# Systematic assessment of various universal machine-learning interatomic potentials

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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

Accuracy





**MLIPs** 

ab initio

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)]





[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 🕜	
372	

Property Instances 🚱 513,959,850

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





# More generally sharing datasets is very useful...



Materials Project Trajectory Dataset He Ne B C S Si Ar A P Zn Ge Se Br Kr Ni Cu Ga Co As Cd Sb Rh Pd Ag Sn Те Xe In Pb Bi Pt Hg Au Tb Eu Gd Dy Er Ho Tm Yb Lu

Magmom	Force	Stress
7,944,833	49,295,660	14,223,555
0.336 µ <sub>B</sub>	0.158 eV Å <sup>-1</sup>	7.553 GPa



10<sup>6</sup>



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





[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	$\mathbf{N}_1$	$N_2$	$N_3$	N <sub>tot</sub>
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	<b>4,451,056</b> (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	<mark>58,718</mark> (58,718)	<mark>690</mark> (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)	<b>296</b> (296)	<mark>662</mark> (660)	2,922
2DMatpedia	1,172	739	255	6,351

# Then, universal MLIPs started to appear...





#### nature computational science

Article

# A universal graph deep learning interatomic potential for the periodic table

Received: 18 March 2022

Chi Chen 🕲 🖂 & Shyue Ping Ong 🕲 🖂

Accepted: 5 October 2022

#### npj | computational materials

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

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

Ji Qi 🖸 <sup>1,2</sup> 🖂, Tsz Wai Ko 🕲 <sup>3</sup>, Brandon C. Wood<sup>2,4</sup>, Tuan Anh Pham<sup>2,4</sup> 🖂 & Shyue Ping Ong 🕲 <sup>1,3</sup> 🖂

https://github.com/materialsvirtuallab/m3gnet

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



Article

0

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





# **CHGNet (Crystal Hamiltonian Graph neural Network) CHGNet** nature machine intelligence

Article

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

Received: 2 March 2023

Bowen Deng<sup>1,2</sup>, Peichen Zhong  $\mathbf{O}^{1,2}$ , KyuJung Jun  $\mathbf{O}^{1,2}$ , Janosh Riebesell<sup>2,3</sup>, Kevin Han<sup>2</sup>, Christopher J. Bartel  $\mathbf{O}^{1,4}$  & Gerbrand Ceder  $\mathbf{O}^{1,2}$ 

Accepted: 4 August 2023

https://github.com/CederGroupHub/chgnet https://chgnet.lbl.gov/

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



# **ALIGNN (Atomistic Line Graph Neural Network)**

# Digital Discovery

### PAPER

Check for updates

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, (1)\*\*\* Brian DeCost, (1)<sup>c</sup> Lily Major, (1)<sup>de</sup> Keith Butler, (1)<sup>e</sup> Jeyan Thiyagalingam (1)<sup>e</sup> and Francesca Tavazza (1)<sup>c</sup>

https://github.com/usnistgov/alignn





View Article Online View Journal | View Issue

### MACE-MP-0

### A foundation model for atomistic materials chemistry

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

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

#### arXiv:2401.00096v2

### TeaNet



#### 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

Akihide Hayashi₀<sup>1</sup>, Nontawat Charoenphakdee₀<sup>1</sup> & Takeshi Ibuka₀<sup>2⊠</sup>



Contents lists available at ScienceDirect

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

#### Towards universal neural network interatomic potential

So Takamoto<sup>a</sup>, Daisuke Okanohara<sup>a</sup>, Qing-Jie Li<sup>b</sup>, Ju Li<sup>b,\*</sup>

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# Check for updates

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#### Journal of Materiomics







# **GNoME (Graph Networks for Materials Exploration)**

### Article Scaling deep learning for materials discovery

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

Received: 8 May 2023

Amil Merchant<sup>1,3</sup>, Simon Batzner<sup>1,3</sup>, Samuel S. Schoenholz<sup>1,3</sup>, Muratahan Aykol<sup>1</sup>, Gowoon Cheon<sup>2</sup> & Ekin Dogus Cubuk<sup>1,3</sup>

Accepted: 10 October 2023

https://github.com/google-deepmind/materials\_discovery



### MatterSim





- MatterSim: A Deep Learning Atomistic Model Across
  - Elements, Temperatures and Pressures
- Han Yang<sup>1\*†</sup>, Chenxi Hu<sup>1†</sup>, Yichi Zhou<sup>1†</sup>, Xixian Liu<sup>1†</sup>, Yu Shi<sup>1†</sup>, Jielan Li<sup>1\*†</sup>, Guanzhi Li<sup>1†</sup>, Zekun Chen<sup>1†</sup>, Shuizhou Chen<sup>1†</sup>, Claudio Zeni $\mathbb{D}^1$ , Matthew Horton $\mathbb{D}^1$ , Robert Pinsler $\mathbb{D}^1$ , Andrew Fowler<sup>1</sup>, Daniel Zügner<sup>D</sup><sup>1</sup>, Tian Xie<sup>D</sup><sup>1</sup>, Jake Smith<sup>D</sup><sup>1</sup>, Lixin Sun<sup>D</sup><sup>1</sup>, Qian Wang<sup>D</sup><sup>1</sup>, Lingyu Kong $\mathbb{D}^1$ , Chang Liu $\mathbb{D}^1$ , Hongxia Hao $\mathbb{D}^{1^*}$ , Ziheng Lu $\mathbb{D}^{1^*}$ 
  - <sup>1\*</sup>Microsoft Research AI for Science.

#### arXiv:2405.04967v2

# SevenNet (Scalable EquiVariance Enabled Neural Network)



pubs.acs.org/JCTC

### 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

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



Article





# **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:

```
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

y configuration



# Matbench-Discovery

	<b>F1</b> ↑	DAF 1	Prec 1	Acc 1	TPR 1	TNR 1	MAE ↓	RMSE ↓	<b>R</b> <sup>2</sup> ↑	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	Е	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)	Е	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	Е	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 Intensity



• Validation against all-electron results for elemental crystals





New methods Mutual agreement



Old methods **Different values** 

#### 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)]

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



(a) FCC crystal (conventional cell).



(c) SC crystal (conventional cell).



**(b) BCC** crystal (conventional cell).



(d) Diamond crystal (conventional cell).



(a) X<sub>2</sub>O crystal (conventional cell).



(d) XO<sub>2</sub> crystal (conventional cell).



**(b)** XO crystal (conventional cell).



(e)  $X_2O_5$  crystal (conventional cell).



(c)  $X_2O_3$  crystal (conventional cell).



(f) XO<sub>3</sub> crystal (conventional cell).



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

• With 2 new metrics:

 $\bullet$  a revised version of the  $\Delta$ -factor

 $\bullet$  a metric dependent on the physically measurable quantities  $V_0$ ,  $B_0$ , and  $B_1$ 

 $\nu_{W_{V_0}, W_{B_0}, W_{B_1}}(a, b) = 100$ 

$$\epsilon(a,b) = \sqrt{\frac{\sum_{i} \left[E_{a}(V_{i}) - E_{b}(V_{i})\right]^{2}}{\sqrt{\sum_{i} \left[E_{a}(V_{i}) - \left\langle E_{a}\right\rangle\right]^{2} \sum_{i} \left[E_{b}(V_{i}) - \left\langle E_{b}\right\rangle\right]^{2}}}}$$

$$\sum_{Y=V_0,B_0,B_1} \left[ \frac{Y_a - Y_b}{(Y_a + Y_b)/2} \right]^2$$

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

#### ε for ABINIT@PWIPseudoDojo-v0.5 vs. all-electron average



La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Ac	Th	Ра	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

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

#### v for ABINIT@PWIPseudoDojo-v0.5 vs. all-electron average



La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Ac	Th	Ра	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

### • The results for uMLIPs are not fantastic!

#### ε for chgnet@UIPIv0.2.2 vs. all-electron average





#### ε for chgnet@UIPIv0.2.2 vs. all-electron average $X_2O_3 X_2O_5$ 5 X<sub>2</sub>O XO<sub>2</sub> 4.5 XO XO3 4 3.5 3 2.5 2 Fr R Lr Rf Db Sg Bh Hs Mt Ds Rg Cn Nh Fl Mc Lv Ts Og 1.5 1 0.5 Am Cm Bk Cf Es Fm Md No Ρ 0



### • The results for uMLIPs are not fantastic!

#### v for chgnet@UIPIv0.2.2 vs. all-electron average





#### v for chgnet@UIPIv0.2.2 vs. all-electron average $X_2O_3$ X<sub>2</sub>O<sub>5</sub> X<sub>2</sub>O XO2 7 XO XO3 6 5 4 Rf Db Sg Bh Hs Mt Ds Rg Cn Nh FI Mc Lv Ts Og Lr 3 2 1 Am Cm Bk Cf Es Fm Md No 0



• The results for uMLIPs are not fantastic!





- 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:
  - 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)]

• their predictions should be taken with some caution and, if possible, validated a

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

<b>H</b> 352				C	ompo	ositio	ons a	mou	nt								<b>He</b> 4
<b>Li</b> 425	<b>Be</b> 209					,		,				<b>B</b> 431	<b>C</b> 605	<b>N</b> 876	<b>O</b> 2353	<b>F</b> 493	<b>Ne</b> 1
<b>Na</b>	<b>Mg</b>	0 500 1000 1500 2000										<b>AI</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>Cl</b>	<b>Ar</b>
347	2233	3 Sc Ti V Cr Mn Fe Co Ni C										666	1598	474	1027	404	2
<b>K</b>	<b>Ca</b>	<b>Sc</b>	<b>Ti</b>	<b>V</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>	<b>Co</b>	<b>Ni</b>	<b>Cu</b>	<b>Zn</b>	<b>Ga</b>	<b>Ge</b>	<b>As</b>	<b>Se</b>	<b>Br</b>	<b>Kr</b>
380	426	305	621	533	444	428	582	480	570	475	717	671	559	446	740	309	7
<b>Rb</b>	<b>Sr</b>	<b>Y</b>	<b>Zr</b>	<b>Nb</b>	<b>Mo</b>	<b>Tc</b>	<b>Ru</b>	<b>Rh</b>	<b>Pd</b>	<b>Ag</b>	<b>Cd</b>	<b>In</b>	<b>Sn</b>	<b>Sb</b>	<b>Te</b>	<b> </b>	<b>Xe</b>
326	424	446	498	387	349	146	234	365	493	400	541	490	647	552	567	436	15
<b>Cs</b>	<b>Ba</b>		<b>Hf</b>	<b>Ta</b>	<b>W</b>	<b>Re</b>	<b>Os</b>	<b>lr</b>	<b>Pt</b>	<b>Au</b>	<b>Hg</b>	<b>TI</b>	<b>Pb</b>	<b>Bi</b>	Po	At	Rn
187	332		326	327	278	224	193	341	485	431	380	301	324	472	-	-	-
Fr -	Ra -		Rf -	Db -	Sg -	Bh -	Hs -	Mt -	Ds -	Rg	Cn -	Nh -	FI -	Mc -	Lv -	Ts -	Og -

<b>La</b>	<b>Ce</b>	<b>Pr</b>	<b>Nd</b>	<b>Pm</b>	<b>Sm</b>	<b>Eu</b>	<b>Gd</b>	<b>Tb</b>	<b>Dy</b>	<b>Ho</b>	<b>Er</b>	<b>Tm</b> 277	<b>Yb</b>	<b>Lu</b>
391	567	357	384	188	364	293	184	360	329	334	316		400	235
<b>Ac</b>	<b>Th</b>	<b>Pa</b>	<b>U</b>	<b>Np</b>	<b>Pu</b>	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
141	300	110	277	155	208	-	-	-	-	-	-	-	-	-

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

ionic- and cell-relaxations



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

<b>H</b> 46.92							(a)	CH	IGN	Net							<b>He</b> 12.54	<b>⊩</b> 122
<b>Li</b> 34.95	<b>Be</b> 44.49	M	ean F	orma	tion I	Energ	y Diff	erend	ce me	V/ato	m	<b>B</b> 53.47	<b>C</b> 57.30	<b>N</b> 61.24	<b>0</b> 75.06	<b>F</b> 51.17	Ne -	<b>L</b> 57.
<b>Na</b> 39.67	<b>Mg</b> 39.10	0	50	) 10	0 15	50 2	00 2	50 3	зоо	350	400	<b>Al</b> 61.46	<b>Si</b> 63.82	<b>P</b> 48.71	<b>S</b> 57.33	<b>CI</b> 42.97	<b>Ar</b> 0.26	<b>N</b> 73.
<b>K</b> 36.08	<b>Ca</b> 33.99	<b>Sc</b> 50.97	<b>Ti</b> 60.65	<b>V</b> 67.23	<b>Cr</b> 92.41	<b>Mn</b> 90.40	<b>Fe</b> 139.09	<b>Co</b> 89.89	<b>Ni</b> 52.93	<b>Cu</b> 28.78	<b>Zn</b> 30.49	<b>Ga</b> 36.24	<b>Ge</b> 102.07	<b>As</b> 60.70	<b>Se</b> 38.86	<b>Br</b> 53.35	<b>Kr</b> 11.77	<b>K</b> 85.
<b>Rb</b> 29.54	<b>Sr</b> 35.84	<b>Y</b> 41.82	<b>Zr</b> 50.09	<b>Nb</b> 70.79	<b>Mo</b> 91.47	<b>Tc</b> 61.30	<b>Ru</b> 95.38	<b>Rh</b> 46.22	<b>Pd</b> 36.74	<b>Ag</b> 36.16	<b>Cd</b> 25.37	<b>In</b> 46.89	<b>Sn</b> 52.76	<b>Sb</b> 58.60	<b>Te</b> 50.34	<b>3</b> 5.77	<b>Xe</b> 27.63	<b>R</b> 100
<b>Cs</b> 36.05	<b>Ba</b> 44.28		<b>Hf</b> 46.18	<b>Ta</b> 52.79	<b>W</b> 93.68	<b>Re</b> 67.17	<b>Os</b> 69.69	<b>lr</b> 49.95	<b>Pt</b> 47.80	<b>Au</b> 44.46	<b>Hg</b> 32.83	<b>TI</b> 34.06	<b>Pb</b> 43.49	<b>Bi</b> 59.32	Ро -	At -	Rn -	<b>C</b> 109
Fr	Ra		Rf -	Db -	Sg -	Bh -	Hs -	Mt	Ds -	Rg	Cn -	Nh -	FI -	Mc -	Lv -	Ts -	Og _	F

<b>La</b>	<b>Ce</b>	<b>Pr</b>	<b>Nd</b>	<b>Pm</b> 27.75	<b>Sm</b>	<b>Eu</b>	<b>Gd</b>	<b>Tb</b>	<b>Dy</b>	<b>Ho</b>	<b>Er</b>	<b>Tm</b>	<b>Yb</b>	<b>Lu</b>
37.60	39.50	39.77	40.64		38.56	58.48	88.30	43.25	39.77	37.15	34.97	32.21	36.51	41.27
<b>Ac</b> 44.93	<b>Th</b> 40.60	<b>Pa</b> 58.17	<b>U</b> 81.79	<b>Np</b> 96.15	<b>Pu</b> 169.87	Am -	Cm	Bk -	Cf -	Es -	Fm	Md	No	Lr -

<b>H</b> 122.90							(b)	M.	3GI	Net							<b>He</b> 1.00
<b>Li</b> 57.65	<b>Be</b> 102.53	M	lean F	orma	tion I	Energ	y Diff	ferenc	ce me	V/ato	om	<b>B</b> 118.06	<b>C</b> 101.13	<b>N</b> 210.18	<b>0</b> 623.52	<b>F</b> 444.05	Ne
<b>Na</b> 73.05	<b>Mg</b> 65.83	0	50	) 10	0 15	50 2	00 2	50 3	300	350	400	<b>Al</b> 107.18	<b>Si</b> 167.30	<b>P</b> 81.46	<b>S</b> 279.60	<b>CI</b> 399.05	<b>Ar</b> 0.25
<b>K</b> 85.80	<b>Ca</b> 65.66	<b>Sc</b> 90.47	<b>Ti</b> 145.84	<b>V</b> 442.41	<b>Cr</b> 329.89	<b>Mn</b> 266.96	<b>Fe</b> 381.93	<b>Co</b> 211.46	<b>Ni</b> 150.04	<b>Cu</b> 99.28	<b>Zn</b> 97.70	<b>Ga</b> 68.97	<b>Ge</b> 66.75	<b>As</b> 76.83	<b>Se</b> 290.76	<b>Br</b> 313.45	<b>Kr</b> 86.14
<b>Rb</b> 100.44	<b>Sr</b> 82.49	<b>Y</b> 72.84	<b>Zr</b> 113.39	<b>Nb</b> 140.43	<b>Mo</b> 380.36	<b>Tc</b> 103.25	<b>Ru</b> 80.62	<b>Rh</b> 69.02	<b>Pd</b> 59.96	<b>Ag</b> 74.42	<b>Cd</b> 95.26	<b>In</b> 77.78	<b>Sn</b> 87.97	<b>Sb</b> 137.78	<b>Te</b> 218.87	<b> </b> 241.47	<b>Xe</b> 179.62
<b>Cs</b> 109.58	<b>Ba</b> 78.42		<b>Hf</b> 95.68	<b>Ta</b> 157.95	<b>W</b> 635.47	<b>Re</b> 123.12	<b>Os</b> 91.90	<b>lr</b> 85.42	<b>Pt</b> 74.27	<b>Au</b> 55.12	<b>Hg</b> 56.40	<b>Tl</b> 75.61	<b>Pb</b> 101.81	<b>Bi</b> 140.01	Ро -	At -	Rn
Fr	Ra		Rf	Db -	Sg	Bh	Hs -	Mt -	Ds -	Rg	Cn -	Nh -	FI	Mc -	Lv -	Ts	Og

<b>H</b> 176.13				
Li	Be	Μ	ean F	orm
68.14	122.00			
<b>Na</b> 91.46	<b>Mg</b> 84.81	0	50	) 1
<b>K</b> 101.90	<b>Ca</b> 86.38	<b>Sc</b> 89.37	<b>Ti</b> 95.20	<b>V</b> 186.6
<b>Rb</b> 97.19	<b>Sr</b> 86.49	<b>¥</b> 80.28	<b>Zr</b> 98.85	<b>Nb</b> 144.3
<b>Cs</b> 141.18	<b>Ba</b> 91.11		<b>Hf</b> 97.94	<b>Ta</b> 158.2
Fr	Ra		Rf	Db

<b>La</b>	<b>Ce</b>	<b>Pr</b>
103.08	150.81	77.41
<b>Ac</b> 70.11	<b>Th</b> 146.13	<b>Pa</b> 105.78

<b>H</b> 7.86	(c) MACE										<b>He</b> 6.94						
<b>Li</b> 20.04	<b>Be</b> 27.66	M	ean F	orma	tion E	Energ	y Diff	erenc	e me	V/ato	m	<b>B</b> 49.55	<b>C</b> 42.02	<b>N</b> 48.98	<b>O</b> 56.38	<b>F</b> 45.40	Ne -
<b>Na</b> 24.51	<b>Mg</b> 26.25	0	50	) 10	0 15	50 20	00 2	50 3	300	350	400	<b>Al</b> 33.49	<b>Si</b> 46.57	<b>P</b> 36.75	<b>S</b> 43.97	<b>CI</b> 36.97	<b>Ar</b> 0.23
<b>K</b> 80.63	<b>Ca</b> 22.96	<b>Sc</b> 29.75	<b>Ti</b> 43.36	<b>∨</b> 38.84	<b>Cr</b> 129.89	<b>Mn</b> 79.55	<b>Fe</b> 125.97	<b>Co</b> 59.34	<b>Ni</b> 49.85	<b>Cu</b> 23.16	<b>Zn</b> 18.11	<b>Ga</b> 25.41	<b>Ge</b> 61.33	<b>As</b> 45.11	<b>Se</b> 36.06	<b>Br</b> 164.99	<b>Kr</b> 6.91
<b>Rb</b> 88.89	<b>Sr</b> 26.85	<b>Y</b> 28.61	<b>Zr</b> 34.69	<b>Nb</b> 54.32	<b>Mo</b> 85.20	<b>Tc</b> 35.77	<b>Ru</b> 42.15	<b>Rh</b> 31.17	<b>Pd</b> 26.65	<b>Ag</b> 22.43	<b>Cd</b> 28.11	<b>In</b> 37.00	<b>Sn</b> 34.44	<b>Sb</b> 52.21	<b>Te</b> 54.33	<b> </b> 58.80	<b>Xe</b> 9.54
<b>Cs</b> 2.37	<b>Ba</b> 36.84		<b>Hf</b> 28.95	<b>Ta</b> 39.42	<b>W</b> 101.46	<b>Re</b> 47.33	<b>Os</b> 33.33	<b>Ir</b> 37.11	<b>Pt</b> 40.15	<b>Au</b> 29.71	<b>Hg</b> 21.67	<b>TI</b> 25.28	<b>Pb</b> 33.75	<b>Bi</b> 43.26	<b>Po</b>	At	Rn
Fr	Ra		Rf	Db -	Sg	Bh _	Hs	Mt	Ds -	Rg	Cn -	Nh -	FI -	Мс	Lv -	Ts	Og

<b>La</b>	<b>Ce</b>	<b>Pr</b> 27.51	<b>Nd</b>	<b>Pm</b>	<b>Sm</b>	<b>Eu</b>	<b>Gd</b>	<b>Tb</b>	<b>Dy</b>	<b>Ho</b>	<b>Er</b>	<b>Tm</b>	<b>Yb</b>	<b>Lu</b>
29.65	28.97		25.88	19.80	32.93	54.00	84.39	31.81	30.42	29.05	23.57	29.30	36.62	28.18
<b>Ac</b> 26.70	<b>Th</b> 31.51	<b>Pa</b> 50.60	<b>U</b> 69.30	<b>Np</b> 102.02	<b>Pu</b> 175.37	Am -	Cm	Bk -	Cf -	Es -	Fm	Md	No -	Lr

<b>L</b>	. <b>a</b>	<b>Ce</b>	<b>Pr</b>	<b>Nd</b>	<b>Pm</b>	<b>Sm</b>	<b>Eu</b>	<b>Gd</b>	<b>Tb</b>	<b>Dy</b>	<b>Ho</b>	<b>Er</b>	<b>Tm</b>	<b>Yb</b>	<b>Lu</b>
78.	.60	185.40	76.07	93.84	70.48	71.61	101.31	157.13	86.46	74.47	71.93	60.44	81.07	88.34	73.29
<b>A</b> 74.	.74	<b>Th</b> 72.19	<b>Pa</b> 117.02	<b>U</b> 178.66	<b>Np</b> 140.21	<b>Pu</b> 201.51	Am	Cm	Bk	Cf	Es -	Fm	Md	No	Lr

	(d) ALIGNN												<b>He</b> 2.46
าล	tion l	Energ	y Diff	erend	ce me	V/ato	m	<b>B</b> 233.35	<b>C</b> 264.30	<b>N</b> 159.31	<b>0</b> 233.95	<b>F</b> 161.94	Ne
10	0 15	50 20	00 2	50 3	300	350	400	<b>Al</b> 87.08	<b>Si</b> 164.37	<b>P</b> 131.86	<b>S</b> 218.83	<b>CI</b> 283.07	<b>Ar</b> 0.35
59	<b>Cr</b> 161.27	<b>Mn</b> 150.99	<b>Fe</b> 181.40	<b>Co</b> 155.67	<b>Ni</b> 115.82	<b>Cu</b> 86.67	<b>Zn</b> 84.01	<b>Ga</b> 71.91	<b>Ge</b> 86.48	<b>As</b> 144.97	<b>Se</b> 237.66	<b>Br</b> 285.19	<b>Kr</b> 72.25
) 32	<b>Mo</b> 169.48	<b>Tc</b> 85.77	<b>Ru</b> 87.04	<b>Rh</b> 77.35	<b>Pd</b> 80.33	<b>Ag</b> 72.51	<b>Cd</b> 103.69	<b>In</b> 74.53	<b>Sn</b> 86.56	<b>Sb</b> 110.44	<b>Te</b> 215.45	<b> </b> 251.27	<b>Xe</b> 101.04
27	<b>W</b> 249.47	<b>Re</b> 122.55	<b>Os</b> 124.69	<b>Ir</b> 103.05	<b>Pt</b> 89.48	<b>Au</b> 83.15	<b>Hg</b> 68.22	<b>Tl</b> 71.68	<b>Pb</b> 94.39	<b>Bi</b> 125.71	Ро -	At	Rn
,	Sg	Bh	Hs	Mt -	Ds -	Rg	Cn	Nh -	FI	Mc -	Lv -	Ts -	Og
1	<b>Nd</b> 85.65	<b>Pm</b> 75.51	<b>Sm</b> 79.20	<b>Eu</b> 191.58	<b>Gd</b> 144.54	<b>Tb</b> 88.00	<b>Dy</b> 78.19	<b>Ho</b> 84.25	<b>Er</b> 78.87	<b>Tm</b> 86.09	<b>Yb</b> 98.33	<b>Lu</b> 88.91	

Pu Am Cm Bk Cf Es Fm Md No Li

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



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



• We compute  $E_{\text{form}}[A_a B_b] = E[A_a B_b] - x_a E[A] - x_b E[B]$  with one-shot energies

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



uMLIP	V	a	b	C	α	β	
CHGNet	3.16	2.03	2.07	2.44	0.75	0.62	1
M3GNet	2.97	2.04	2.09	2.46	0.89	0.73	1
MACE	5.22	2.01	2.11	2.58	0.73	0.59	1
ALIGNN	7.85	3.42	3.42	3.61	0.94	0.86	1

MARE (%)



- 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

$\Lambda F_{\alpha}$ –	$_{F}MP$	_ <sub>F</sub> uMLIP
$\Delta L$ form –	form	form

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

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

### MARE (%)

uMLIP	V	а	b	С	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



### **Test #3: Phonon band structures**

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



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

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



# **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)



8)	(19)	(3)	(36)	(25)	(25)	(24)	(12)	(19)	(3)	(25)
0.045	0.316	0.007	0.095	0.120	0.248	0.926	0.620	0.153	0.496	1.045
.37	0.025	0.019	0.019	0.015	0.023	0.101	0.076	0.117	0.014	0.063
0.056	0.505	0.008	0.057	0.135	0.442	1.094	0.159	0.599	1.178	1.314
.06	0.004	0.025	0.009	0.029	0.043	0.094	0.002	0.072	0.051	0.075
0.056	0.548	0.014	0.090	0.101	0.484	0.748	0.632	1.252	1.559	1.295
08	0.017	0.028	0.008	0.007	0.027	0.025	0.002	0.020	0.006	0.008
Si	Р	S	К	Ca	Sc	Ti	V	Cr	Mn	Fe
3)	(78)	(47)	(27)	(26)	(27)	(13)	(24)	(26)	(13)	(13)
0.005	0.094	0.097	0.215	0.383	0.365	0.633	0.621	1.558	0.772	0.258
109	0.032	0.005	0.014	0.012	0.142	0.219	0.001	0.111	0.039	0.019
0.088	0.048	0.152	0.266	0.342	0.489	0.754	0.896	0.913	0.471	0.374
44	0.017	0.016	0.020	0.027	0.141	0.166	0.016	0.093	0.046	0.025
0.000	0.095	0.210	0.670	0.701	1.624	1.014	1.537	1.602	1.073	0.620
0.029	0.028	0.006	0.013	0.034	0.006	0.012	0.004	0.055	0.007	0.002
e	Rb	Sr	Y	Zr	Nb	Мо	Tc	Ru	Rh	Pd
3)	(12)	(14)	(13)	(12)	(12)	(12)	(20)	(7)	(30)	(19)
0.019	0.075	0.042	0.085	0.066	0.122	0.068	0.142	0.042	0.078	0.079
163	0.035	0.045	0.013	0.039	0.006	0.017	0.027	0.022	0.016	0.017
0.045	0.206	0.539	0.218	0.187	0.217	0.200	0.238	0.209	0.196	0.202
42	0.032	0.059	0.026	0.031	0.039	0.029	0.020	0.040	0.033	0.043
	0.485	0.770	0.469	0.562	0.561	0.573	0.407	0.562	0.513	0.758
.62	0.002	0.011	0.009	0.206	0.006	0.019	0.012	0.024	0.005	0.012
a	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy
(1	.2) (1	2) (14	4) (14	) (15)	(12)	(24)	(25)	(24)	(13)	(13)
1.109	1.769	0.831	0.041	0.111	0.007	0.063	0.149	0.105	0.127	0.136
0.0	0.138	0.230	0.122	1 0.025	0.018	0.031	0.019	0.047	0.006	0.001
1.04	5 1.492	0.801	0.419	0.379	0.051	0.045	0.173	0.121	0.287	0.317
1	0.172	0.176	0.090	0.097	0.034 0.033	.022 0.022	0.031	0.05	8 0.067	0.002
1.558	3 2.012	1.199	0.785	0.478	0.012	0.178	0.241	0.197	0.495	0.652
4	0.235	0.283	0.160	0.118	0.066	.008 0.0	0.00	59 0.04 0.052	5 0.164	0.0134
F	Re O	rs Ir	- Pt	Au	Hg	TI	Pb	Bi	Ac	Th
	Sytem cl	hemistry								

0.1 0.2 0.3 0.4 0.5 0.6 0.7 Bulk total energy RMSE (eV atom<sup>-1</sup>) 0.1 0.2 0.3 0.4 0.5 0.6 0.7 Surface total energy RMSE (eV atom<sup>-1</sup>)

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



[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

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> 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-

## **Possible use cases**

. . . .

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

ionic-relaxations with CHGNet

1.8																
Li 1.7	<b>Be</b> 1.7				mean	Speedl	Jp via c	hgnet				<b>B</b> 1.4	<b>C</b> 1.5	<b>N</b> 1.7	<b>O</b> 2.3	
<b>Na</b> 1.3	<b>Mg</b> 1.5		0	0.5		1		1.5	2			<b>Al</b> 1.6	<b>Si</b> 1.1	<b>P</b> 1.4	<b>S</b> 1.3	
<b>K</b> 1.4	<b>Ca</b> 1.6	<b>Sc</b> 1.6	<b>Ti</b> 1.3	<b>V</b> 1.7	<b>Cr</b> 1.4	<b>Mn</b> 1.1	<b>Fe</b> 1.0	<b>Co</b>	<b>Ni</b> 1.7	<b>Cu</b> 1.3	<b>Zn</b> 1.7	<b>Ga</b> 1.2	<b>Ge</b> 1.9	<b>As</b> 1.1	<b>Se</b> 1.6	
<b>Rb</b> 1.3	<b>Sr</b> 1.3	<b>Y</b> 1.5	<b>Zr</b> 1.3	<b>Nb</b> 1.2	<b>Mo</b> 1.4	<b>Tc</b> 1.8	<b>Ru</b> 1.5	<b>Rh</b> 1.2	<b>Pd</b> 1.4	<b>Ag</b> 1.3	<b>Cd</b>	<b>In</b> 1.2	<b>Sn</b> 1.2	<b>Sb</b> 1.5	<b>Te</b> 0.8	
<b>Cs</b> 1.2	<b>Ba</b> 1.8		<b>Hf</b> 1.4	<b>Ta</b> 1.1	<b>W</b> 1.1	<b>Re</b> 1.7	<b>Os</b> 1.4	<b>Ir</b> 1.7	<b>Pt</b> 1.4	<b>Au</b> 1.4	<b>Hg</b> 1.3	<b>TI</b> 1.5	<b>Pb</b> 2.3	<b>Bi</b> 1.2	Ро	
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	FI	Мс	Lv	•

Elements in ionmove 31 none

<b>La</b> 1.8	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Тb	Dy	Но	Er	Tm	Yb	
Ac	Th	Ра	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	

#### ionic-relaxations with MACE



**H** 1.7

Elements in ionmove 31 none

<b>Li</b> 2.1	<b>Be</b> 2.4				mean	Speed		<b>B</b> 1.5	<b>C</b> 2.0	<b>N</b> 1.9	<b>O</b> 1.9	<b>F</b> 2.4				
<b>Na</b> 1.3	<b>Mg</b> 1.7		0	0.5		1	1.5		2	2.5		<b>Al</b> 1.7	<b>Si</b> 1.3	<b>P</b> 1.7	<b>S</b> 2.0	<b>CI</b> 1.8
<b>K</b> 1.5	<b>Ca</b> 1.9	<b>Sc</b> 1.8	<b>Ti</b> 1.9	<b>V</b> 1.7	<b>Cr</b> 1.4	<b>Mn</b> 1.6	<b>Fe</b> 1.5	<b>Co</b> 1.8	<b>Ni</b> 1.9	<b>Cu</b> 2.5	<b>Zn</b> 1.9	<b>Ga</b> 1.5	<b>Ge</b> 2.2	<b>As</b> 1.7	<b>Se</b> 2.0	<b>Br</b> 1.7
<b>Rb</b> 1.6	<b>Sr</b> 1.8	<b>Y</b> 1.8	<b>Zr</b> 1.9	<b>Nb</b> 1.8	<b>Mo</b> 1.4	<b>Tc</b> 1.6	<b>Ru</b> 1.7	<b>Rh</b> 1.6	<b>Pd</b> 1.9	<b>Ag</b> 2.2	<b>Cd</b> 2.1	<b>In</b> 1.7	<b>Sn</b> 1.8	<b>Sb</b> 1.5	<b>Te</b> 2.2	<b>I</b> 2.2
<b>Cs</b> 1.2	<b>Ba</b> 1.8		<b>Hf</b> 1.5	<b>Ta</b> 1.6	<b>W</b> 1.4	<b>Re</b> 2.0	<b>Os</b> 1.6	<b>Ir</b> 2.0	<b>Pt</b> 2.1	<b>Au</b> 1.8	<b>Hg</b> 1.7	<b>TI</b> 1.5	<b>Pb</b> 1.8	<b>Bi</b> 1.6	Ро	At
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	FI	Мс	Lv	Ts

<b>La</b> 2.3	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Тb	Dy	Но	Er	Tm	Yb	Lu
Ac	Th	Ра	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr



## **Possible use cases**

**–** Ц

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

cell-relaxations with CHGNet

1	.0																
<b>I</b> 1	Li .0	<b>Be</b> 1.2				mean	Speed	Jp via c	hgnet				<b>B</b> 1.0	<b>C</b> 0.8	<b>N</b> 0.7	<b>O</b> 1.0	1
<b>N</b> 0	<b>la</b> ).9	<b>Mg</b> 1.0		0		0.5	5		<b>Al</b> 0.9	<b>Si</b> 1.0	<b>P</b> 0.9	<b>S</b> 1.0	1				
1	<b>K</b> .0	<b>Ca</b> 1.2	<b>Sc</b> 1.1	<b>Ti</b> 1.1	<b>V</b> 1.1	<b>Cr</b> 1.0	<b>Mn</b> 1.1	<b>Fe</b> 0.9	<b>Co</b> 0.9	<b>Ni</b> 1.1	<b>Cu</b> 0.8	<b>Zn</b> 1.1	<b>Ga</b> 0.8	<b>Ge</b> 0.3	<b>As</b> 0.9	<b>Se</b> 1.1	E
<b>R</b> 1	<b>₹b</b> 1.0	<b>Sr</b> 1.1	<b>Y</b> 1.3	<b>Zr</b> 1.2	<b>Nb</b> 1.1	<b>Mo</b> 1.0	<b>Tc</b> 0.9	<b>Ru</b> 0.8	<b>Rh</b> 1.0	<b>Pd</b> 0.9	<b>Ag</b> 1.0	<b>Cd</b> 1.1	<b>In</b> 1.0	<b>Sn</b> 0.9	<b>Sb</b> 1.0	<b>Te</b> 1.0	C
<b>C</b>	<b>.</b> 0	<b>Ba</b> 1.1		<b>Hf</b> 1.2	<b>Ta</b> 0.8	<b>W</b> 0.8	<b>Re</b> 1.0	<b>Os</b> 1.0	<b>ir</b> 1.1	<b>Pt</b> 1.0	<b>Au</b> 0.9	<b>Hg</b> 1.0	<b>TI</b> 0.9	<b>Pb</b> 0.7	<b>Bi</b> 0.8	Ро	ŀ
F	۶r	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	FI	Мс	Lv	٦

Elements in ionmove 31 none

<b>La</b> 1.4	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Тb	Dy	Но	Er	Tm	Yb	Lu 1.1
Ac	Th	Ра	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

#### cell-relaxations with MACE

Elements in ionmove 31 none

<b>Li</b> 1.1	<b>Be</b> 1.4				mear	) Speed	Up via N	Mace				<b>B</b> 1.1	<b>C</b> 0.9	<b>N</b> 0.8	<b>0</b> 1.2	<b>F</b> 1.3
<b>Na</b> 1.1	<b>Mg</b> 1.3		0		0.5		1			1.5		<b>Al</b> 1.1	<b>Si</b> 1.2	<b>P</b> 1.1	<b>S</b> 1.5	<b>Cl</b> 1.0
<b>K</b> 1.0	<b>Ca</b> 1.5	<b>Sc</b> 1.3	<b>Ti</b> 1.3	<b>V</b> 1.2	<b>Cr</b> 1.1	<b>Mn</b> 0.9	<b>Fe</b> 1.1	<b>Co</b> 1.2	<b>Ni</b> 1.2	<b>Cu</b> 1.3	<b>Zn</b> 1.1	<b>Ga</b> 1.3	<b>Ge</b> <sub>0.4</sub>	<b>As</b> 1.3	<b>Se</b> 1.3	<b>Br</b> 1.0
<b>Rb</b> 1.1	<b>Sr</b> 1.4	<b>Y</b> 1.4	<b>Zr</b> 1.2	<b>Nb</b> 1.4	<b>Mo</b> 1.1	<b>Tc</b> 1.0	<b>Ru</b> 1.1	<b>Rh</b> 1.2	<b>Pd</b> 1.1	<b>Ag</b> 1.2	<b>Cd</b> 1.5	<b>In</b> 1.4	<b>Sn</b> 1.3	<b>Sb</b> 1.1	<b>Te</b> 0.9	<b>I</b> 1.0
<b>Cs</b> 1.2	<b>Ba</b> 1.3		<b>Hf</b> 1.3	<b>Ta</b> 1.2	<b>W</b> 1.2	<b>Re</b> 1.0	<b>Os</b> 0.9	<b>Ir</b> 1.0	<b>Pt</b> 1.3	<b>Au</b> 1.0	<b>Hg</b> 1.2	<b>TI</b> 1.1	<b>Pb</b> 1.3	<b>Bi</b> 0.9	Ро	At
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	FI	Мс	Lv	Ts

<b>La</b> 1.6	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Тb	Dy	Но	Er	Tm	Yb	<b>Lu</b> 1.2
Ac	Th	Ра	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr



**H** 1.0



# uMLIPs clearly show significant interest but further improvement is still needed

#### • Many thanks to my collaborators:





Haochen Yu

Matteo Giantomassi

### • Thank you for your attention



### Giuliana Materzanini



Junjie Wang