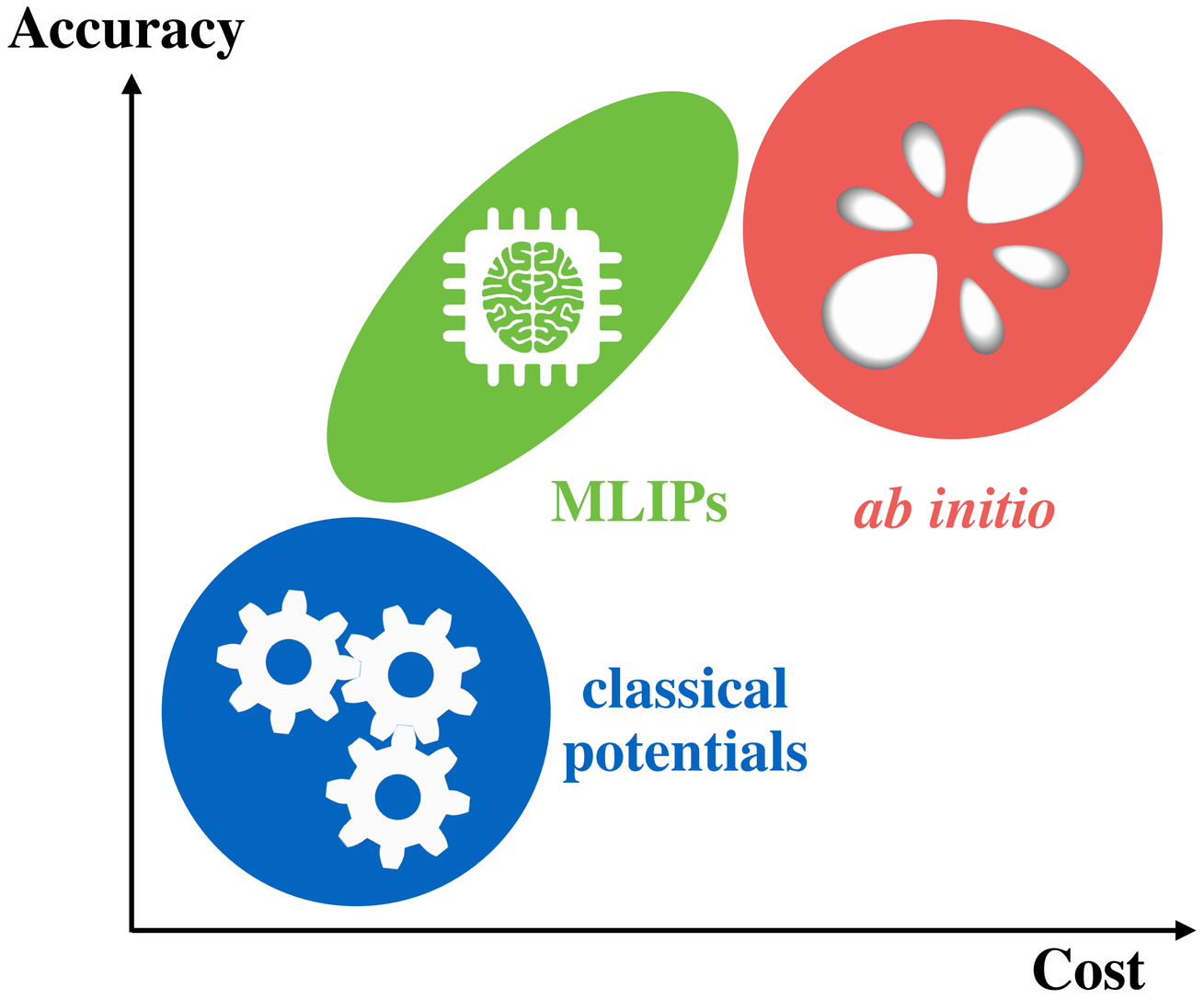
Systematic assessment of various universal machine-learning interatomic potentials

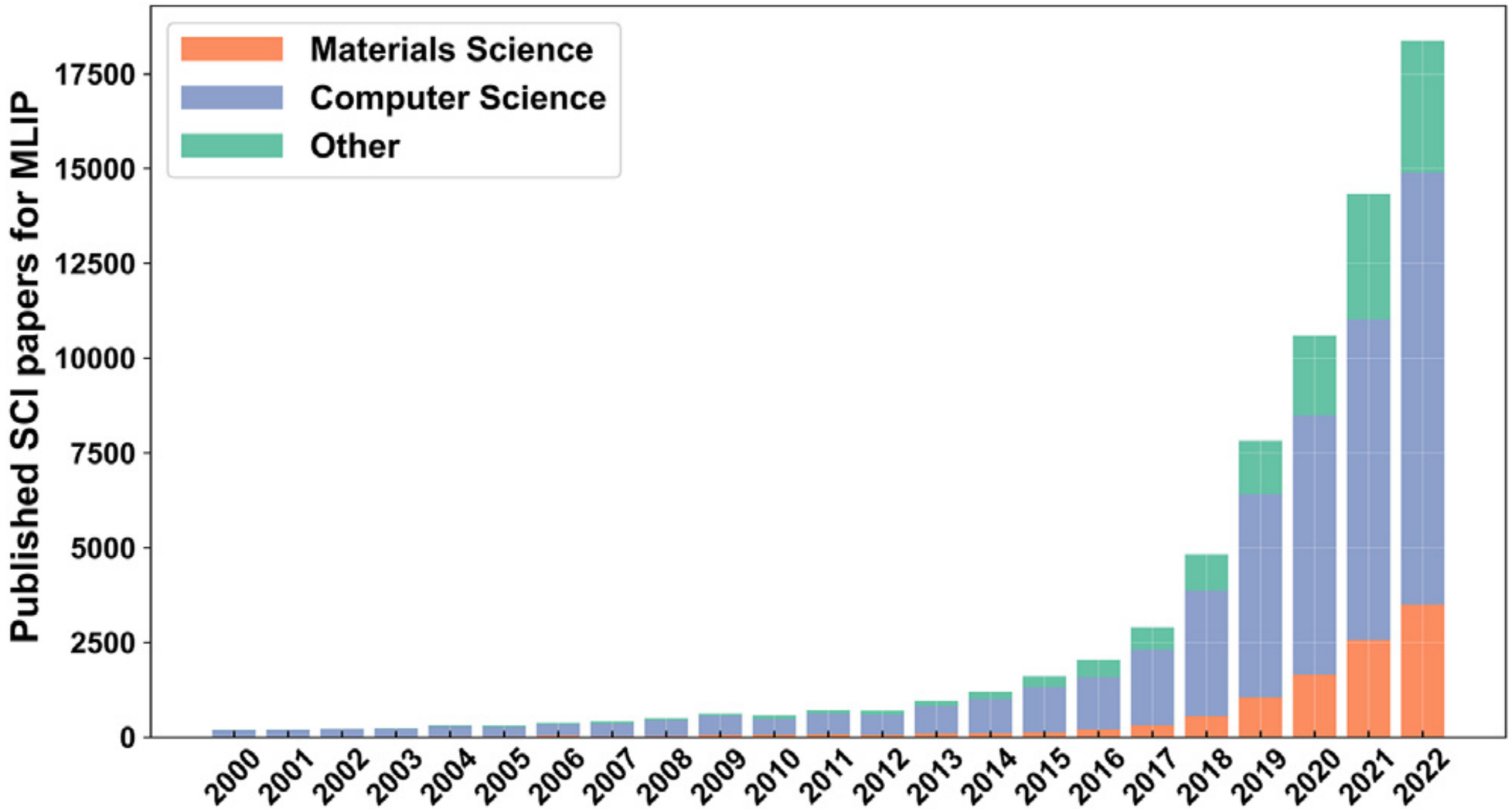
Gian-Marco Rignanese

CECAM Workshop on "Machine Learning Interatomic Potentials and Accessible Databases"
Grenoble, 10-12 September, 2024

For MD simulations, MLIPs bridge the gap between costly *ab initio* and low-accuracy classical potentials

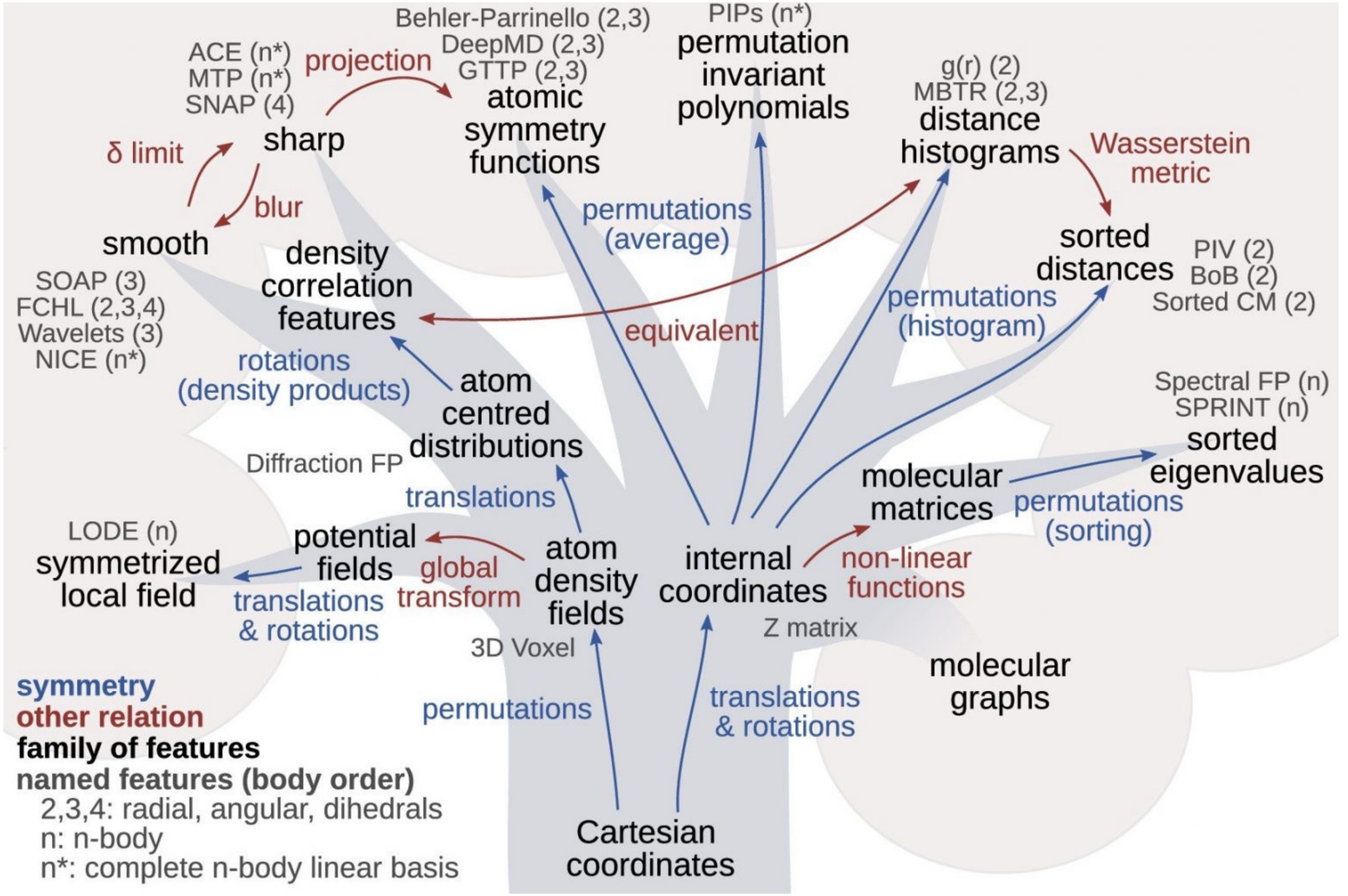


As a result, the usage of MLIPs has increased exponentially in the last few years



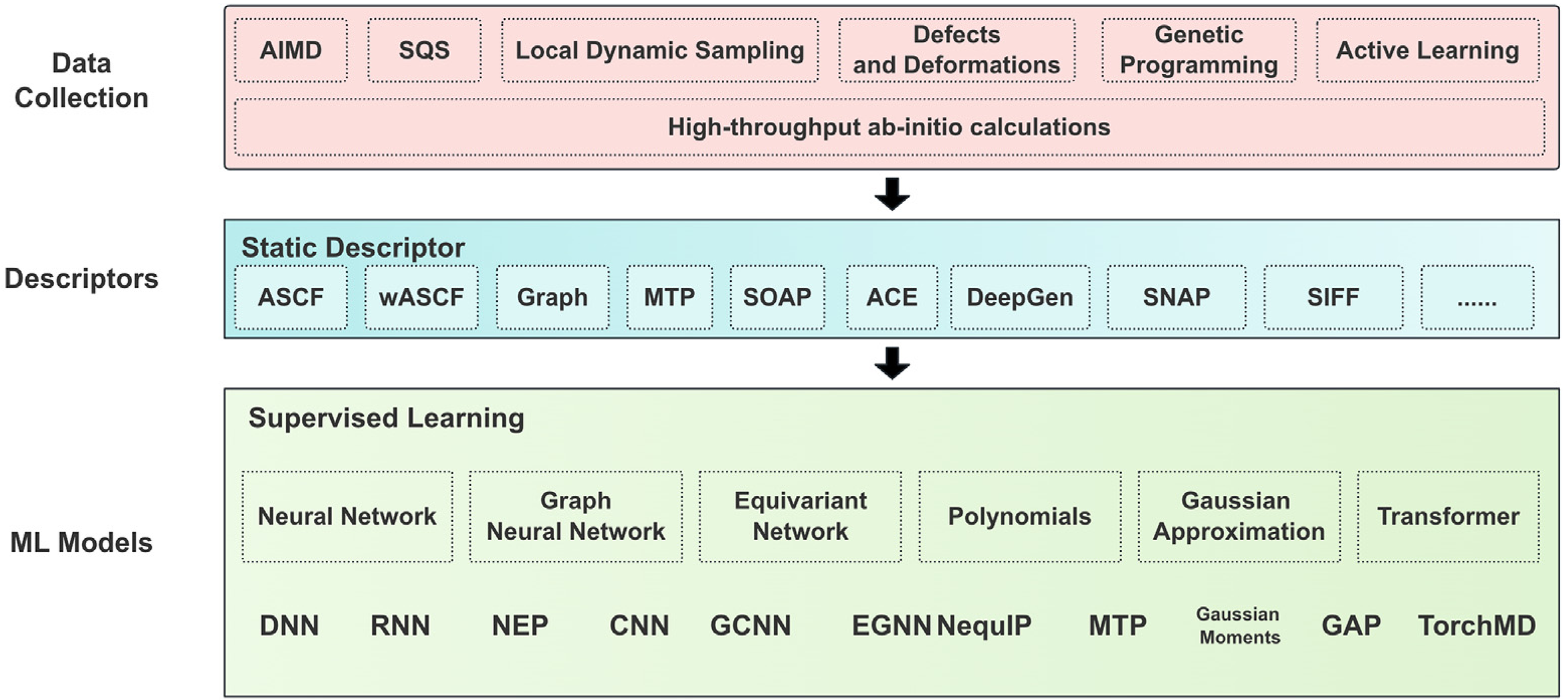
[G. Wang *et al.*, iScience **27**, 109673 (2024)]

Many papers were indeed first dedicated to the development of the MLIPs (descriptors and models)



[F. Musil *et al.*, Chem. Rev. **121**, 9759 (2021)]

Another key component of MLIPs is the data collection for training the potentials and for their transferability



[G. Wang *et al.*, iScience **27**, 109673 (2024)]

From that standpoint, efforts like ColaFit are crucial

The ColabFit Exchange: Data for Advanced Materials Science

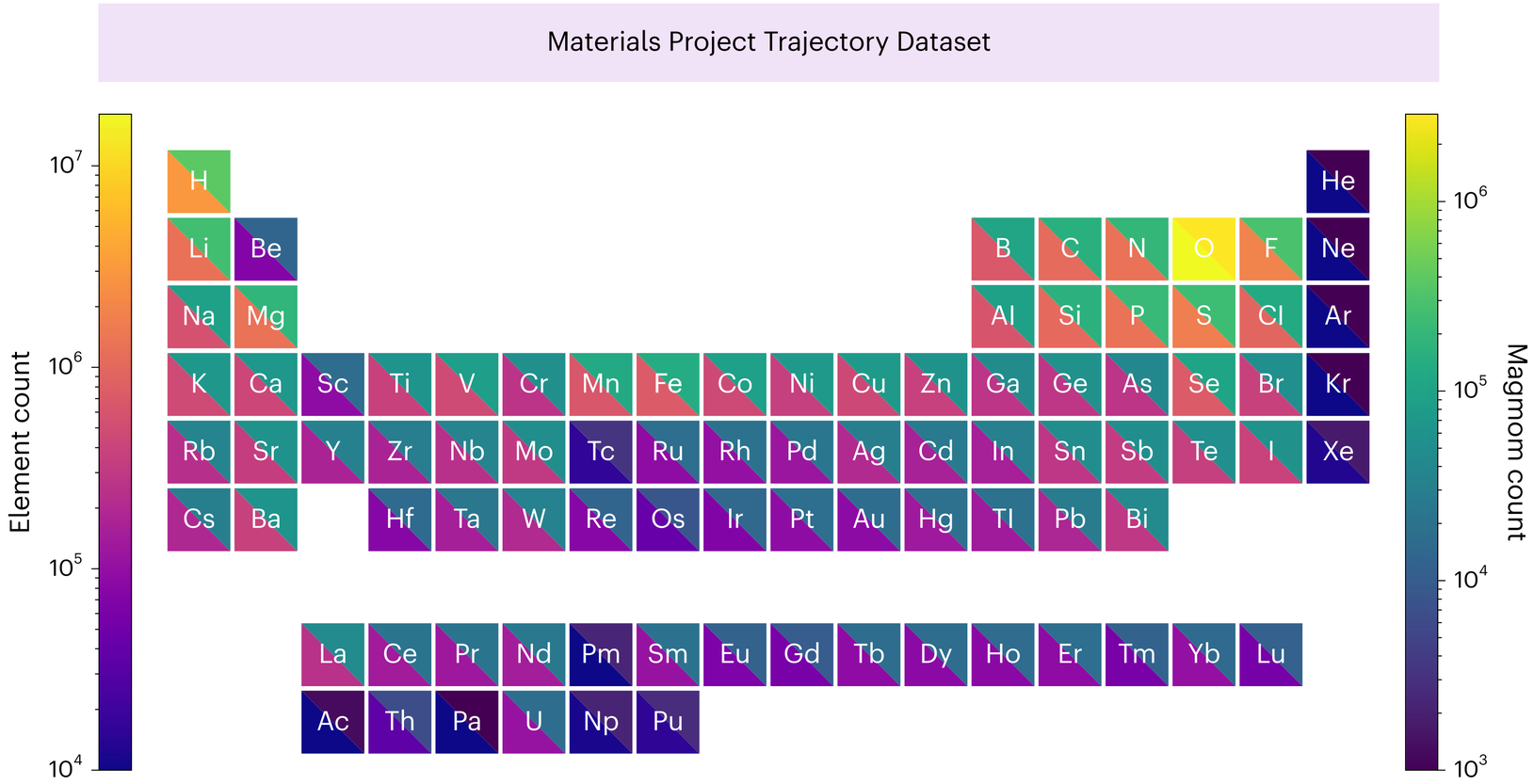
Welcome to the ColabFit Exchange! This is an online resource for the discovery, exploration and submission of datasets for data-driven interatomic potential (DDIP) development for materials science and chemistry applications. ColabFit's goal is to increase the Findability, Accessibility, Interoperability, and Reusability (FAIR) of DDIP data by providing convenient access to well-curated and standardized first-principles and experimental datasets. Content on the ColabFit Exchange is open source and freely available.

Datasets	Configuration Sets
372	1,327

Property Instances	Configurations
513,959,850	180,074,146

[J.A. Vita *et al.*, J. Chem. Phys. **159**, 154802 (2023)]

More generally sharing datasets is very useful...

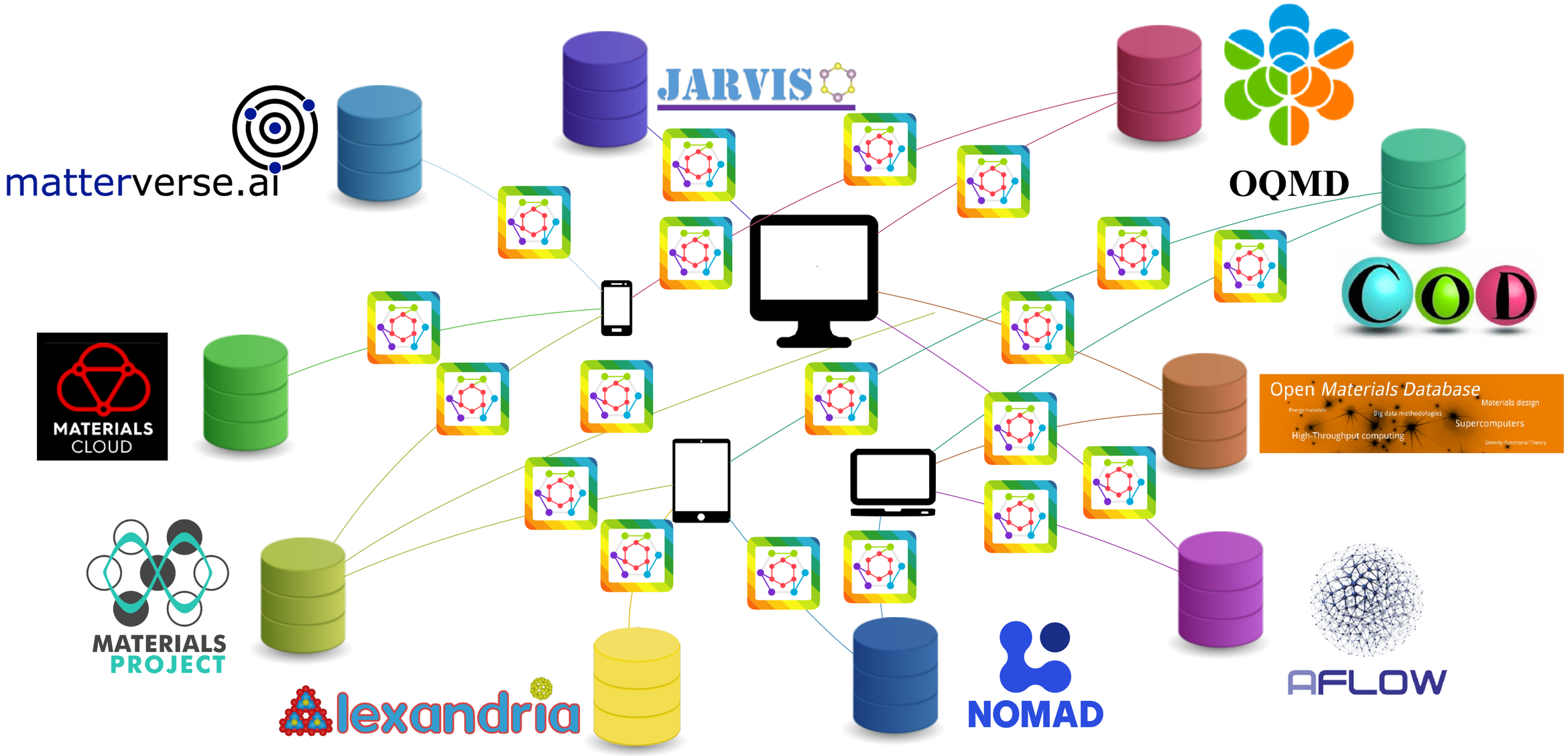


	Compounds	Energy	Magmom	Force	Stress
Count	145,923	1,580,395	7,944,833	49,295,660	14,223,555
MAD		1,480 eV atom^{-1}	0.336 μ_B	0.158 eV Å^{-1}	7.553 GPa

[B. Deng *et al.*, Nat. Mach. Intel. **5**, 1031 (2023)]

figshare

More generally sharing datasets is very useful...



[C.W. Andersen *et al.*, Sci. Data **8**, 217 (2021); M.L. Evans *et al.,* Digital Discovery, 2024, DOI: 10.1039/D4DD00039K]

Users are now able to search

more materials DBs with the same query…

- simple query on Group 14 compounds (1):
  /v1/structures?filter=elements HAS ANY "C", "Si", "Ge", "Sn", "Pb"
- with a focus on binary materials (2):
  /v1/structures?filter=elements HAS ANY "C", "Si", "Ge", "Sn", "Pb" AND nelements=2
- with a focus on ternary materials without Pb (3):
  /v1/structures?filter=elements HAS ANY "C", "Si", "Ge", "Sn" AND NOT elements HAS "Pb"
  AND elements LENGTH 3

PROVIDER	N_1	N_2	N_3	N_{tot}
AFLOW	704,302 (700,192)	63,017 (62,293)	413,797 (382,554)	3,530,330
Alexandria*	939,084	48,510	437,768	5,055,842
COD	452,574 (416,314)	4,046 (3,896)	34,739 (32,420)	506,394
CMR	147	147	0	1,536
JARVIS-DFT	9,017	1,426	-	77,096
Materials Cloud*	961,564	4,218	136,176	4,515,120
MPDD	811,136	80,195	490,900	3,975,666
MPOD	91	8	16	401
MPDS	-	-	-	507,178
NOMAD	4,451,056 (3,359,594)	587,923 (532,123)	2,092,989 (1,611,302)	12,116,021
odbx*	14,490 (55)	2,921 (54)	7,684 (0)	138,278
omdb	58,718 (58,718)	690 (690)	7,428 (7,428)	68,566
OQMD	204,143 (153,113)	12,467 (11,011)	81,673 (70,252)	1,022,603
TCOD	2,634 (2,631)	296 (296)	662 (660)	2,922
2DMatpedia	1,172	739	255	6,351

Then, universal MLIPs started to appear...

M3GNet

nature computational science

Article

https://doi.org/10.1038/s43588-022-00349-3

A universal graph deep learning interatomic potential for the periodic table

Received: 18 March 2022

Accepted: 5 October 2022

Chi Chen ✉ & Shyue Ping Ong ✉

npj | computational materials

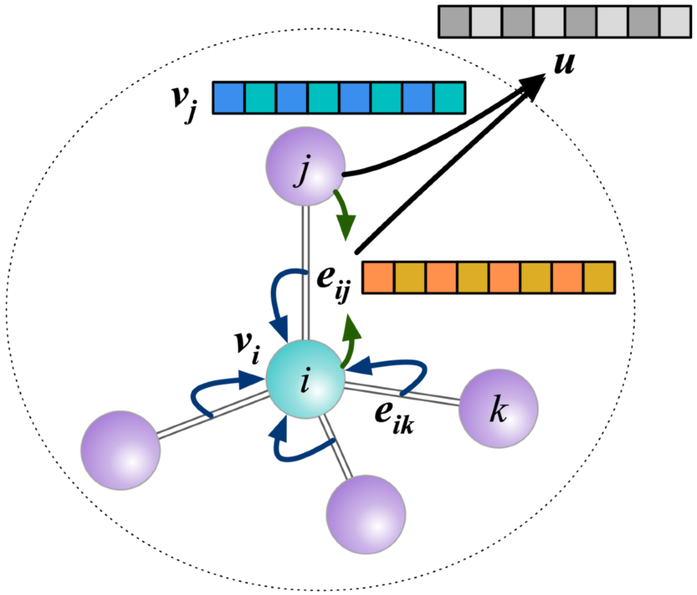
Article

Published in partnership with the Shanghai Institute of Ceramics of the Chinese Academy of Sciences

https://doi.org/10.1038/s41524-024-01227-4

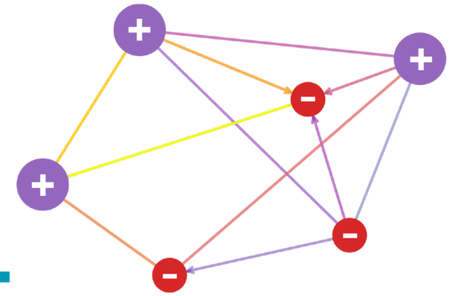
Robust training of machine learning interatomic potentials with dimensionality reduction and stratified sampling

Ji Qi [1,2] ✉, Tsz Wai Ko [3], Brandon C. Wood [2,4], Tuan Anh Pham [2,4] ✉ & Shyue Ping Ong [1,3] ✉



https://github.com/materialsvirtuallab/m3gnet

CHGNet (Crystal Hamiltonian Graph neural Network)



nature machine intelligence

Article

https://doi.org/10.1038/s42256-023-00716-3

CHGNet as a pretrained universal neural network potential for charge-informed atomistic modelling

Received: 2 March 2023

Accepted: 4 August 2023

Bowen Deng[1,2], Peichen Zhong[1,2] ✉, KyuJung Jun[1,2], Janosh Riebesell[2,3], Kevin Han[2], Christopher J. Bartel[1,4] & Gerbrand Ceder[1,2] ✉

https://github.com/CederGroupHub/chgnet

https://chgnet.lbl.gov/

ALIGNN (Atomistic Line Graph Neural Network)

Digital Discovery

PAPER

View Article Online
View Journal | View Issue

Cite this: *Digital Discovery*, 2023, **2**, 346

Received 12th September 2022
Accepted 12th January 2023

DOI: 10.1039/d2dd00096b

Unified graph neural network force-field for the periodic table: solid state applications

Kamal Choudhary, *[ab] Brian DeCost, [c] Lily Major, [de] Keith Butler, [e] Jeyan Thiyagalingam [e] and Francesca Tavazza [c]

https://github.com/usnistgov/alignn

MACE-MP-0

A foundation model for atomistic materials chemistry

Ilyes Batatia[†1], Philipp Benner[†2], Yuan Chiang[†3,4], Alin M. Elena[†17], Dávid P. Kovács[†1], Janosh Riebesell[†4,13], Xavier R. Advincula[12,13], Mark Asta[3,4], William J. Baldwin[1], Noam Bernstein[11], Arghya Bhowmik[25], Samuel M. Blau[10], Vlad Cărare[1,13], James P. Darby[1], Sandip De[18], Flaviano Della Pia[12], Volker L. Deringer[16], Rokas Elijošius[1], Zakariya El-Machachi[16], Edvin Fako[18], Andrea C. Ferrari[26], Annalena Genreith-Schriever[12], Janine George[2,6], Rhys E. A. Goodall[15], Clare P. Grey[12], Shuang Han[18], Will Handley[13,19], Hendrik H. Heenen[9], Kersti Hermansson[23], Christian Holm[22], Stephan Hofmann[1], Jad Jaafar[1], Konstantin S. Jakob[9], Hyunwook Jung[9], Venkat Kapil[12, 21], Aaron D. Kaplan[4], Nima Karimitari[20], Namu Kroupa[13,19,1], Jolla Kullgren[23], Matthew C. Kuner[3,4], Domantas Kuryla[12], Guoda Liepuoniute[1,26], Johannes T. Margraf[8], Ioan-Bogdan Magdău[24], Angelos Michaelides[12], J. Harry Moore[1], Aakash A. Naik[2,6], Samuel P. Niblett[12], Sam Walton Norwood[25], Niamh O'Neill[12,13], Christoph Ortner[5], Kristin A. Persson[3,4,7], Karsten Reuter[9], Andrew S. Rosen[3,4], Lars L. Schaaf[1], Christoph Schran[13], Eric Sivonxay[10], Tamás K. Stenczel[1], Viktor Svahn[23], Christopher Sutton[20], Cas van der Oord[1], Eszter Varga-Umbrich[1], Tejs Vegge[25], Martin Vondrák[8,9], Yangshuai Wang[5], William C. Witt[14], Fabian Zills[22], and Gábor Csányi[*1]

arXiv:2401.00096v2

https://github.com/ACEsuit/mace-mp

TeaNet

nature COMMUNICATIONS

ARTICLE

https://doi.org/10.1038/s41467-022-30687-9 OPEN

Towards universal neural network potential for material discovery applicable to arbitrary combination of 45 elements

So Takamoto[1✉], Chikashi Shinagawa[1], Daisuke Motoki[1], Kosuke Nakago[1], Wenwen Li[1], Iori Kurata[1], Taku Watanabe[2], Yoshihiro Yayama[2], Hiroki Iriguchi[2], Yusuke Asano[2], Tasuku Onodera[2], Takafumi Ishii[2], Takao Kudo[2], Hideki Ono[2], Ryohto Sawada[1], Ryuichiro Ishitani[1], Marc Ong[1], Taiki Yamaguchi[1], Toshiki Kataoka[1], Akihide Hayashi[1], Nontawat Charoenphakdee[1] & Takeshi Ibuka[2✉]

MATLANTIS

Contents lists available at ScienceDirect

Journal of Materiomics

journal homepage: www.journals.elsevier.com/journal-of-materiomics/

Towards universal neural network interatomic potential

So Takamoto [a], Daisuke Okanohara [a], Qing-Jie Li [b], Ju Li [b, *]

[a] Preferred Networks, Inc., 100-0004, 1-6-1 Otemachi, Chiyoda-ku, Tokyo, Japan
[b] Department of Nuclear Science and Engineering and Department of Materials Science and Engineering, MIT, Cambridge, MA, 02139, USA

GNoME (Graph Networks for Materials Exploration)

Google DeepMind

Article

Scaling deep learning for materials discovery

https://doi.org/10.1038/s41586-023-06735-9

Received: 8 May 2023

Accepted: 10 October 2023

Amil Merchant[1,3]✉, Simon Batzner[1,3], Samuel S. Schoenholz[1,3], Muratahan Aykol[1], Gowoon Cheon[2] & Ekin Dogus Cubuk[1,3]✉

https://github.com/google-deepmind/materials_discovery

MatterSim

MatterSim: A Deep Learning Atomistic Model Across Elements, Temperatures and Pressures

Han Yang[1*†], Chenxi Hu[1†], Yichi Zhou[1†], Xixian Liu[1†], Yu Shi[1†], Jielan Li[1*†], Guanzhi Li[1†], Zekun Chen[1†], Shuizhou Chen[1†], Claudio Zeni[1], Matthew Horton[1], Robert Pinsler[1], Andrew Fowler[1], Daniel Zügner[1], Tian Xie[1], Jake Smith[1], Lixin Sun[1], Qian Wang[1], Lingyu Kong[1], Chang Liu[1], Hongxia Hao[1*], Ziheng Lu[1*]

[1*]Microsoft Research AI for Science.

arXiv:2405.04967v2

SevenNet (Scalable EquiVariance Enabled Neural Network)

JCTC Journal of Chemical Theory and Computation

pubs.acs.org/JCTC Article

Scalable Parallel Algorithm for Graph Neural Network Interatomic Potentials in Molecular Dynamics Simulations

Yutack Park, Jaesun Kim, Seungwoo Hwang, and Seungwu Han*

Cite This: *J. Chem. Theory Comput.* 2024, 20, 4857–4868 Read Online

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

Orbital Materials - Pretrained models for atomic simulations

You can use this calculator with any ASE calculator-compatible code. For example, you can use it to perform a geometry optimization:

```python
from ase.optimize import BFGS

# Rattle the atoms to get them out of the minimum energy configuration
atoms.rattle(0.5)
print("Rattled Energy:", atoms.get_potential_energy())

calc = ORBCalculator(orbff, device="cpu")
dyn = BFGS(atoms)
dyn.run(fmax=0.01)
print("Optimized Energy:", atoms.get_potential_energy())
```

Citing

We are currently preparing a preprint for publication.

License

ORB models are licensed under the ORB Community License Agreement, Version 1. Please see the LICENSE file for details.

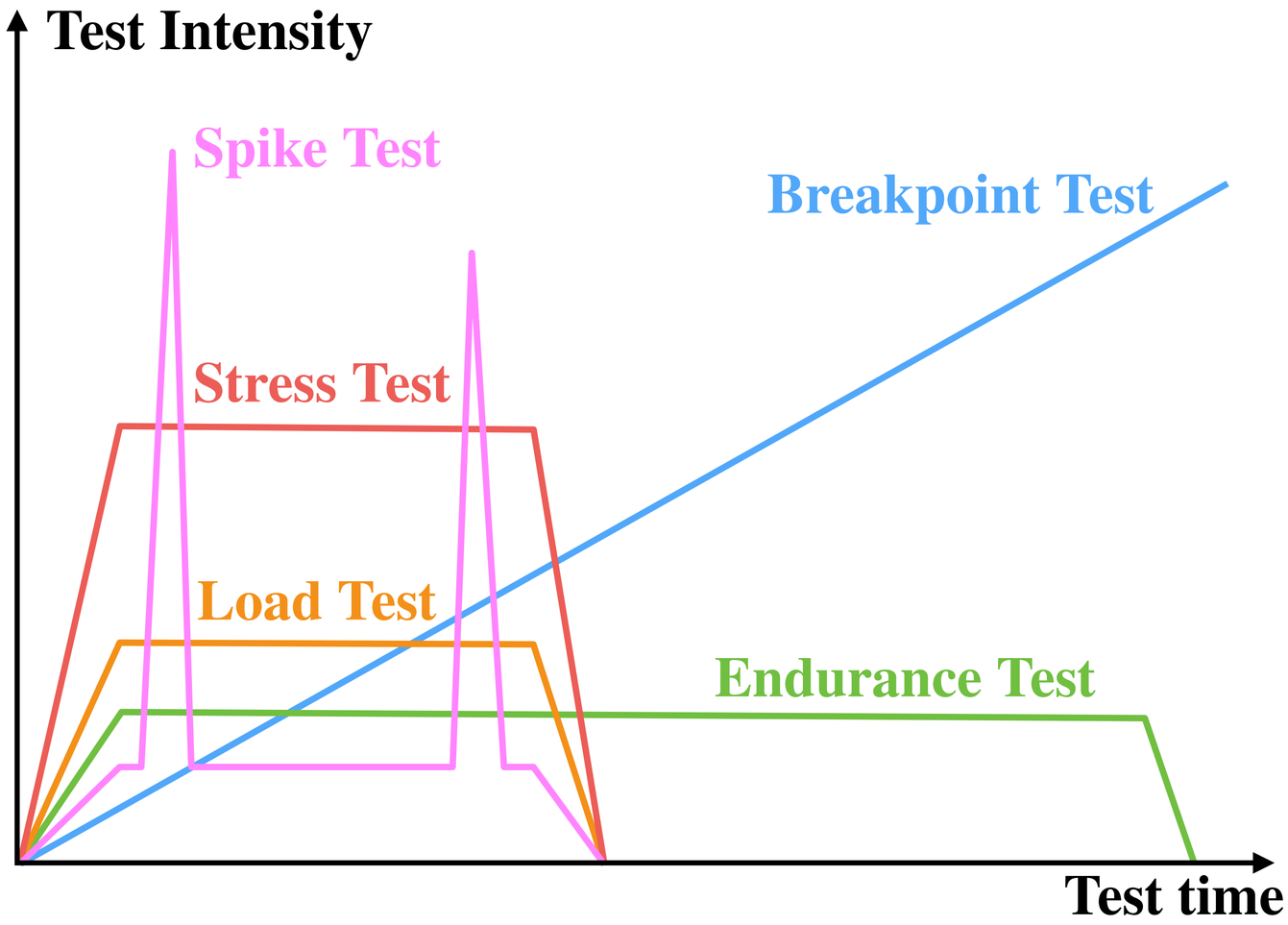
https://github.com/orbital-materials/orb-models

Matbench-Discovery

	F1 ↑	DAF ↑	Prec ↑	Acc ↑	TPR ↑	TNR ↑	MAE ↓	RMSE ↓	R^2 ↑	Training Set	Model Params	Targets	Date Added
ORB	0.867	6.020	0.920	0.961	0.819	0.987	0.031	0.079	0.816	3M (32.1M) (MPtrj+Alex)	25.2M	EFS	2024-09-02
MatterSim	0.859	5.646	0.863	0.957	0.856	0.975	0.026	0.080	0.812	17M (MatterSim)	182.0M	EFS	2024-06-16
GNoME	0.829	5.523	0.844	0.955	0.814	0.972	0.035	0.085	0.785	6M (89.0M) (GNoME)	16.2M	EF	2024-02-03
ORB-MPtrj	0.763	4.679	0.715	0.921	0.817	0.940	0.046	0.094	0.740	146K (1.6M) (MPtrj)	25.2M	EFS	2024-09-02
SevenNet	0.724	4.252	0.650	0.904	0.818	0.919	0.048	0.092	0.750	146K (1.6M) (MPtrj)	842.4K	EFS	2024-07-13
MACE	0.669	3.777	0.577	0.878	0.796	0.893	0.057	0.101	0.697	146K (1.6M) (MPtrj)	4.7M	EFS	2023-07-14
CHGNet	0.613	3.361	0.514	0.851	0.758	0.868	0.063	0.103	0.689	146K (1.6M) (MPtrj)	412.5K	EFSM	2023-03-03
M3GNet	0.569	2.882	0.441	0.813	0.803	0.813	0.075	0.118	0.585	63K (188.3K) (MPF)	227.5K	EFS	2022-09-20
ALIGNN	0.567	3.206	0.490	0.841	0.672	0.872	0.093	0.154	0.297	155K (MP 2022)	4.0M	E	2023-06-02
MEGNet	0.510	2.959	0.452	0.826	0.585	0.870	0.130	0.206	-0.248	133K (MP Graphs)	167.8K	E	2022-11-14
CGCNN	0.507	2.855	0.436	0.818	0.605	0.857	0.138	0.233	-0.603	155K (MP 2022)	128.4K (N=10)	E	2022-12-28
CGCNN+P	0.500	2.563	0.392	0.786	0.693	0.803	0.113	0.182	0.019	155K (MP 2022)	128.4K (N=10)	E	2023-02-03
Wrenformer	0.466	2.256	0.345	0.745	0.719	0.750	0.110	0.186	-0.018	155K (MP 2022)	5.2M (N=10)	E	2022-11-26
BOWSR	0.423	1.964	0.300	0.712	0.718	0.693	0.118	0.167	0.151	133K (MP Graphs)	167.8K	E	2022-11-17
Voronoi RF	0.333	1.579	0.241	0.668	0.535	0.692	0.148	0.212	-0.329	155K (MP 2022)	0.0	E	2022-11-26
Dummy	0.185	1	0.154	0.687	0.232	0.769	0.124	0.184	0				

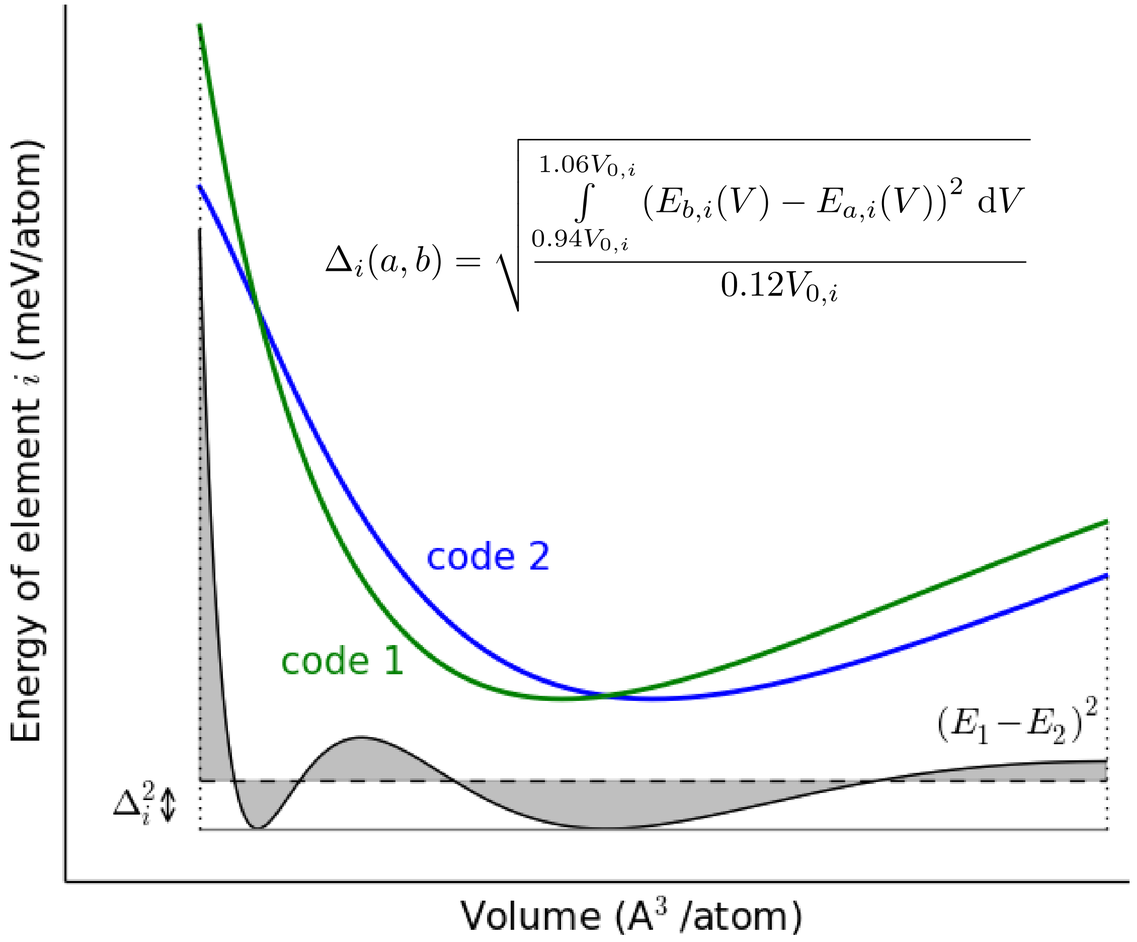
https://matbench-discovery.materialsproject.org/

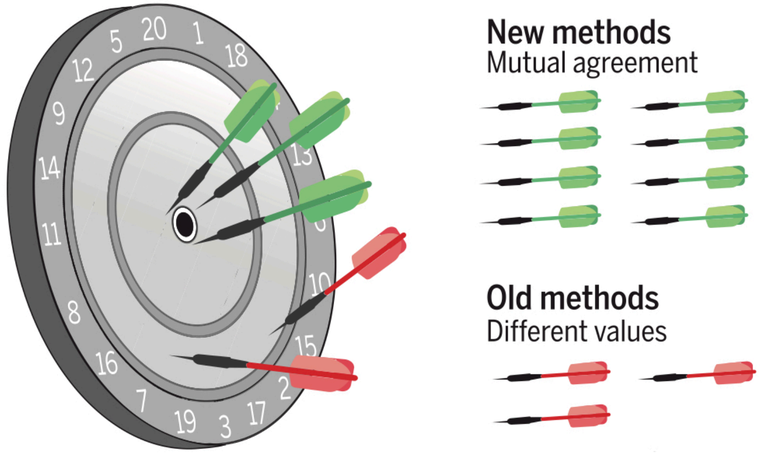
There clearly was a need for some assessment...



Test #1: Equation of state

- Validation against all-electron results for elemental crystals





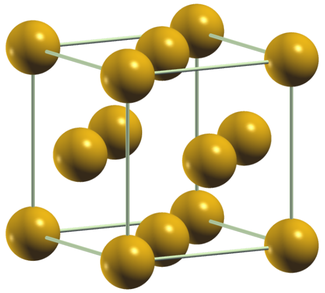
Scorecard

	0.3	0.3	0.6	1.0	0.9	0.3
0.3		0.1	0.5	0.9	0.8	0.2
0.3	0.1		0.5	0.9	0.8	0.2
0.6	0.5	0.5		0.8	0.6	0.4
1.0	0.9	0.9	0.8		0.9	0.9
0.9	0.8	0.8	0.6	0.9		0.8
0.3	0.2	0.2	0.4	0.9	0.8	

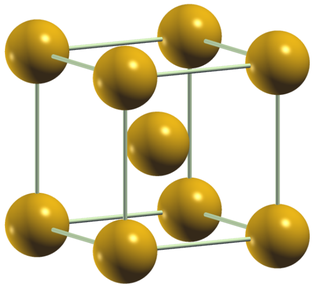
[K. Lejaeghere *et al.*, Science **351**, aad3000 (2016)]

Test #1: Equation of state

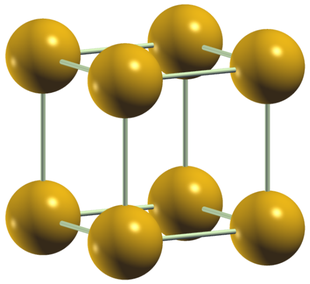
- Validation against all-electron results for 4 elemental and 6 oxide crystals



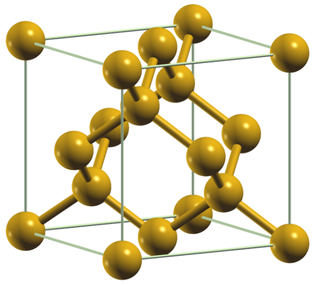
(a) FCC crystal (conventional cell).



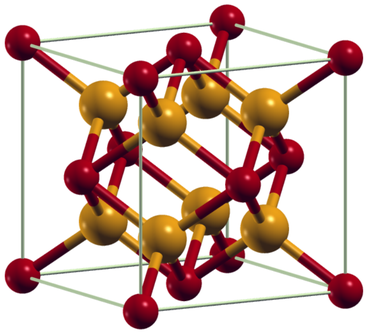
(b) BCC crystal (conventional cell).



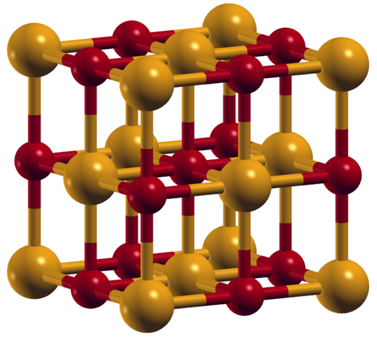
(c) SC crystal (conventional cell).



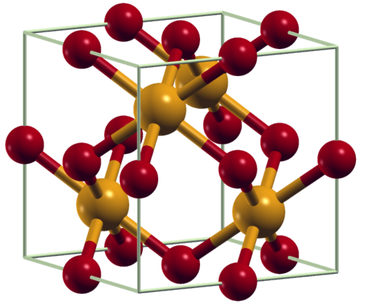
(d) Diamond crystal (conventional cell).



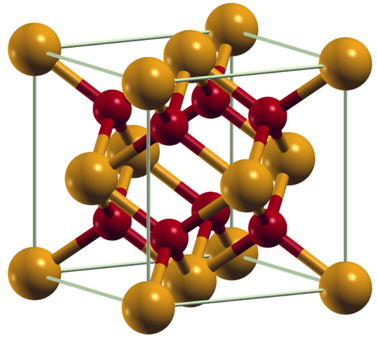
(a) X_2O crystal (conventional cell).



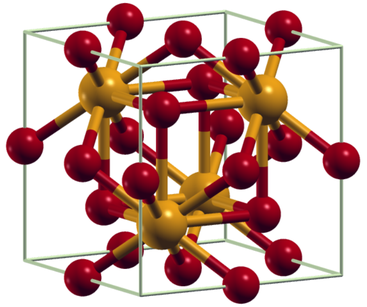
(b) XO crystal (conventional cell).



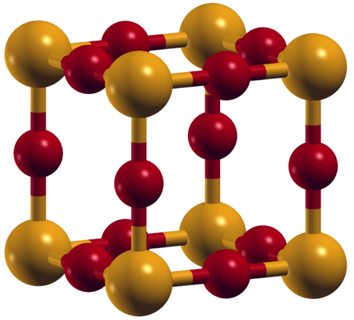
(c) X_2O_3 crystal (conventional cell).



(d) XO_2 crystal (conventional cell).



(e) X_2O_5 crystal (conventional cell).



(f) XO_3 crystal (conventional cell).

[E. Bosoni *et al.*, Nat. Rev. Phys. **6**, 45 (2024)]

Test #1: Equation of state

- Validation against all-electron results for 4 elemental and 6 oxide crystals
- With 2 new metrics:
  - a revised version of the Δ-factor

$$\epsilon(a,b) = \frac{\sum_i \left[E_a(V_i) - E_b(V_i)\right]^2}{\sqrt{\sum_i \left[E_a(V_i) - \left\langle E_a \right\rangle\right]^2 \sum_i \left[E_b(V_i) - \left\langle E_b \right\rangle\right]^2}}$$

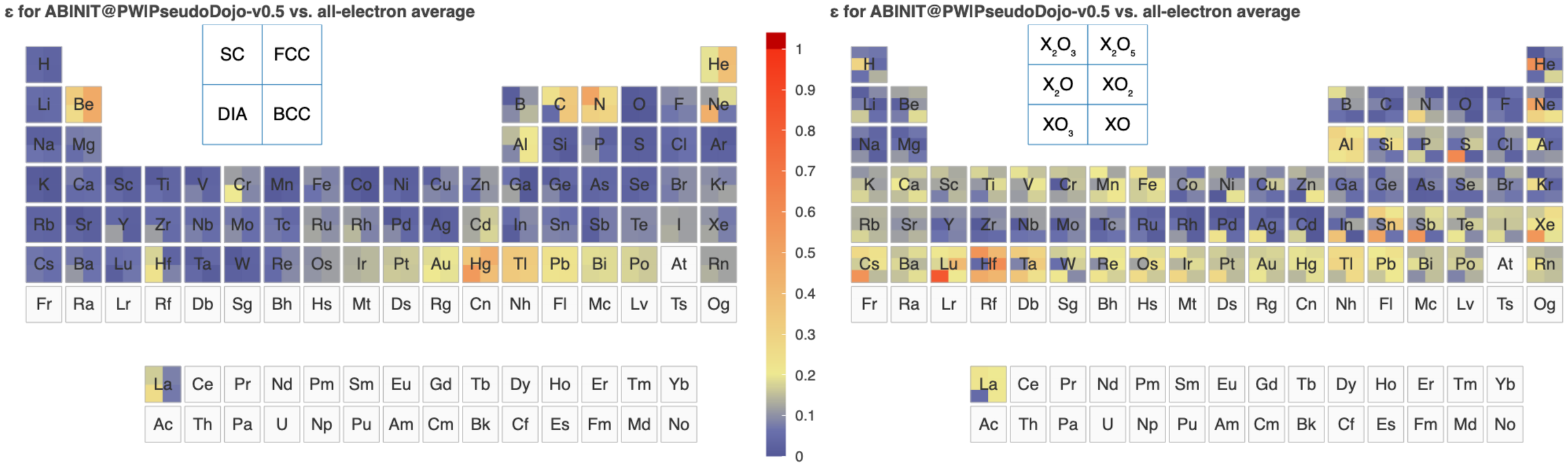
  - a metric dependent on the physically measurable quantities V_0, B_0, and B_1

$$\nu_{w_{V_0},w_{B_0},w_{B_1}}(a,b) = 100 \sqrt{\sum_{Y=V_0,B_0,B_1} \left[w_Y \frac{Y_a - Y_b}{(Y_a + Y_b)/2} \right]^2}$$

[E. Bosoni *et al.*, Nat. Rev. Phys. **6**, 45 (2024)]

Test #1: Equation of state

- Validation against all-electron results for 4 elemental and 6 oxide crystals



[E. Bosoni *et al.*, Nat. Rev. Phys. **6**, 45 (2024)]

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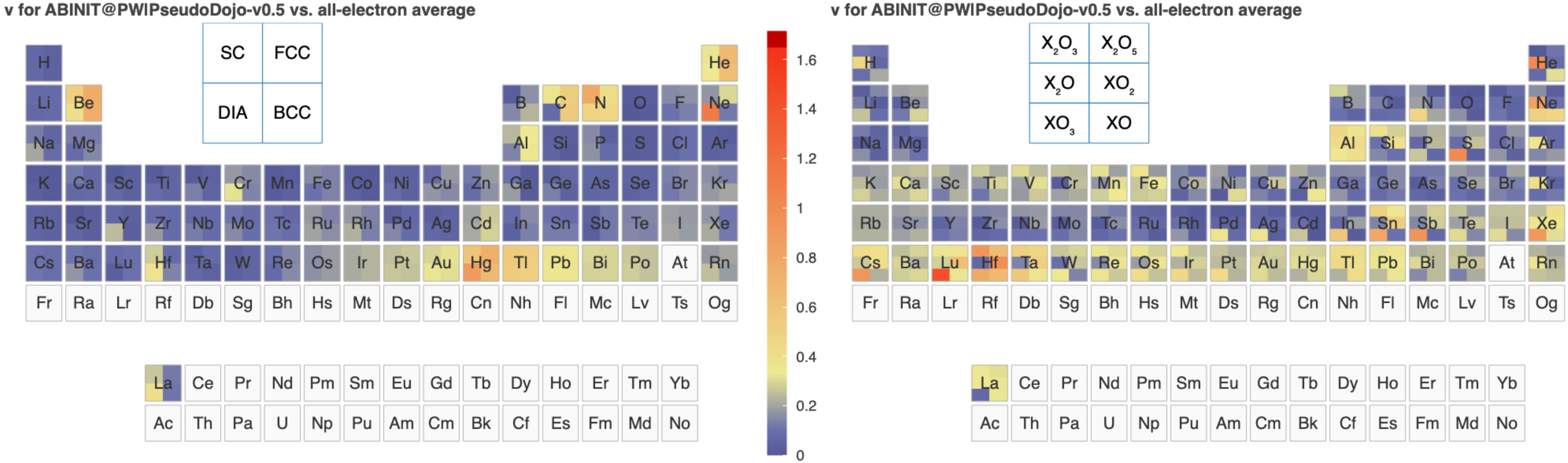
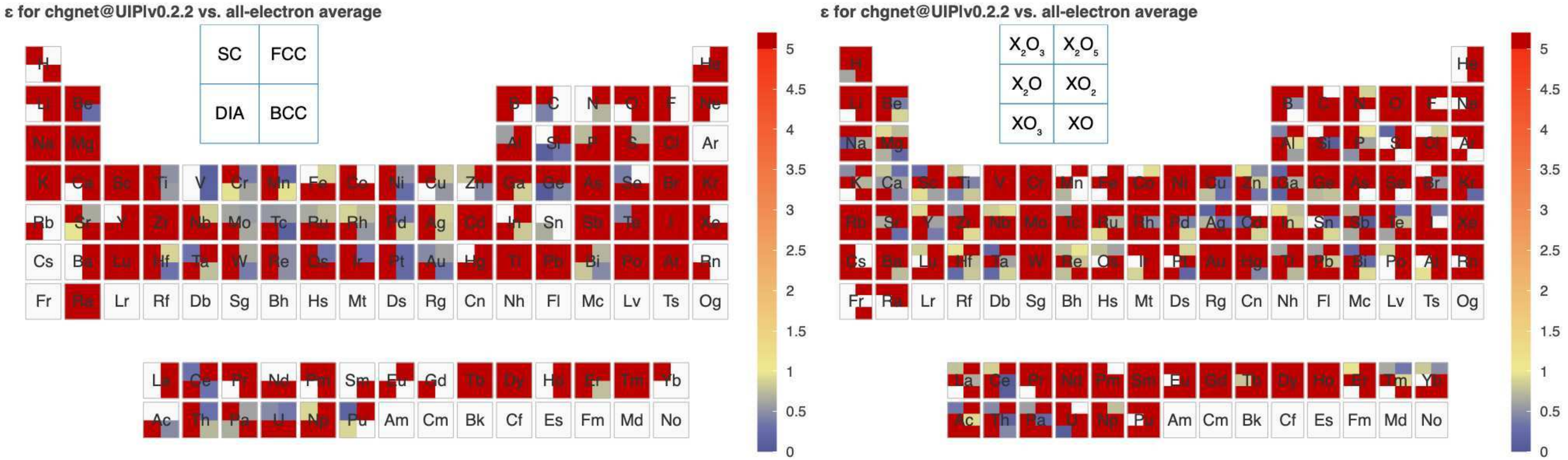


[E. Bosoni *et al.*, Nat. Rev. Phys. **6**, 45 (2024)]

Test #1: Equation of state

- The results for uMLIPs are not fantastic!



[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

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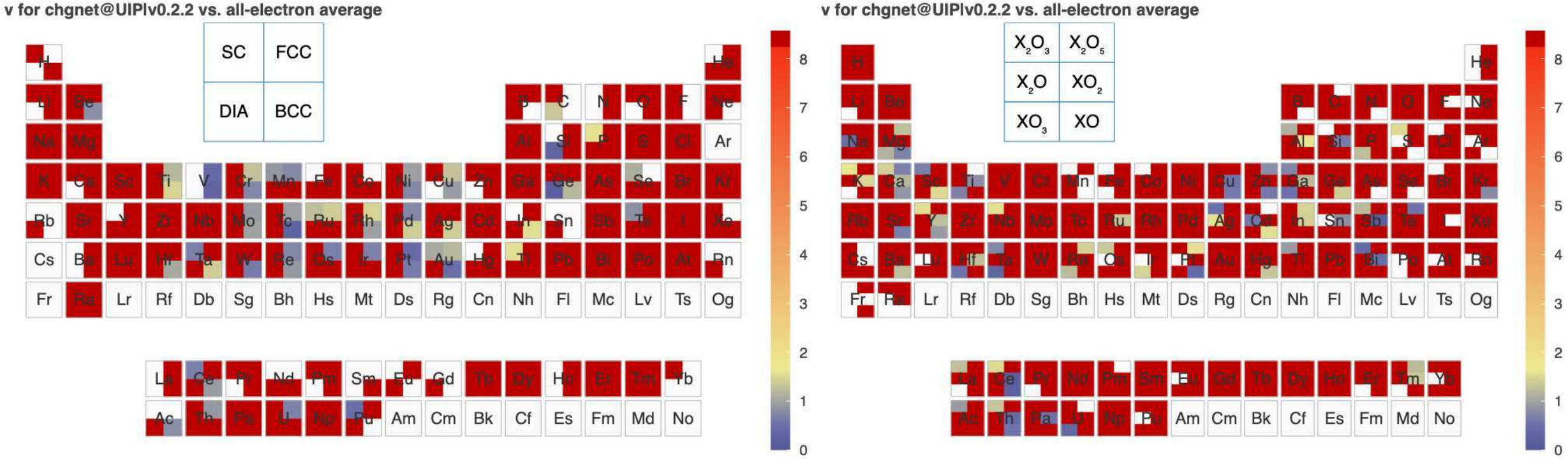

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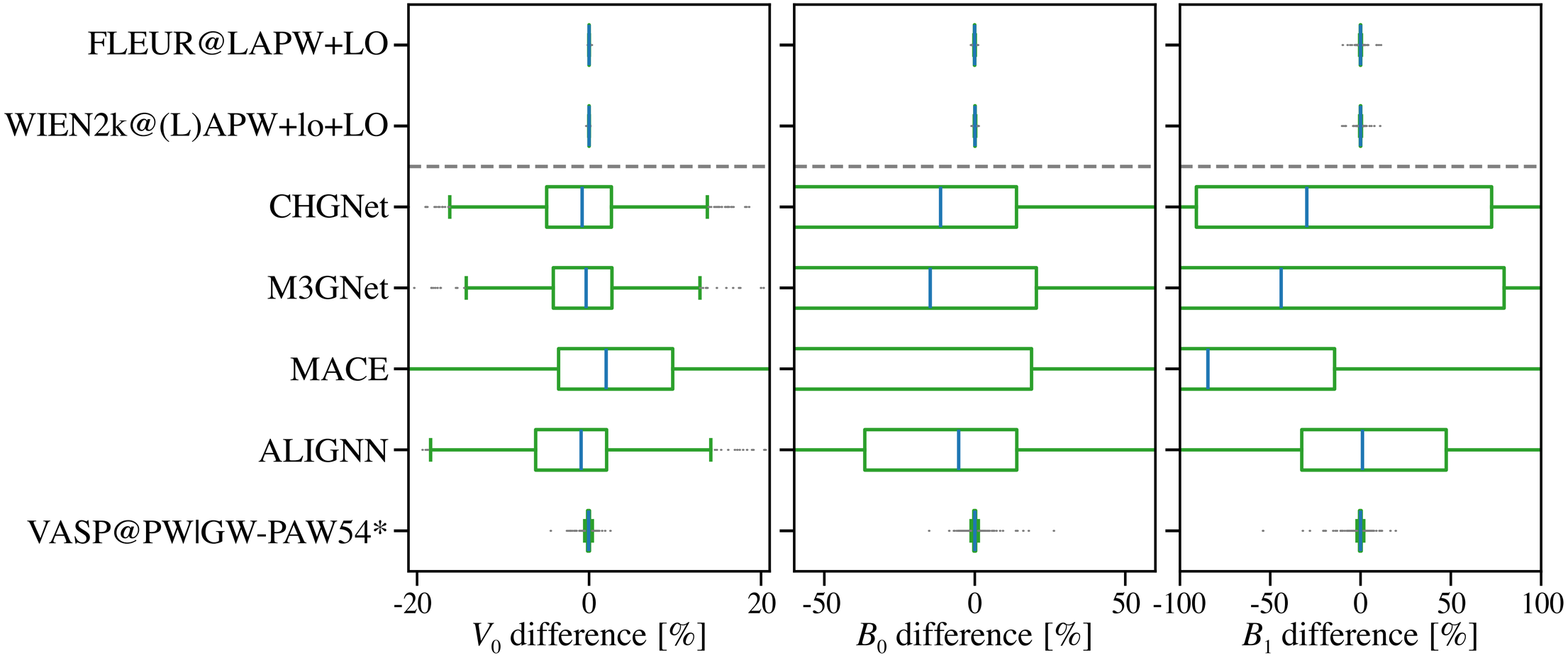


[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

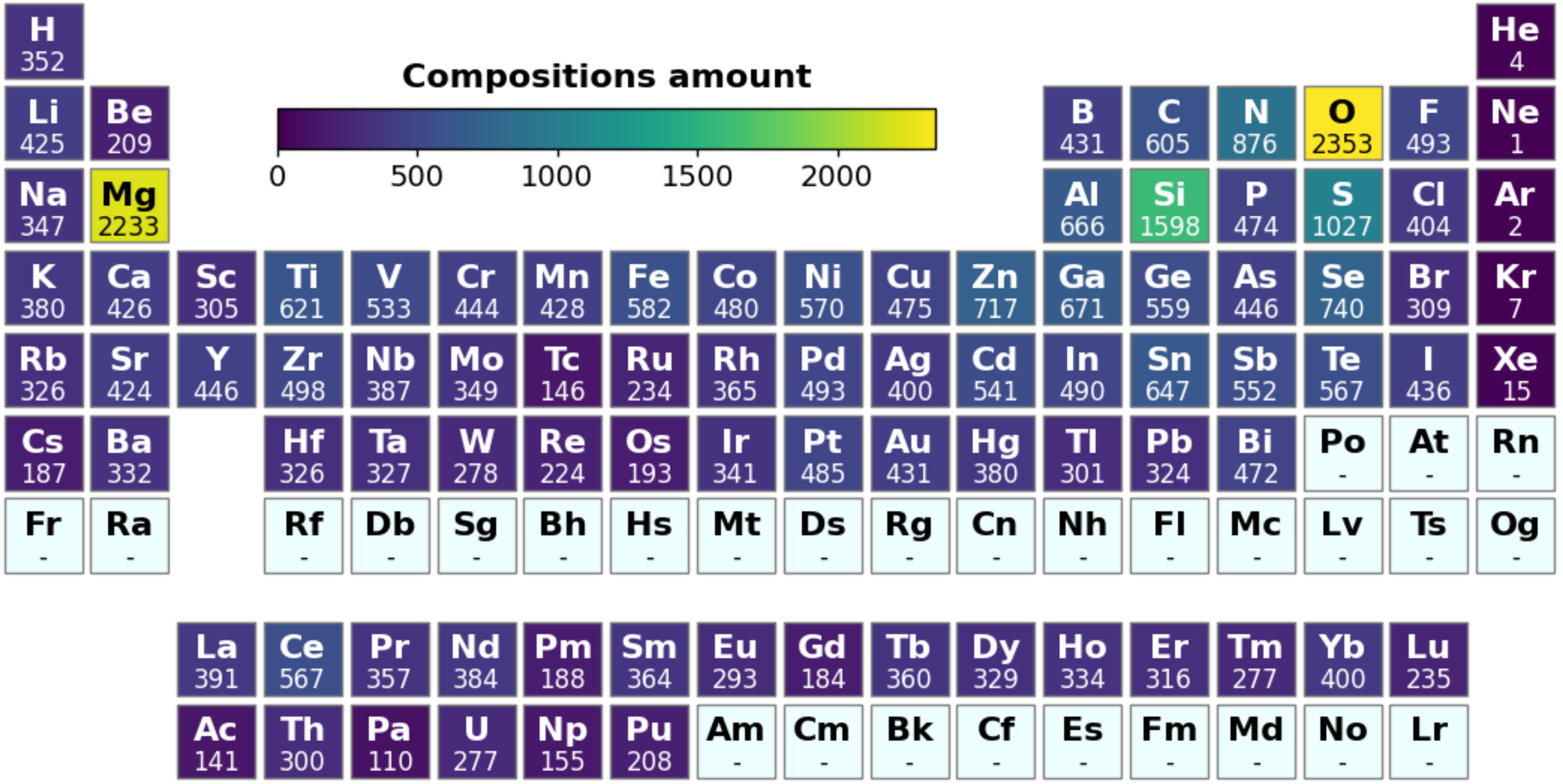
Test #1: Equation of state

- The results for uMLIPs are not fantastic!
- However, most structures in the dataset are not stable in nature...
- This is a very stringent test for uMLIPs. But it indicates that:
  - their predictions should be taken with some caution and, if possible, validated a posteriori via *ab initio* calculations
  - it might be appropriate to retrain them by including additional *ab initio* data capturing the chemical/physical configurations under investigation

[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

Test #2: Structural optimization and formation energy

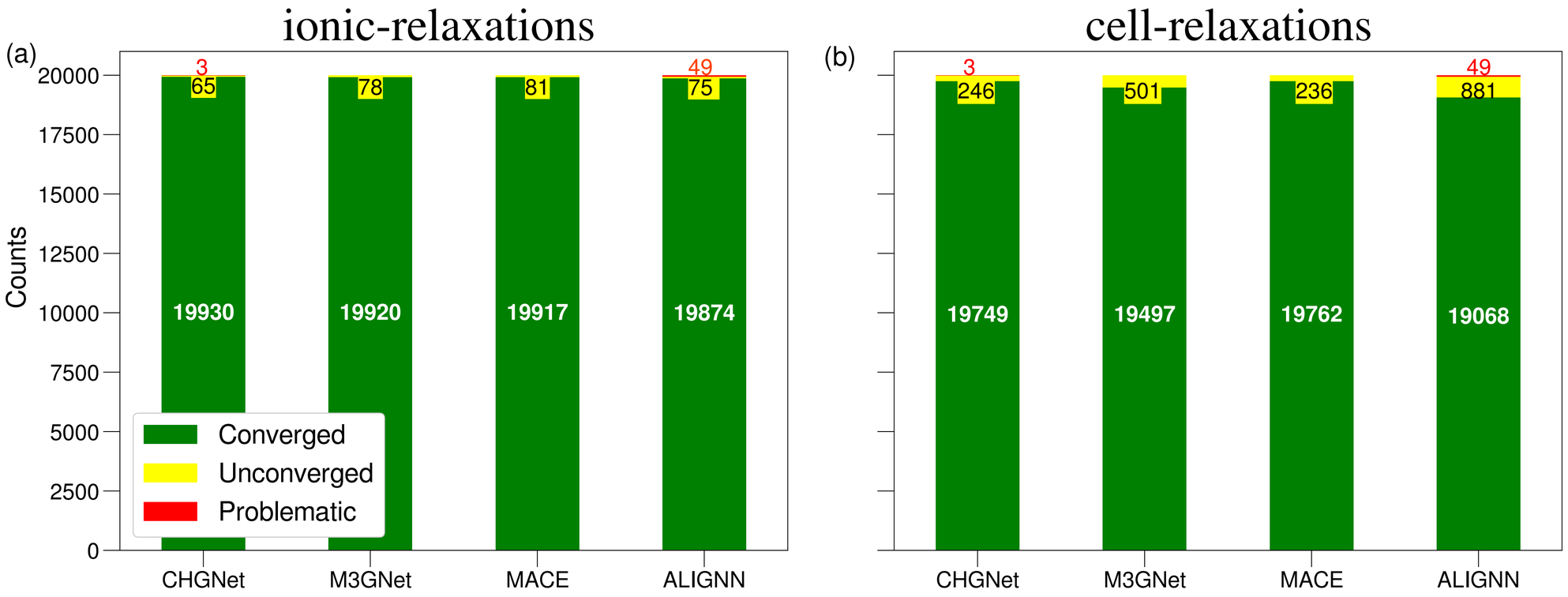
- Dataset #1 from the Materials Project (19998 unary and binary compounds)



[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

Test #2: Structural optimization and formation energy

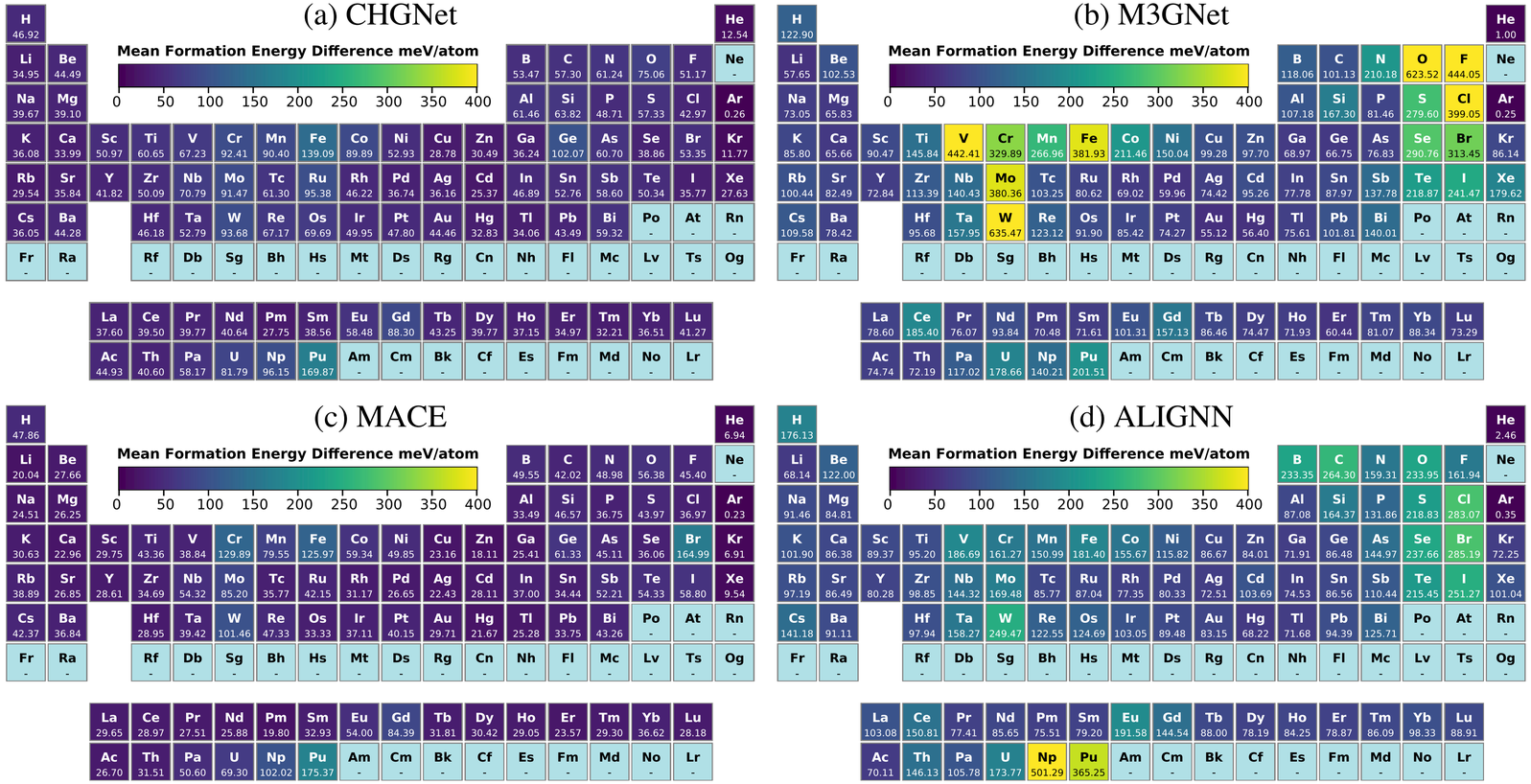
- Dataset #1 from the Materials Project (19998 unary and binary compounds)
  - one-shot calculations of the energy (without any relaxation)
  - ionic- and cell-relaxations



[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

Test #2: Structural optimization and formation energy

- Dataset #1 from the Materials Project (19998 unary and binary compounds)
- We compute $E_{\text{form}}[A_aB_b] = E[A_aB_b] - x_aE[A] - x_bE[B]$ with one-shot energies



$$\Delta E_{\text{form}} = E^{\text{MP}}_{\text{form}} - E^{\text{uMLIP}}_{\text{form}}$$

[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

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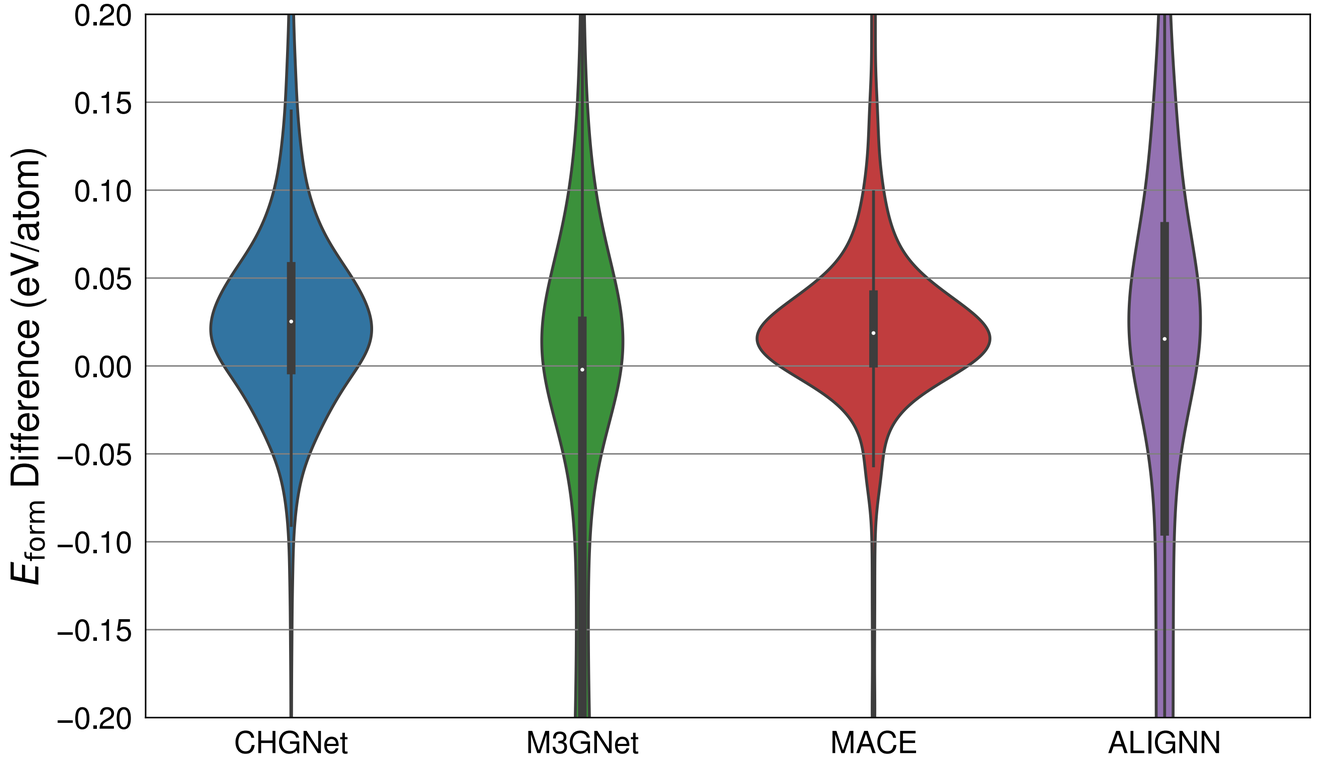


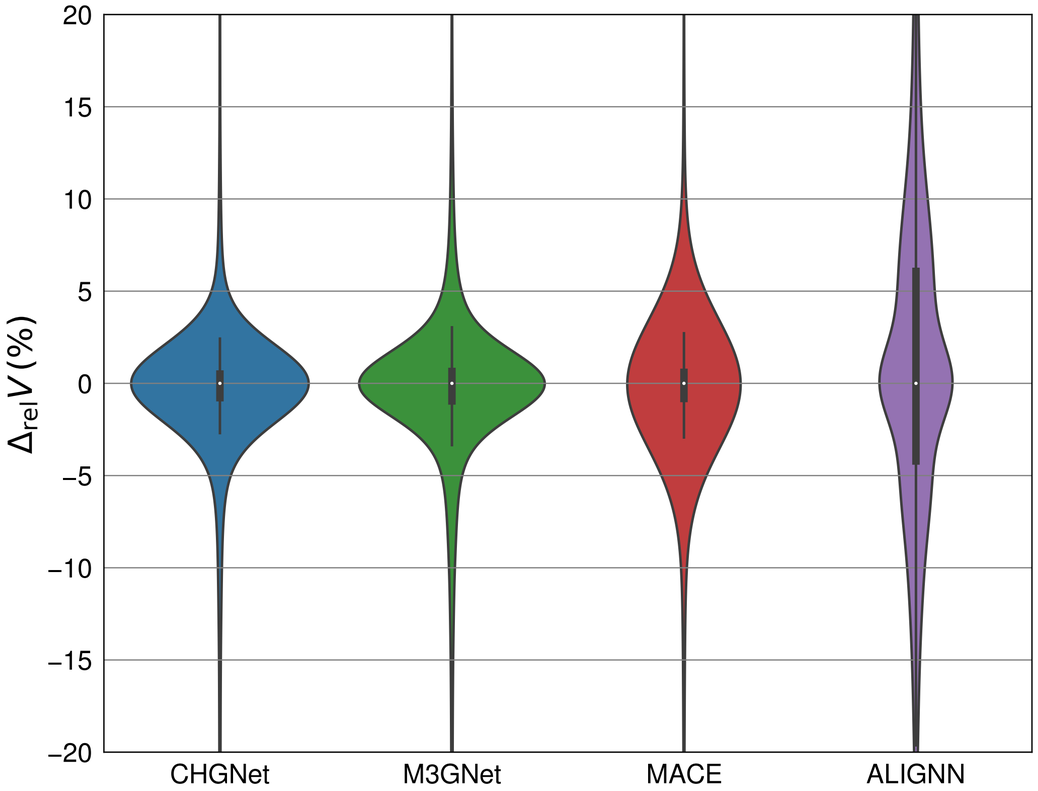
$$\Delta E_{\text{form}} = E_{\text{form}}^{\text{MP}} - E_{\text{form}}^{\text{uMLIP}}$$

uMLIP	MAE	RMSE	R^2
CHGNet	0.054	0.105	0.988
M3GNet	0.172	0.316	0.896
MACE	0.044	0.101	0.989
ALIGNN	0.137	0.223	0.947

[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

Test #2: Structural optimization and formation energy

- Dataset #1 from the Materials Project (19998 unary and binary compounds)
- We compute $\Delta_{\mathrm{rel}} V = 1 - \dfrac{V^{\mathrm{uMLIP}}}{V^{\mathrm{MP}}}$ for the cell-relaxations



MARE (%)

uMLIP	V	a	b	c	α	β	γ
CHGNet	3.16	2.03	2.07	2.44	0.75	0.62	1.19
M3GNet	2.97	2.04	2.09	2.46	0.89	0.73	1.24
MACE	5.22	2.01	2.11	2.58	0.73	0.59	1.13
ALIGNN	7.85	3.42	3.42	3.61	0.94	0.86	1.32

[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

Test #2: Structural optimization and formation energy

- Dataset #2 from the Materials Project (100 randomly chosen quinary materials)
- We perform one-shot and cell-relaxations calculations:
  - 4 unconverged cases (4%) for CHGNet and M3GNet
  - 2 unconverged cases (2%) for MACE and ALIGNN

$$\Delta E_{\text{form}} = E_{\text{form}}^{\text{MP}} - E_{\text{form}}^{\text{uMLIP}}$$

uMLIP	MAE	RMSE	R^2
CHGNet	0.048	0.062	0.995
M3GNet	0.462	0.505	0.678
MACE	0.038	0.054	0.996
ALIGNN	0.157	0.185	0.957

MARE (%)

uMLIP	V	a	b	c	α	β	γ
CHGNet	1.76	1.21	1.12	1.01	0.61	0.31	0.47
M3GNet	3.21	1.15	1.74	1.66	1.63	0.60	0.95
MACE	5.49	1.54	2.57	2.69	1.46	0.48	0.61
ALIGNN	3.74	3.42	3.42	3.61	0.94	0.86	1.32

[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

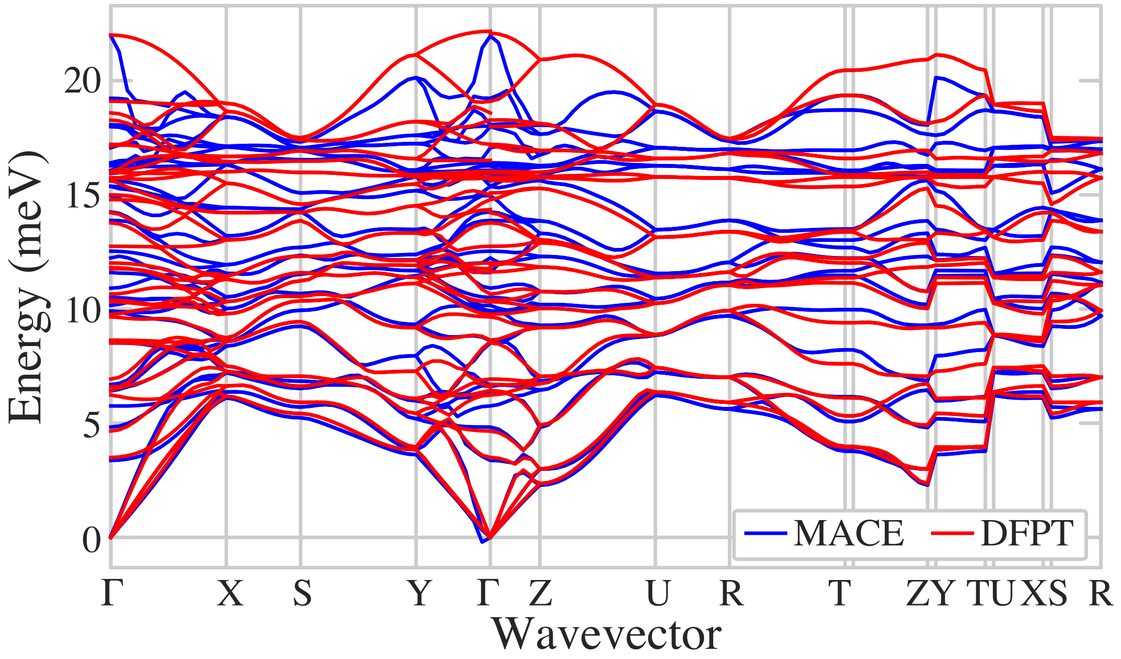
Test #3: Phonon band structures

- Dataset #3 from the Materials Project (101 structures with DFPT phonons)

$$\mathrm{MAE} = \frac{1}{N_{\mathbf{q}}} \sum_{\mathbf{q}\nu} \left| \omega_{\mathbf{q}\nu}^{\mathrm{uMLIP}} - \omega_{\mathbf{q}\nu}^{\mathrm{DFPT}} \right|$$

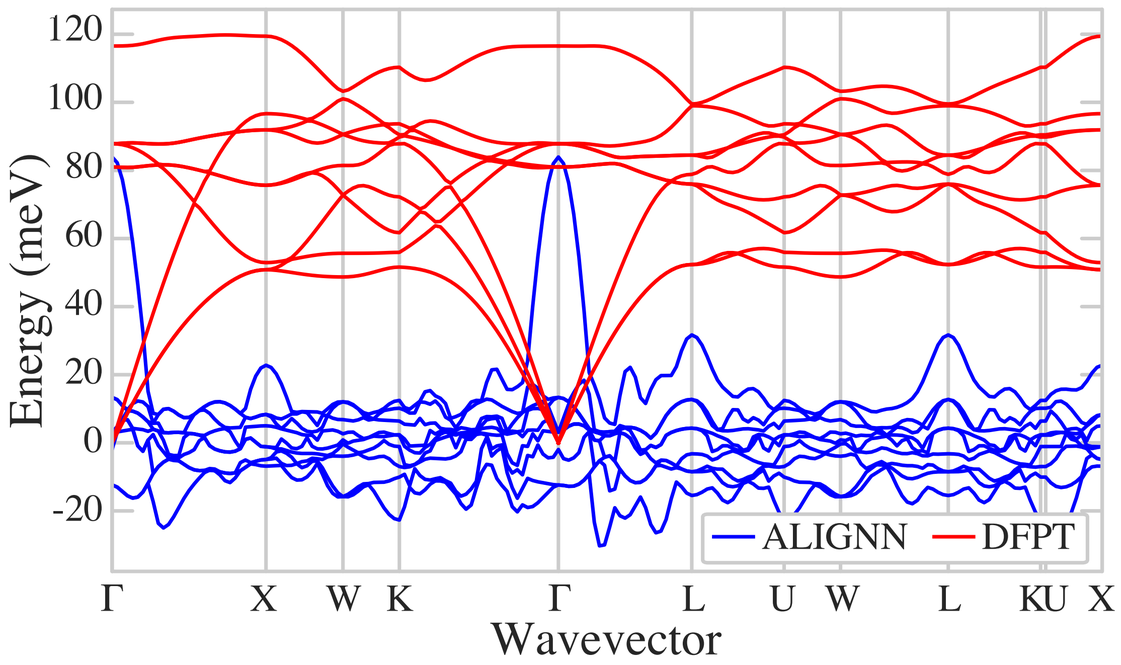
Best result (MAE = 0.3 meV)

MACE for the compound (mp-567744: $SrBr_2$)



Worst result (MAE = 75.4 meV)

ALIGNN for the compound (mp-1569: Be_2C)



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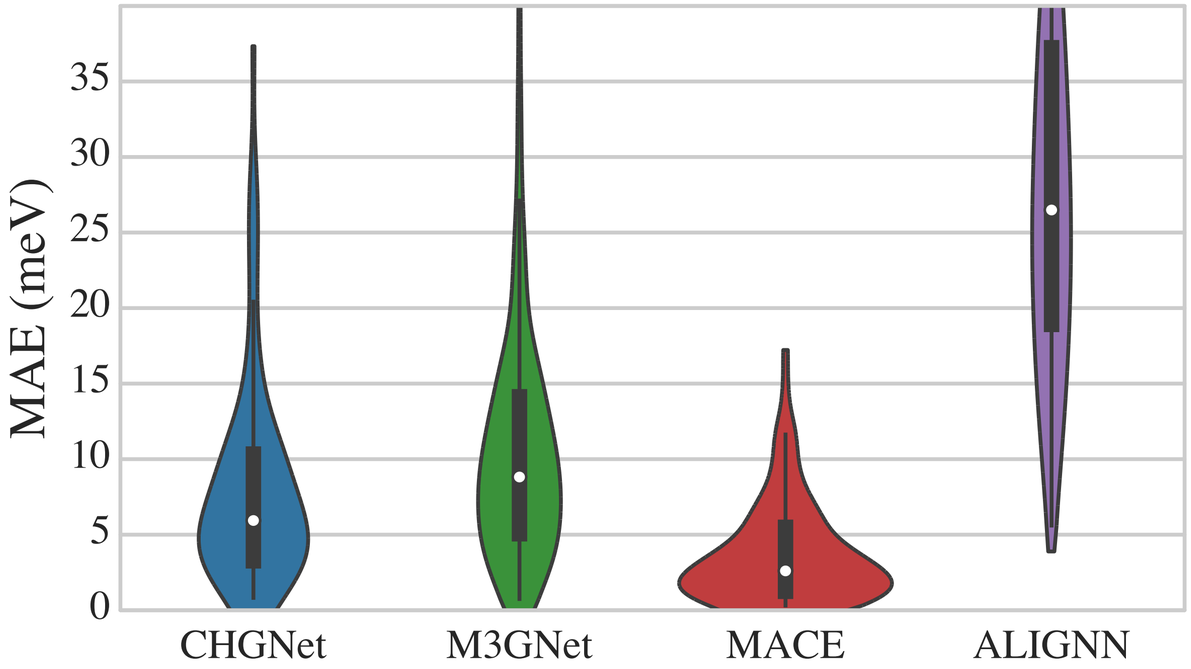


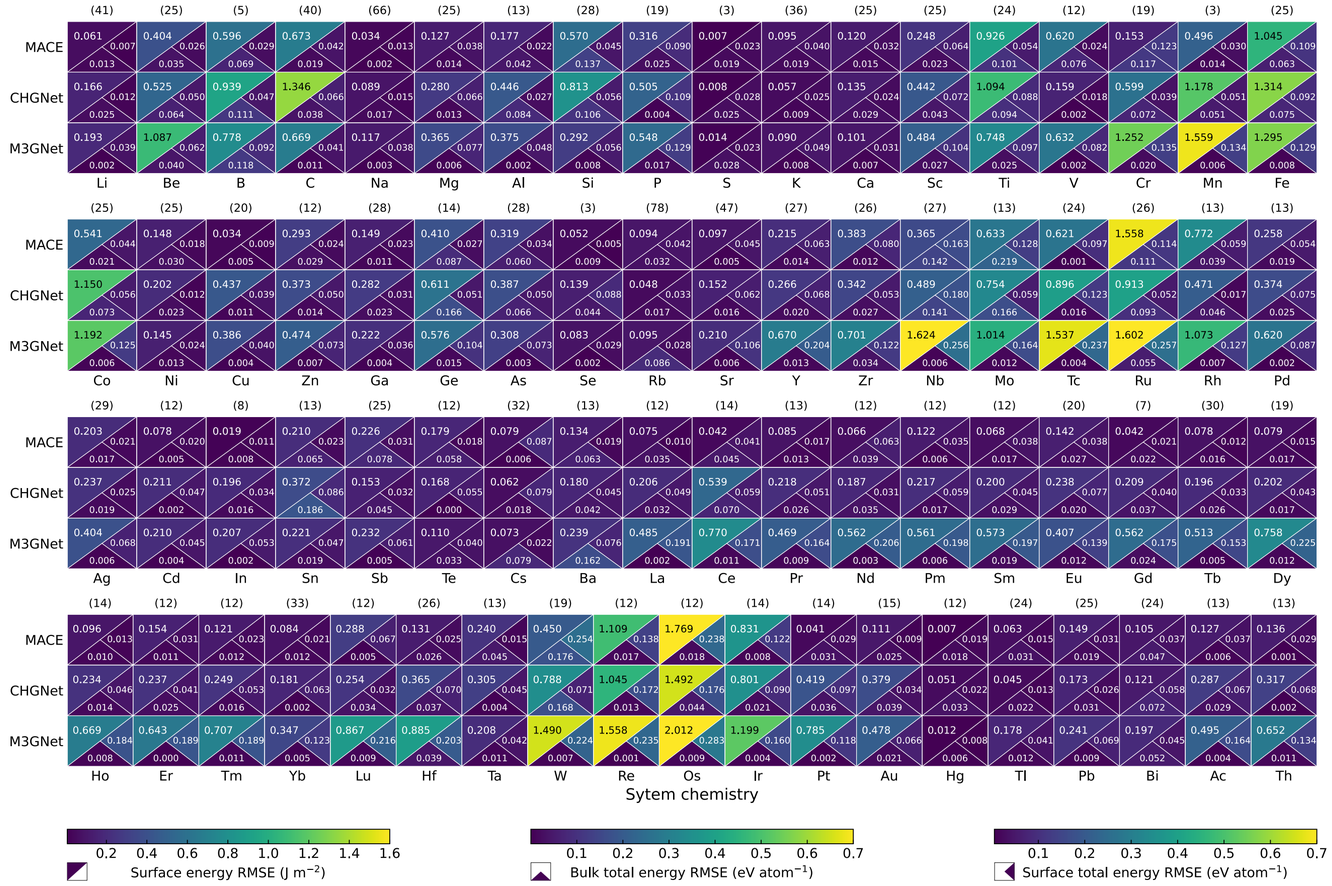
$$\mathrm{MAE} = \frac{1}{N_{\mathbf{q}}} \sum_{\mathbf{q}\nu} \left| \omega_{\mathbf{q}\nu}^{\mathrm{uMLIP}} - \omega_{\mathbf{q}\nu}^{\mathrm{DFPT}} \right|$$

uMLIP	min	max	mean
CHGNet	0.82	37.34	8.12
M3GNet	0.74	40.20	10.41
MACE	0.31	17.22	3.71
ALIGNN	5.60	75.38	29.36

[H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]

Test #4: Surface energy

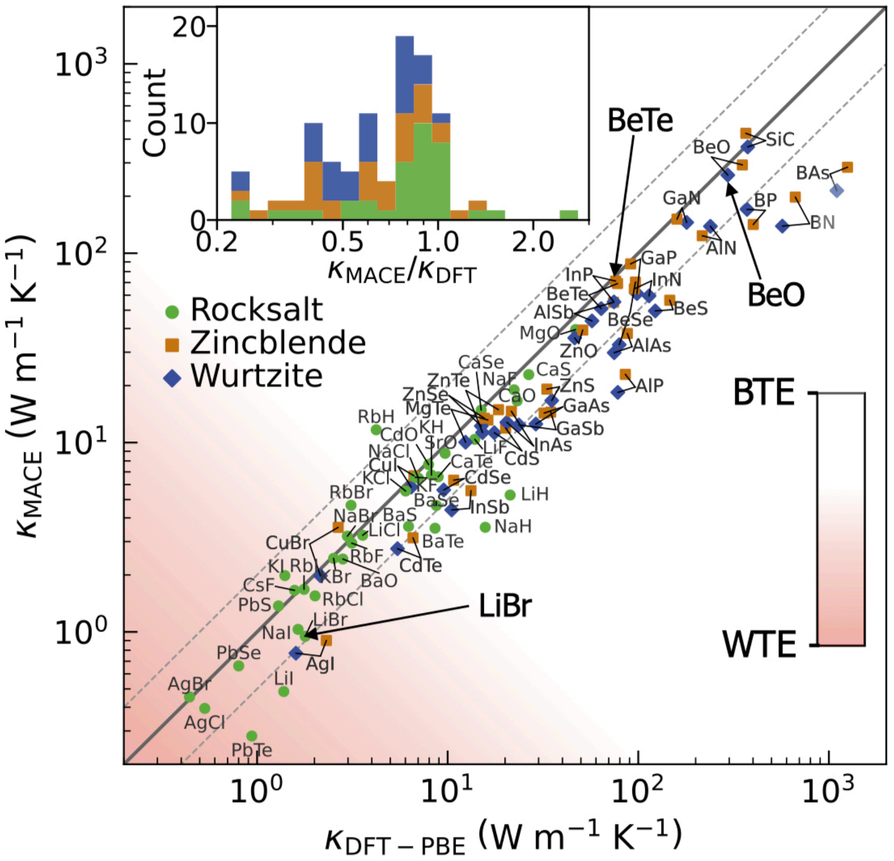
- Dataset #4 from the Materials Project (1497 different surface structures were generated from 138 different bulk systems, 73 different chemical elements)

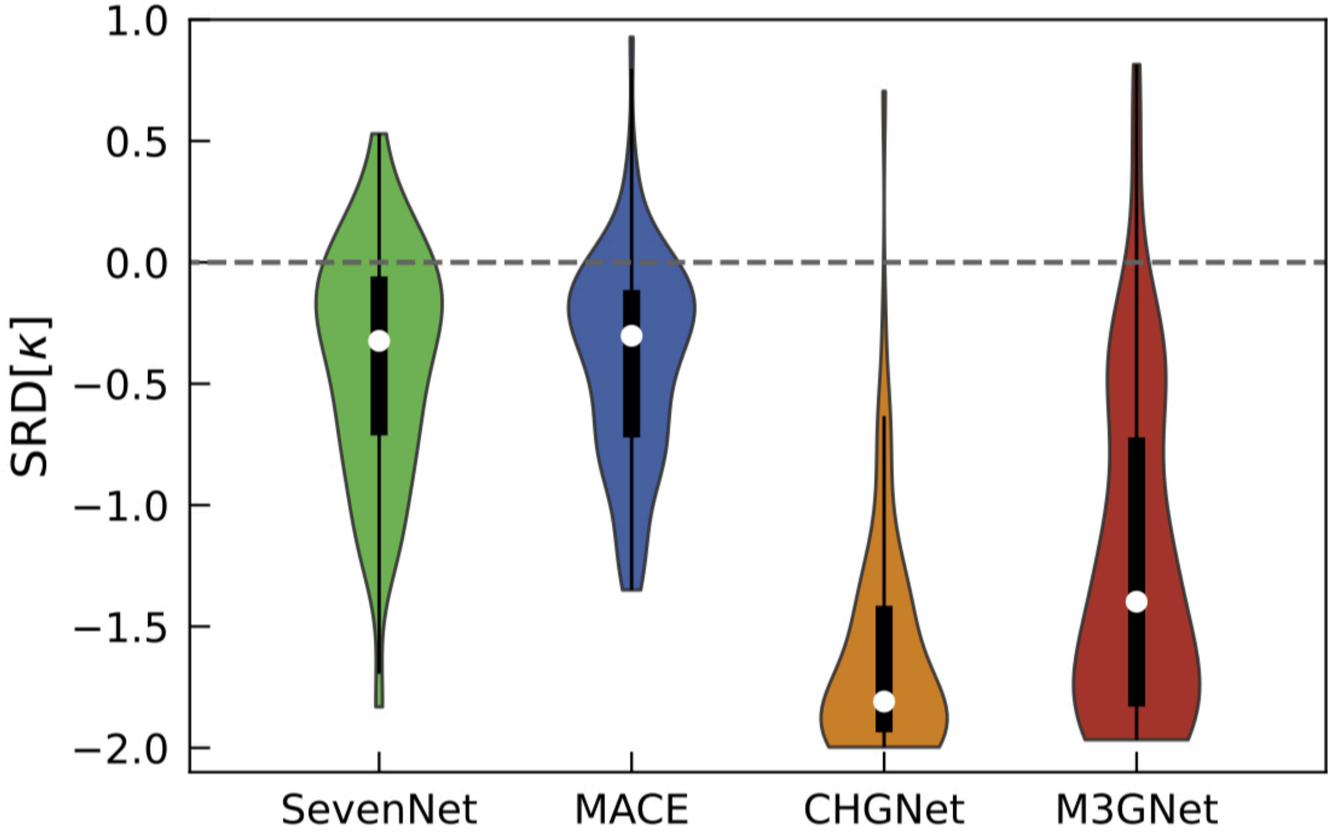


[B. Focassio *et al.*, ACS Appl. Mater. Interfaces (2024)]

Test #5: Thermal conductivity

$$\mathrm{SRD}[\kappa] = 2\frac{\kappa^{\mathrm{uMLIP}} - \kappa^{\mathrm{DFT}}}{\kappa^{\mathrm{uMLIP}} + \kappa^{\mathrm{DFT}}}$$





Note: They show how to achieve first-principles accuracy through foundational model fine-tuning

[B. Póta *et al.*, arXiv:2408.00755v3]

Main conclusions of the tests

- "Among the considered uMLIPs, we find that MACE shows superior accuracy in predicting formation energies and vibrational properties, and CHGNet and M3GNet are outstanding for relaxed geometry predictions."
  [H. Yu *et al.*, MGE Adv. **2**, e58 (2024)]
- "From our results for surface energies, we see that the total energies for surface geometries are modestly accurate, however, not good enough for specific properties."
  [B. Focassio *et al.*, ACS Appl. Mater. Interfaces (2024)]
- There is still a need for further optimization and training of the currently available uMLIPs to fully exploit the capability of ML techniques across a broader range of applications.

Possible use cases

- Sampling of the potential energy surface
- Accelerating *ab initio* relaxations

PHYSICAL REVIEW B **89**, 144110 (2014)

Approximate Hessian for accelerating *ab initio* structure relaxation by force fitting

Zhanghui Chen, Jingbo Li,* and Shushen Li
State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, People's Republic of China

Linwang Wang†
Materials Sciences Division, Lawrence Berkeley National Laboratory, One Cyclotron Road, Mail Stop 50F, Berkeley, California 94720, USA
(Received 28 February 2014; revised manuscript received 8 April 2014; published 22 April 2014)

We present a method to approximate the Hessian matrix of the Born-Oppenheimer energy landscape by using a simple force field model whose parameters are fitted to on-the-flight *ab-initio* results. The inversed Hessian matrix is used as the preconditioner of conjugate gradient algorithms to speed up the atomic structure relaxation, resulting in a speedup factor of 2 to 5 on systems of bulk, slab, sheets, and atomic clusters. Because the force field model employed is simple and general, the parameter fitting is straightforward; the method is applicable to a variety of complicated systems for minimum structure relaxation. In the metal cluster new structure search, the new method yields better structures than the one obtained before with conventional algorithms.

DOI: 10.1103/PhysRevB.89.144110 PACS number(s): 71.15.−m, 31.15.A−

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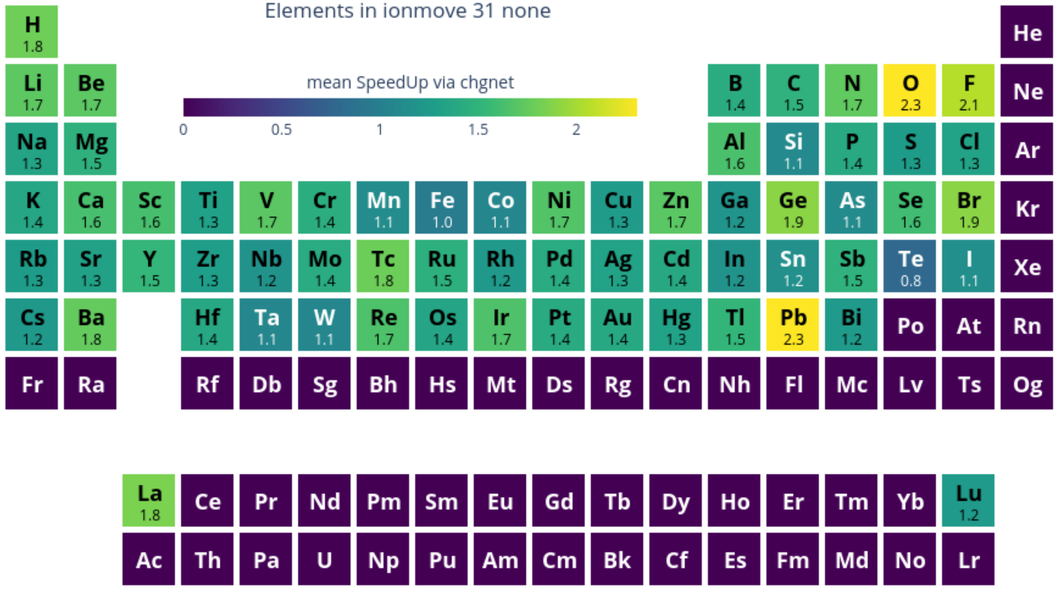
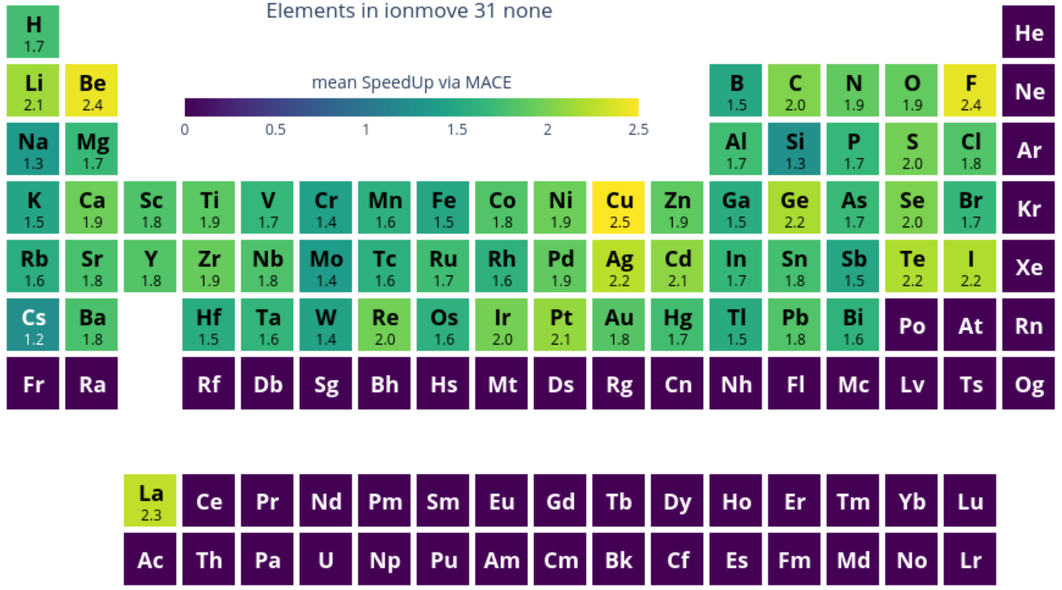
ionic-relaxations with CHGNet



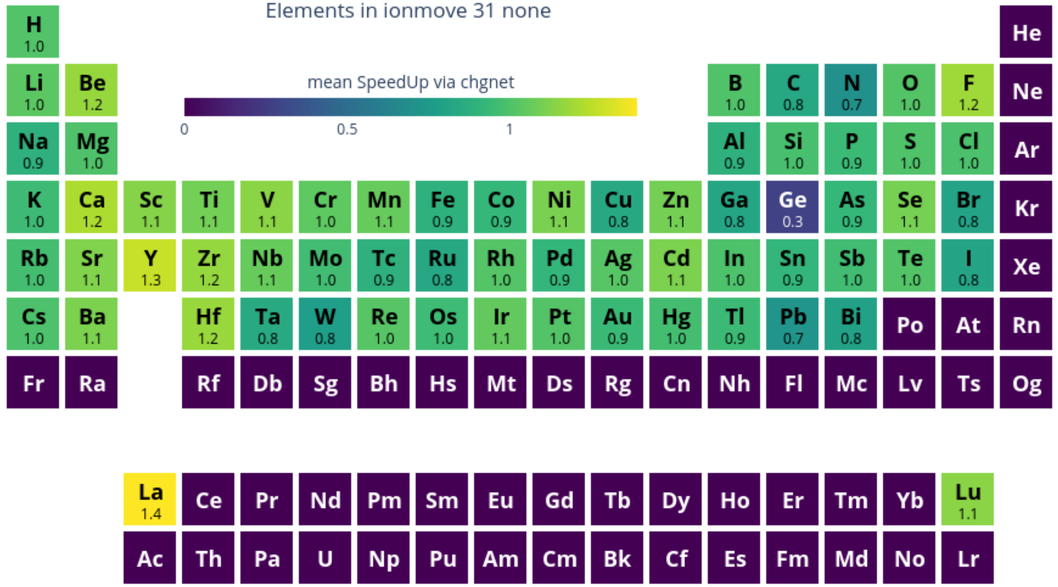
ionic-relaxations with MACE



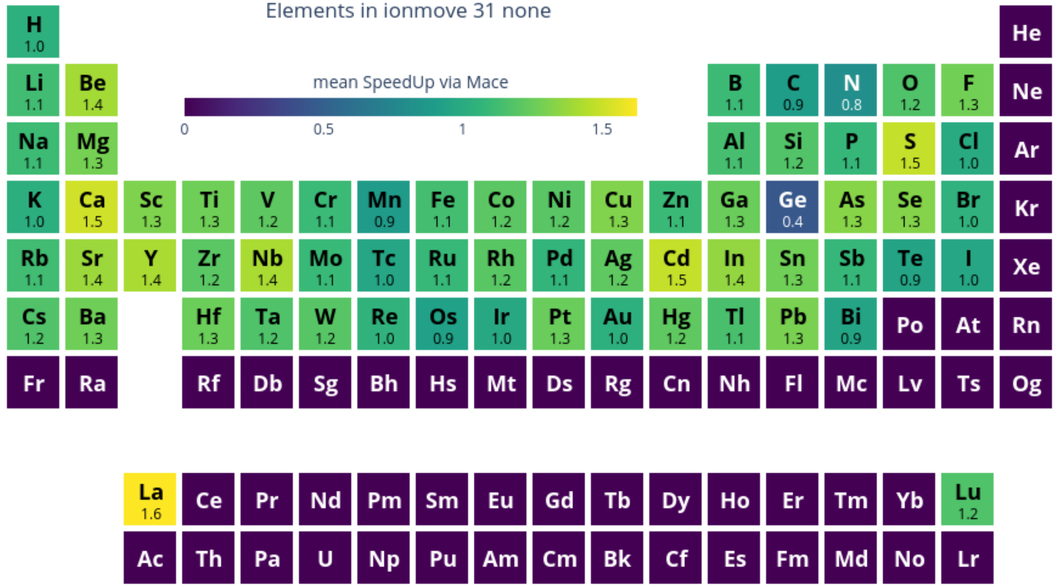
Possible use cases

- Sampling of the potential energy surface
- Accelerating *ab initio* relaxations

cell-relaxations with CHGNet



cell-relaxations with MACE

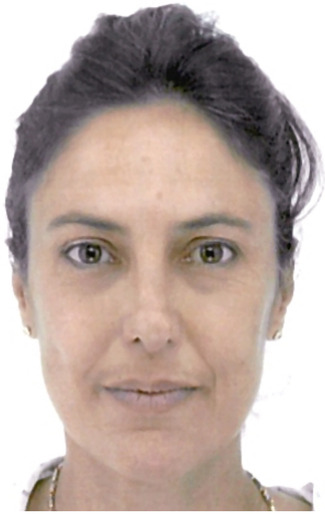


uMLIPs clearly show significant interest but further improvement is still needed

- Many thanks to my collaborators:

Haochen Yu

Matteo Giantomassi



Giuliana Materzanini

Junjie Wang

- Thank you for your attention