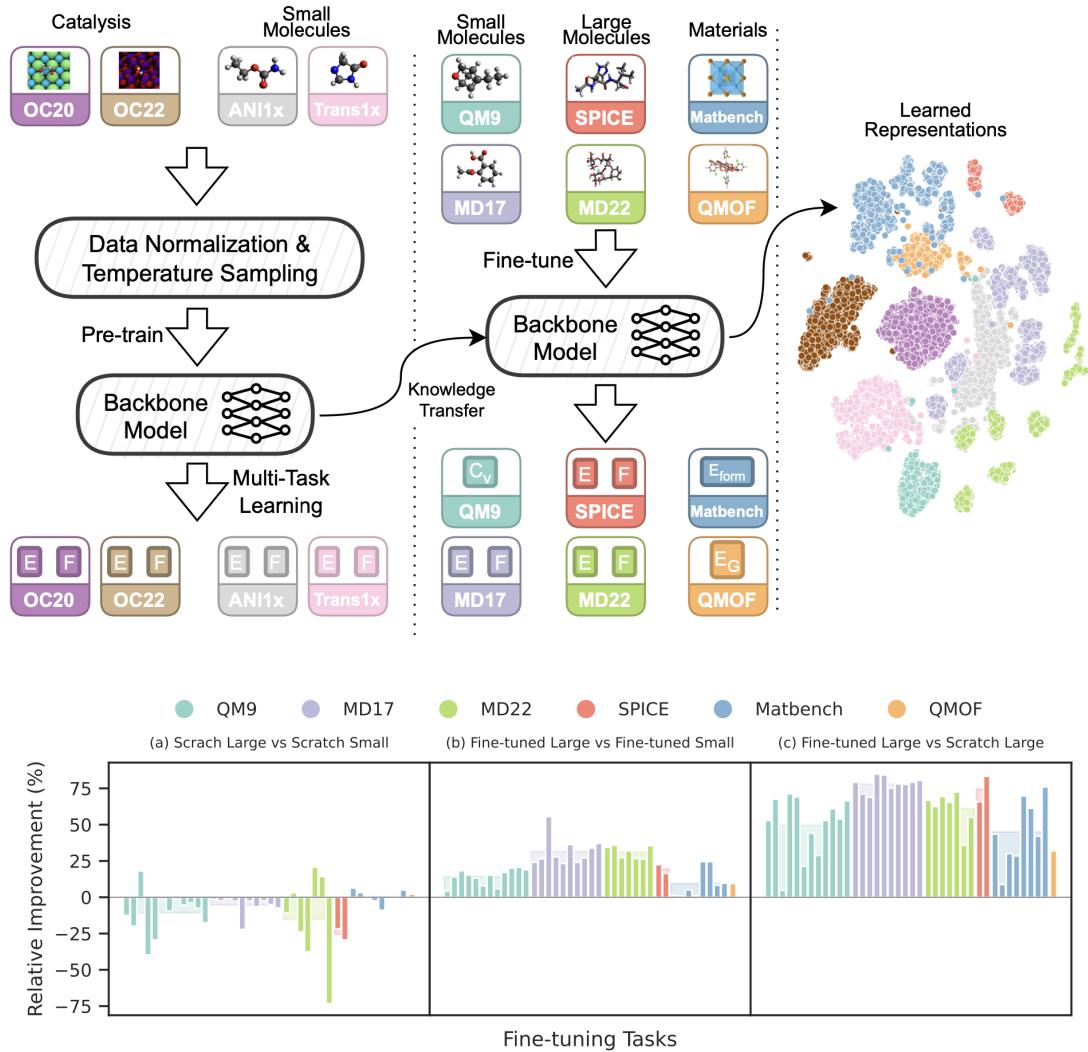
¹Fundamental AI Research (FAIR) at Meta

²Carnegie Mellon University

*Work done while at FAIR

Correspondence to: ns@nima.sh, bmwood@meta.com

ABSTRACT

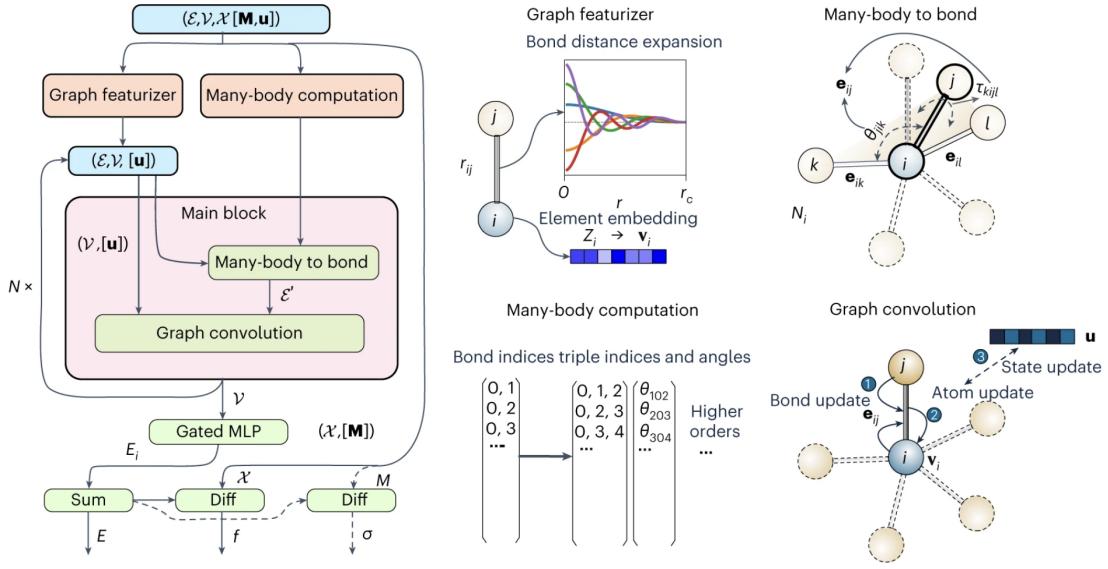


<https://arxiv.org/pdf/2310.16802.pdf>

M3GNET: rich information in edge feature

three-body spherical harmonics features are used to update bond features

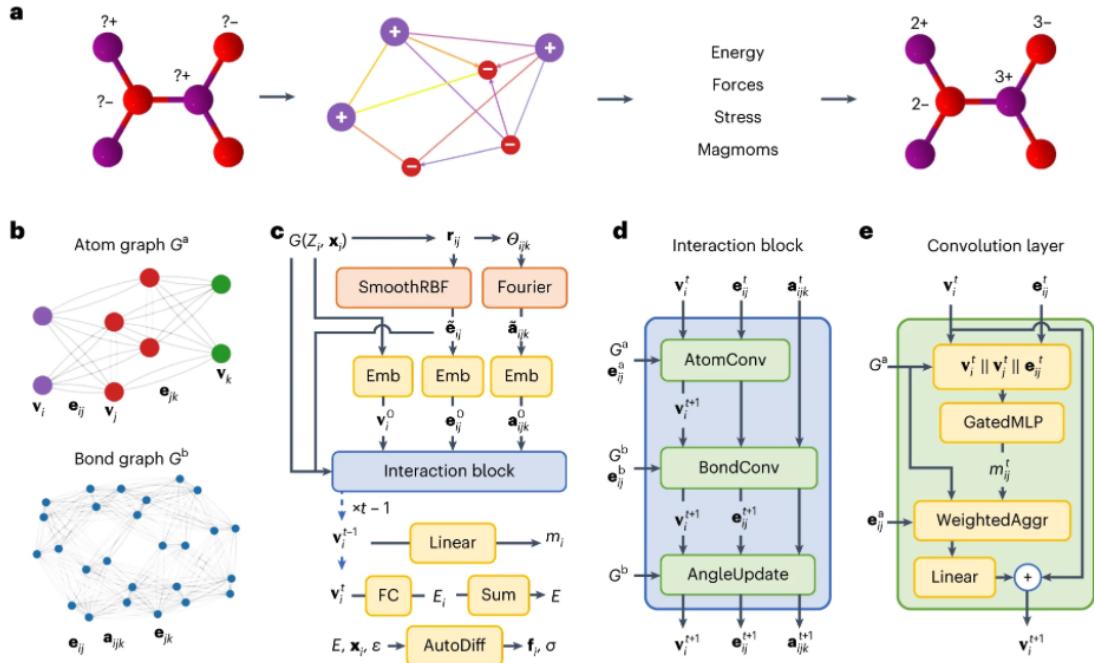
- **Angle-Based Interactions:** angles between atoms and neighbors.
- **Smooth Basis Encoding:** Uses spherical Bessel and harmonics functions to represent distances and angles smoothly.
- **Enhanced Bond Updates:** Bond features are updated with three-body terms for capturing complex atomic interactions.



<https://www.nature.com/articles/s43588-022-00349-3>

CHGNet: rich information in node feature

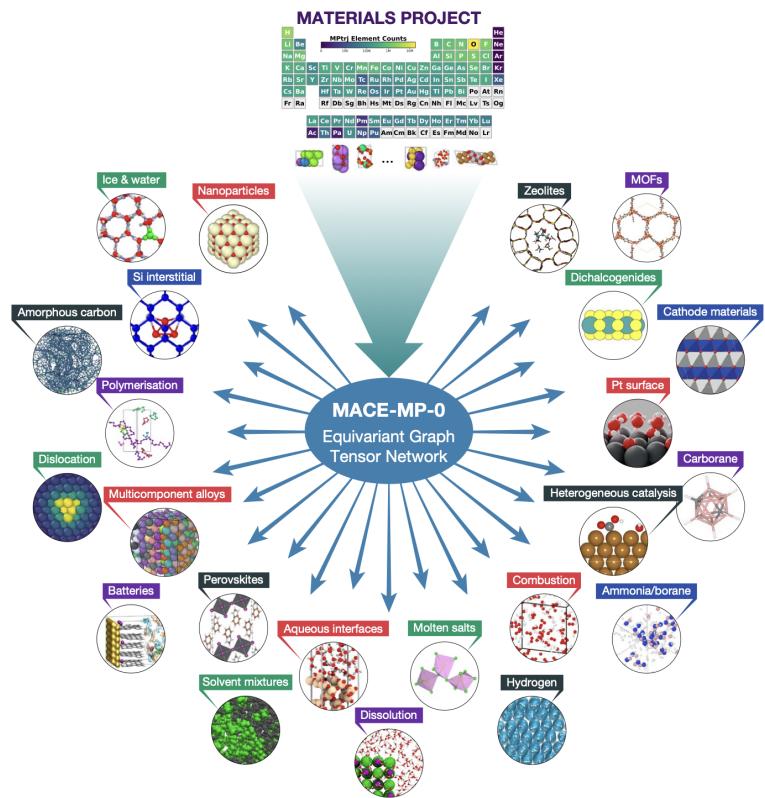
CHGNet incorporates **magnetic moments as node features** in its graph neural network, allowing each node (representing an atom) to encode charge information.



<https://github.com/CederGroupHub/chgnet>

Nature Machine Intelligence volume 5, pages 1031–1041 (2023)

MACE-MP: rich higher order information efficiently



<https://arxiv.org/pdf/2401.00096>

<https://doi.org/10.48550/arXiv.2206.07697>

Characteristics of MACE

- MPNN Interatomic Potentials
- Equivariant Graph Neural Networks

▼ SevenNet: Scale up efficiently

efficient parallelization based on NequIP architecture

large-scale MD simulations, offering researchers a powerful tool to explore complex material systems with high accuracy and efficiency.

J. Chem. Theory Comput. 2024, 20, 11, 4857-4868.

SevenNet Calculator for ASE

[ASE \(Atomic Simulation Environment\)](#) is a set of tools and Python modules for atomistic simulations. SevenNet-0 and SevenNet-trained potentials can be used with ASE for its use in python.

For pre-trained models,

```
from sevenn.sevennet_calculator import SevenNetCalculator  
sevenet_0_cal = SevenNetCalculator("7net-0", device='cpu') # 7net-0, SevenNet-0, 7net-0_22
```

For user trained models,

```
from sevenn.sevennet_calculator import SevenNetCalculator  
checkpoint_path = ### PATH TO CHECKPOINT ###  
sevenet_cal = SevenNetCalculator(checkpoint_path, device='cpu')
```

After the PyTorch installation, run

```
pip install sevenn
```

To download the latest version of SevenNet(not stable!), run

```
pip install https://github.com/MDIL-SNU/SevenNet.git
```

<https://github.com/MDIL-SNU/SevenNet>

Precautions to take when applying a pretrained model to out-of-distribution problems.

*In mathematical folklore, the "**no free lunch**" (**NFL theorem** (sometimes pluralized) of David Wolpert and William Macready, alludes to the saying "no such thing as a free lunch", that is, there are no easy shortcuts to success.*

No Free Lunch Theorems for Optimization

David H. Wolpert and William G. Macready

Abstract—A framework is developed to explore the connection between effective optimization algorithms and the problems they are solving. A number of “no free lunch” (NFL) theorems are presented which establish that for any algorithm, any elevated performance over one class of problems is offset by performance over another class. These theorems result in a geometric interpretation of what it means for an algorithm to be well suited to an optimization problem. Applications of the NFL theorems to information-theoretic aspects of optimization and benchmark measures of performance are also presented. Other issues addressed include time-varying optimization problems and *a priori* “head-to-head” minimax distinctions between optimization algorithms, distinctions that result despite the NFL theorems’ enforcing of a type of uniformity over all algorithms.

Index Terms—Evolutionary algorithms, information theory, optimization.

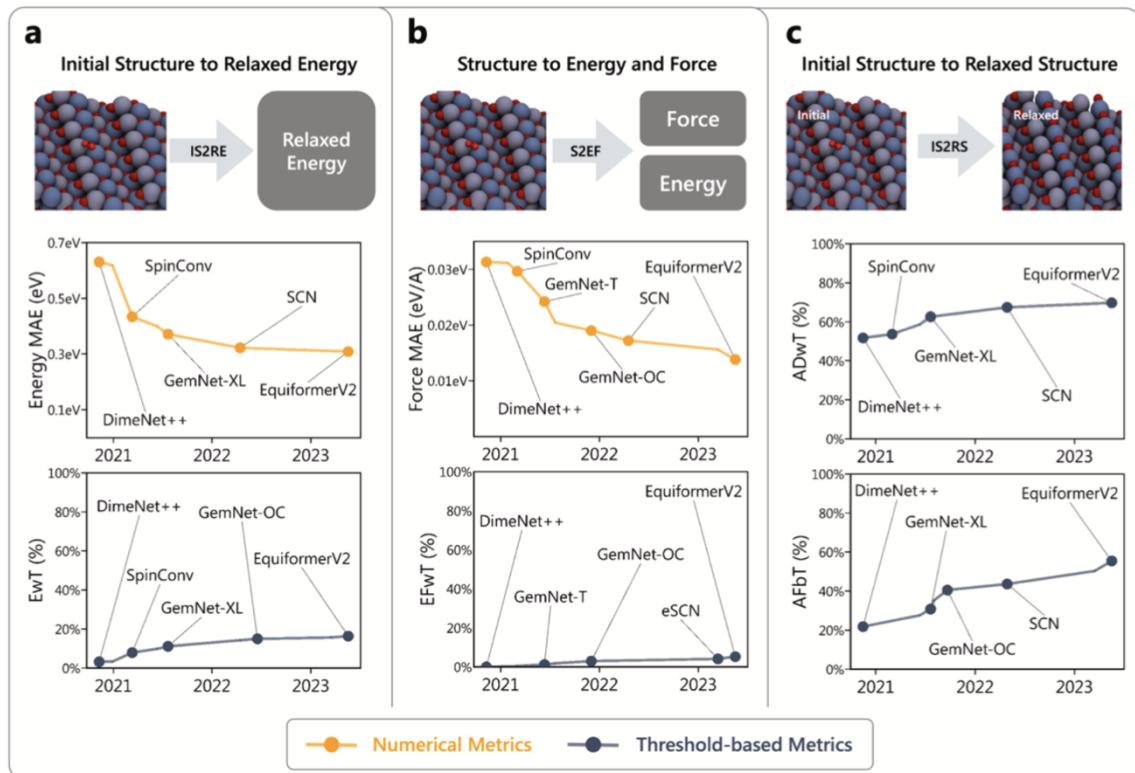
information theory and Bayesian analysis contribute to an understanding of these issues? How *a priori* generalizable are the performance results of a certain algorithm on a certain class of problems to its performance on other classes of problems? How should we even measure such generalization? How should we assess the performance of algorithms on problems so that we may programmatically compare those algorithms?

Broadly speaking, we take two approaches to these questions. First, we investigate what *a priori* restrictions there are on the performance of one or more algorithms as one runs over the set of all optimization problems. Our second approach is to instead focus on a particular problem and consider the effects of running over all algorithms. In the current paper

<https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=585893>

▼ Evaluation of MLP

Open Catalyst project



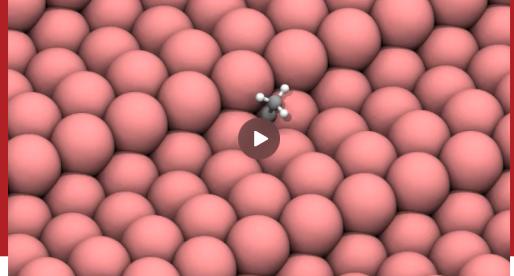
<https://www.sciencedirect.com/science/article/pii/S138589472404244X#da005>

∞ Meta | Carnegie Mellon University

Home Demo Leaderboard Datasets Challenge Discuss

Public Leaderboard OC20

See the latest results and submit your own on the [OC20 evaluation server!](#)
You can also check the [OC22 leaderboard](#).



Task IS2RE Task S2EF Task IS2RS

Test Split

Average ID OOD Ads OOD Cat OOD Both

Team	Method	Average		
		Energy MAE (eV)	EWT (%)	Submitted
Atomic Architects MIT + FAIR at Meta	EquiformerV2 + DeNS (160M, λ _E =4) -- All+MD	0.2933	18.78	2024/06/27
Open Catalyst Project (FAIR+CMU)	EquiformerV2 - 31M - LBFGS Fix	0.3009	16.8	2024/05/05
FAIR at Meta + Atomic Architects MIT	EquiformerV2 + DeNS (160M, λ _E =4) -- All+MD	0.3082	17.03	2023/11/22

<https://opencatalystproject.org/leaderboard.html>

Matbench discovery

<https://matbench-discovery.materialsproject.org/models>

Disclaimer: We evaluate how accurately ML models predict solid-state thermodynamic stability. Although this is an important aspect of high-throughput materials discovery, the ranking cannot give a complete picture of a model's general applicability to materials. A high ranking does not constitute endorsement by the Materials Project.

Matbench Discovery is an [interactive leaderboard](#) and associated [PyPI package](#) which together make it easy to rank ML energy models on a task designed to simulate high-throughput discovery of new stable inorganic crystals.

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	TPR ↑	TNR ↑	MAE ↓	RMSE ↓	R ² ↑	Training Set	Model Params	Targets	Date Added
eqV2 M	0.917	6.05	0.924	0.975	0.91	0.986	0.02	0.072	0.848	3M (102.4M) (OMat24+MPtrj)	86.6M	EFS _D	2024-10-18
ORB	0.88	6.04	0.924	0.965	0.841	0.987	0.028	0.077	0.824	3M (32.1M) (MPtrj+Alex)	25.2M	EFS _D	2024-10-11
MatterSim	0.859	5.65	0.863	0.957	0.856	0.975	0.026	0.08	0.812	17M (MatterSim)	182.0M	EFS _D	2024-06-16
GNoME	0.829	5.52	0.844	0.955	0.814	0.972	0.035	0.085	0.785	6M (89.0M) (GNoME)	16.2M	EF _C	2024-02-03
eqV2 S DeNS	0.815	5.04	0.771	0.941	0.864	0.953	0.036	0.085	0.788	146K (1.6M) (MPtrj)	31.2M	EFS _D	2024-10-18
ORB MPtrj	0.765	4.7	0.719	0.922	0.817	0.941	0.045	0.091	0.756	146K (1.6M) (MPtrj)	25.2M	EFS _D	2024-10-14
SevenNet	0.724	4.25	0.65	0.904	0.818	0.919	0.048	0.092	0.75	146K (1.6M) (MPtrj)	842.4K	EFS _C	2024-07-13
MACE	0.669	3.78	0.577	0.878	0.796	0.893	0.057	0.101	0.697	146K (1.6M) (MPtrj)	4.7M	EFS _C	2023-07-14
CHGNet	0.613	3.36	0.514	0.851	0.758	0.868	0.063	0.103	0.689	146K (1.6M) (MPtrj)	412.5K	EFS _C M	2023-03-03
M3GNet	0.569	2.88	0.441	0.813	0.803	0.813	0.075	0.118	0.585	63K (188.3K) (MPF)	227.5K	EFS _C	2022-09-20
ALIGNN	0.567	3.21	0.49	0.841	0.672	0.872	0.093	0.154	0.297	155K (MP_2022)	4.0M	Energy	2023-06-02
MEGNet	0.51	2.96	0.452	0.826	0.585	0.87	0.13	0.206	-0.248	133K (MP_Graphs)	167.8K	Energy	2022-11-14
CGCNN	0.507	2.85	0.436	0.818	0.605	0.857	0.138	0.233	-0.603	155K (MP_2022)	128.4K (N=10)	Energy	2022-12-28
CGCNN+P	0.5	2.56	0.392	0.786	0.693	0.803	0.113	0.182	0.019	155K (MP_2022)	128.4K (N=10)	Energy	2023-02-03
Wrenformer	0.466	2.26	0.345	0.745	0.719	0.75	0.11	0.186	-0.018	155K (MP_2022)	5.2M (N=10)	Energy	2022-11-26
BOWSR	0.423	1.96	0.3	0.712	0.718	0.693	0.118	0.167	0.151	133K (MP_Graphs)	167.8K	Energy	2022-11-17
Voronoi RF	0.333	1.58	0.241	0.668	0.535	0.692	0.148	0.212	-0.329	155K (MP_2022)	26.2M	Energy	2022-11-26
Dummy	0.185	1	0.154	0.687	0.232	0.769	0.124	0.184	0				

▼ Catalysis-hub

nature > scientific_data > articles > article

Article | [Open access](#) | Published: 28 May 2019

Catalysis-Hub.org, an open electronic structure database for surface reactions

Kirsten T. Winther, Max J. Hoffmann, Jacob R. Boes, Osman Mamun, Michal Bajdich & Thomas Bligaard 

[Scientific Data](#) 6, Article number: 75 (2019) | [Cite this article](#)

14k Accesses | 188 Citations | 10 Altmetric | [Metrics](#)

Abstract

We present a new open repository for chemical reactions on catalytic surfaces, available at <https://www.catalysis-hub.org>. The featured database for surface reactions contains more than 100,000 chemisorption and reaction energies obtained from electronic structure calculations, and is continuously being updated with new datasets. In addition to providing quantum-mechanical results for a broad range of reactions and surfaces from different publications, the database features a systematic, large-scale study of chemical adsorption and hydrogenation on bimetallic alloy surfaces. The database contains reaction specific information, such as the surface composition and reaction energy for each reaction, as well as the surface geometries and calculational parameters, essential for data reproducibility. By providing direct access via the web-interface as well as a Python API, we seek to accelerate the discovery of catalytic materials for sustainable energy applications by enabling researchers to efficiently use the data as a basis for new calculations and model generation.

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

▼ Assignment

Please refer to the following code:

https://github.com/s-choung/Simulation_tutorials/blob/main/handson10.ipynb

using **CatBench library, evaluate MLP energy MAE for at least 5 different cathub benchmark datasets. ex) ComerUnraveling2022, TangRevamped2024, StricklerSystematic2019**