Supporting Information for: Benchmarking Universal Machine Learning Interatomic Potentials on Elemental Systems

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1 Minima Hopping

1.1 MH Performance Summary across all models

1.1.1 MACE-Unary-PBE-0

elements	#optimization attempts	#failed optimization	#visited minima	#accepted minima	#catas. latt. exp.	I (%)
As	42560	0	32556	15561	4	0.01
B	24589	0	16286	7135	106	0.65
Cd	36256	712	31916	15741	1619	7.04
Cu	28542	1556	19199	7366	508	8.1
Li	17262	1197	9821	4758	1384	21.03
Mg	23619	1001	18257	7925	1048	9.98
Nb	40453	534	23460	7240	1818	9.07
Sc	28694	520	21097	9280	768	5.45
Si	42683	4	28484	12277	211	0.75
Ta	29729	64	18116	6137	132	0.94
Te	45917	1	32936	15851	94	0.29
Ti	27171	335	20900	9187	273	2.54
Tl	35442	3861	29246	12851	1686	16.66
W	22956	48	13151	4060	49	0.58
Zr	32672	1165	25886	11248	945	7.22

Table S1 Details of MH calculations with MACE-Unary-PBE-0 across the benchmark elements.

1.1.2 MACE-MATPES-PBE-0

elements	#optimization attempts	#failed optimization	#visited minima	#accepted minima	#catas. latt. exp.	I (%)
As	45217	1	32699	14951	0	0.0
B	25880	0	16260	6983	42	0.26
Cd	39524	473	33190	14302	4393	14.43
Cu	32747	4361	23669	9093	3903	29.81
Li	36026	9961	21968	8421	5540	52.87
Mg	30213	2466	24190	9306	4333	26.07
Nb	45495	1513	28177	9029	2517	12.26
Sc	36861	2077	29115	11679	2810	15.29
Si	45709	48	28586	10878	209	0.84
Ta	32711	765	19414	6168	885	6.9
Te	47462	20	32766	14420	7	0.06
Ti	34730	2909	24539	9445	3051	20.81
Tl	39997	6851	32048	13805	3297	27.42
W	24261	195	13649	4165	419	3.87
Zr	38698	1362	30818	12950	1324	7.82

Table S2 Details of MH calculations with MACE-MATPES-PBE-0 across the benchmark elements.

1.1.3 MACE-OMAT-0

elements	#optimization attempts	#failed optimization	#visited minima	#accepted minima	#catas. latt. exp.	I (%)
As	46253	6	32566	15198	2	0.02
B	20352	0	12184	5052	181	1.49
Cd	39717	251	33317	13970	6360	19.72
Cu	34400	3693	24782	8603	5189	31.67
Li	35171	7627	21968	8470	4982	44.36
Mg	30460	2403	23984	8944	4941	28.49
Nb	45593	1229	28229	9060	2539	11.69
Sc	38465	654	29802	12132	1203	5.74
Si	46079	24	28530	10760	202	0.76
Ta	31626	802	19431	6458	1131	8.36
Te	48505	0	32762	14772	3	0.01
Ti	31724	655	25820	11508	1476	7.78
Tl	39228	6462	31166	13753	4090	29.6
W	23958	132	13736	4216	436	3.73
Zr	37713	1236	30683	13322	1790	9.11

Table S3 Details of MH calculations with MACE-OMAT-0 across the benchmark elements.

1.1.4 PET-OMat

elements	#optimization attempts	#failed optimization	#visited minima	#accepted minima	#catas. latt. exp.	I (%)
As	44200	0	32681	16098	47	0.14
B	22958	0	16290	7704	0	0.0
Cd	36645	164	32495	15437	693	2.58
Cu	33224	4006	26209	10807	2770	22.63
Li	33303	2610	29204	14272	1369	12.52
Mg	30820	1991	25532	11095	682	9.13
Nb	36161	1451	28346	12408	950	7.36
Sc	35374	701	29752	12520	587	3.95
Si	40987	1	28498	12188	197	0.69
Ta	26085	256	19614	8443	245	2.23
Te	42566	0	32568	15956	0	0.0
Ti	25211	192	22154	10728	222	1.76
Tl	35399	193	32573	16131	466	1.98
W	18858	196	13902	6017	179	2.33
Zr	35569	125	31254	14552	93	0.65

Table S4 Details of MH calculations with PET-OMat across the benchmark elements.

1.1.5 PET-MAD

elements	#optimization attempts	#failed optimization	#visited minima	#accepted minima	#catas. latt. exp.	I (%)
As	36079	0	32628	17853	8	0.02
B	23309	15	16099	7515	177	1.16
Cd	36290	36	32559	16696	1001	3.17
Cu	31144	2415	25894	12125	1068	11.88
Li	31227	205	28420	14362	189	1.32
Mg	28585	598	26159	13360	477	3.92
Nb	31625	130	28759	15812	92	0.73
Sc	33310	20	29955	15412	5	0.08
Si	36797	0	28526	14381	182	0.64
Ta	21588	17	19704	10619	16	0.16
Te	34831	11	32565	18104	1	0.03
Ti	29357	74	26258	13734	46	0.43
Tl	36134	1	32549	16668	954	2.93
W	16445	47	13838	7725	27	0.48
Zr	33129	26	31081	16573	30	0.18

Table S5 Details of MH calculations with PET-MAD across the benchmark elements.

1.1.6 MatterSim

elements	#optimization attempts	#failed optimization	#visited minima	#accepted minima	#catas. latt. exp.	I (%)
As	41706	0	32541	16352	40	0.12
B	25581	6	16361	6875	0	0.02
Cd	37938	383	32406	15550	1124	4.48
Cu	34830	2488	25023	9235	5044	27.3
Li	37612	4487	23510	8516	7345	43.17
Mg	32401	1418	25471	10419	2493	14.16
Nb	44178	671	27673	9348	1403	6.59
Sc	34165	532	29248	13902	719	4.02
Si	45423	16	28592	10972	251	0.91
Ta	31071	203	18998	6600	425	2.89
Te	41895	3	32727	16424	17	0.06
Ti	30071	881	25759	13039	1104	7.22
Tl	38395	801	32564	14552	2298	9.14
W	23730	30	13800	4375	670	4.98
Zr	37073	1538	31086	14204	1524	9.05

Table S6 Details of MH calculations with MatterSim across the benchmark elements.

1.2 MH results for all 15 elements

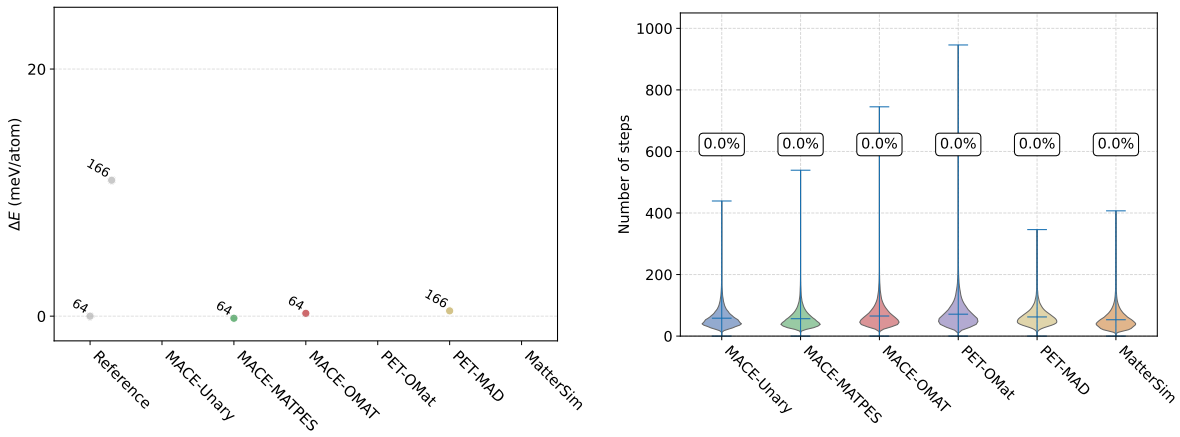

Fig. S1 Left: Comparison of MH results for As using uMLIPs with respect to MP reference data. Right: Violin plots showing the distribution of optimization-step counts during local geometry relaxations in the MH trajectories. Box annotations report the failure rate of structural relaxations.

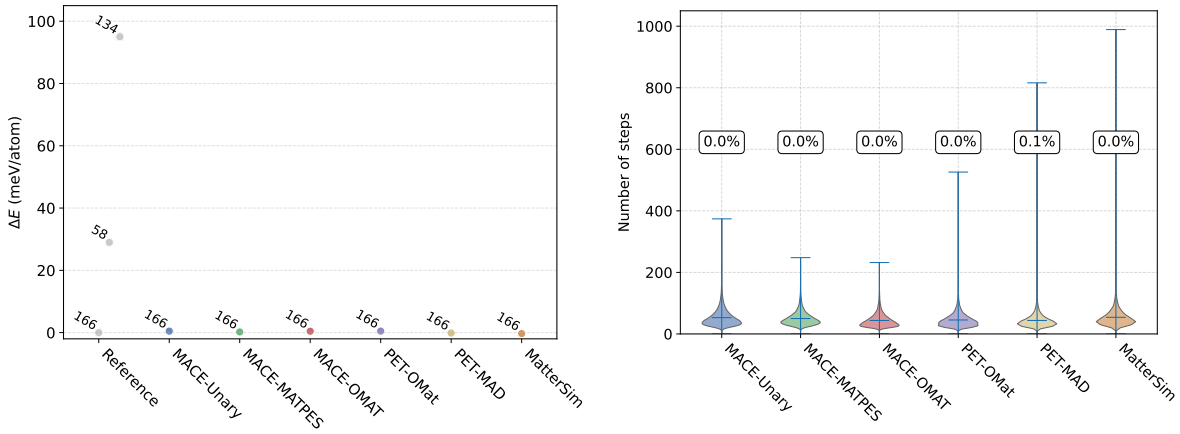

Fig. S2 Same as Fig. S1 for B.

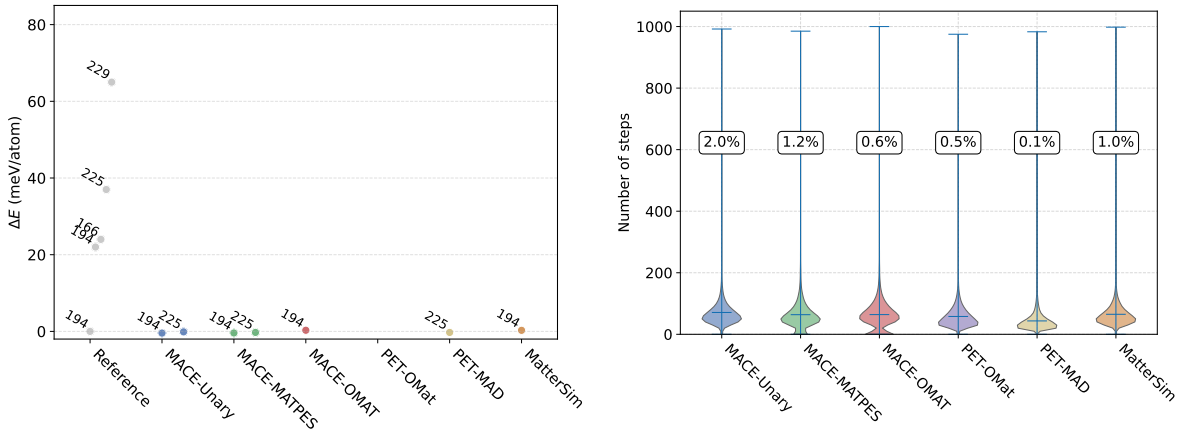

Fig. S3 Same as Fig. S1 for Cd.

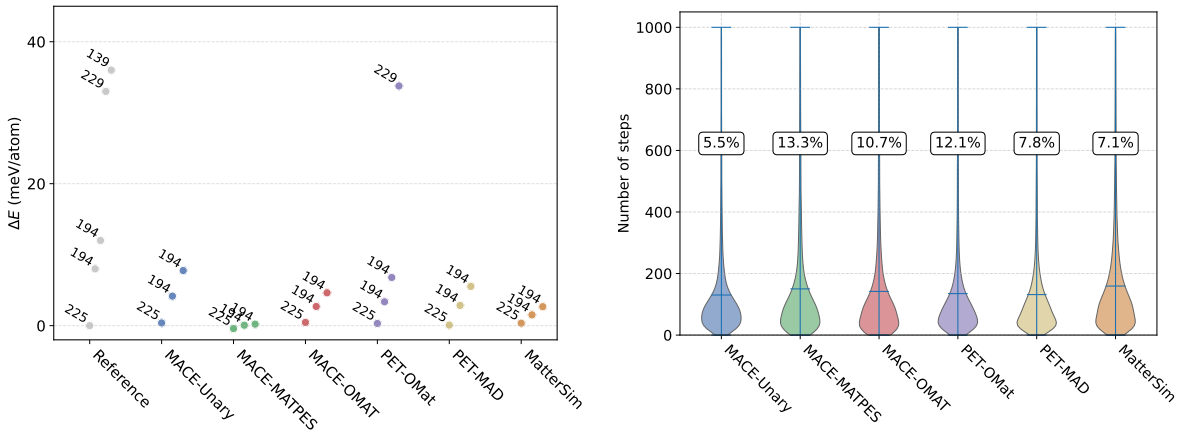

Fig. S4 Same as Fig. S1 for Cu.

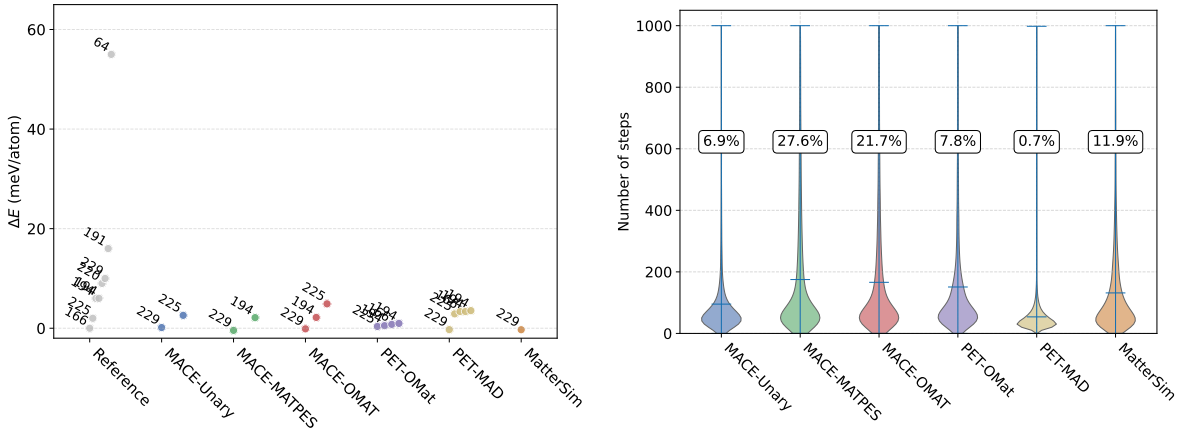

Fig. S5 Same as Fig. S1 for Li.

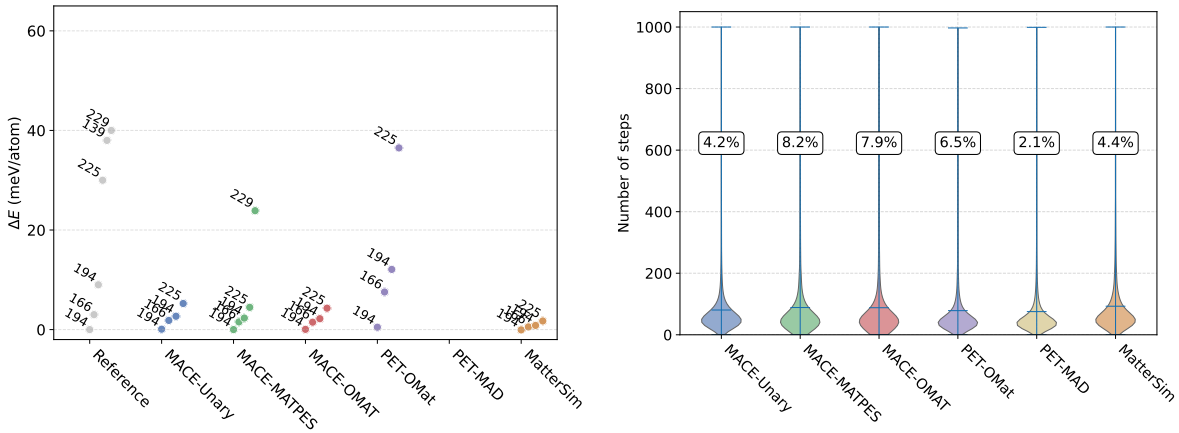

Fig. S6 Same as Fig. S1 for Mg.

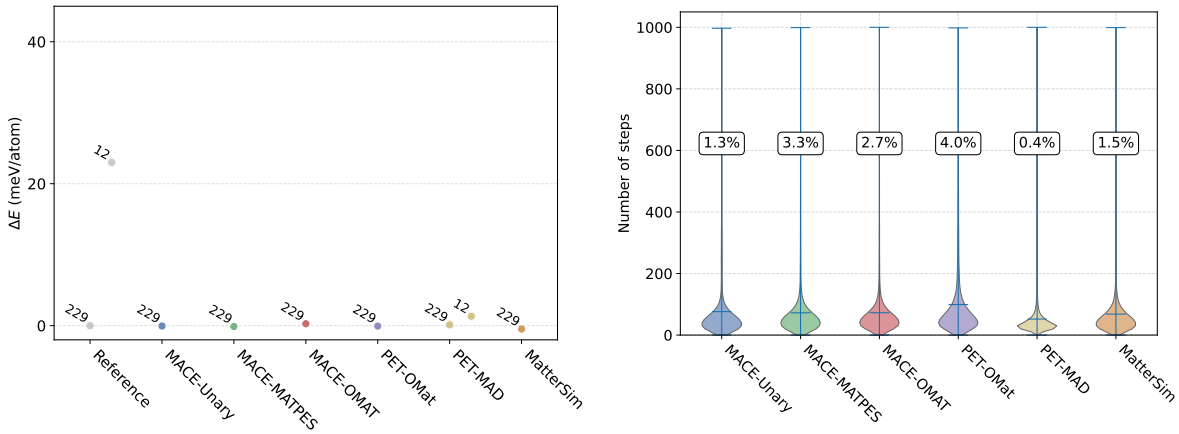

Fig. S7 Same as Fig. S1 for Nb.

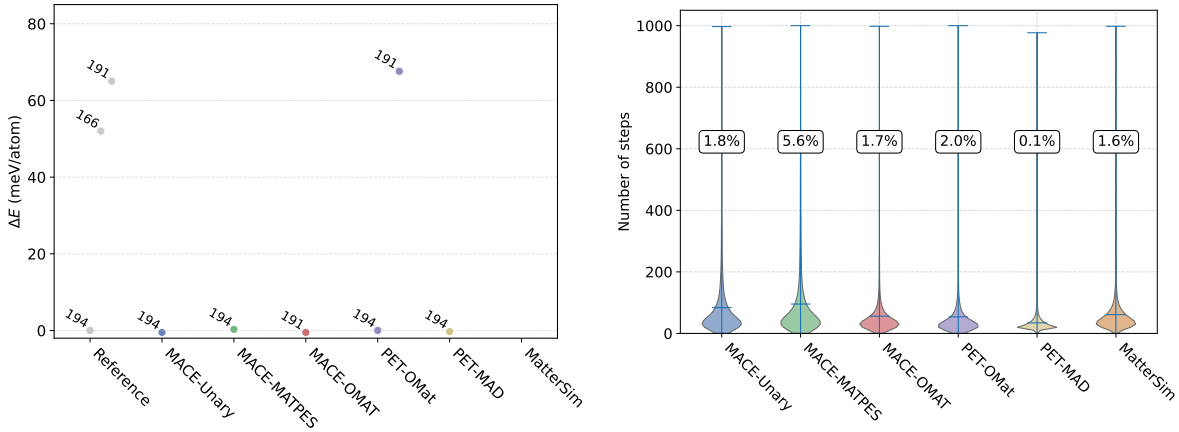

Fig. S8 Same as Fig. S1 for Sc.

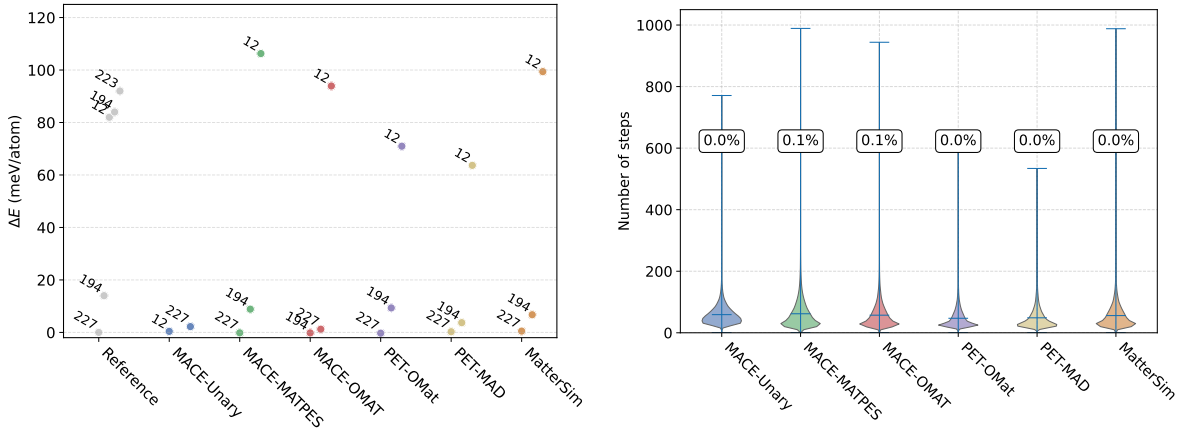

Fig. S9 Same as Fig. S1 for Si.

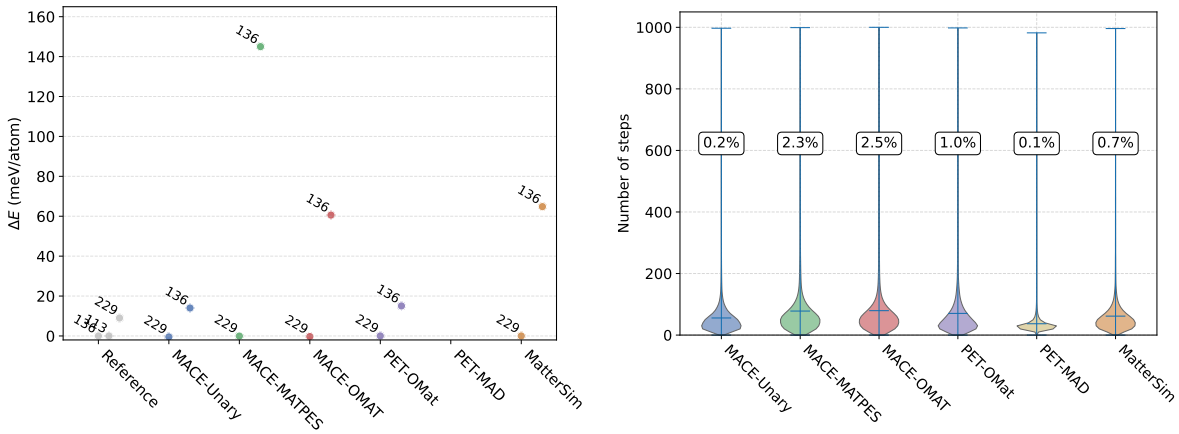

Fig. S10 Same as Fig. S1 for Ta.

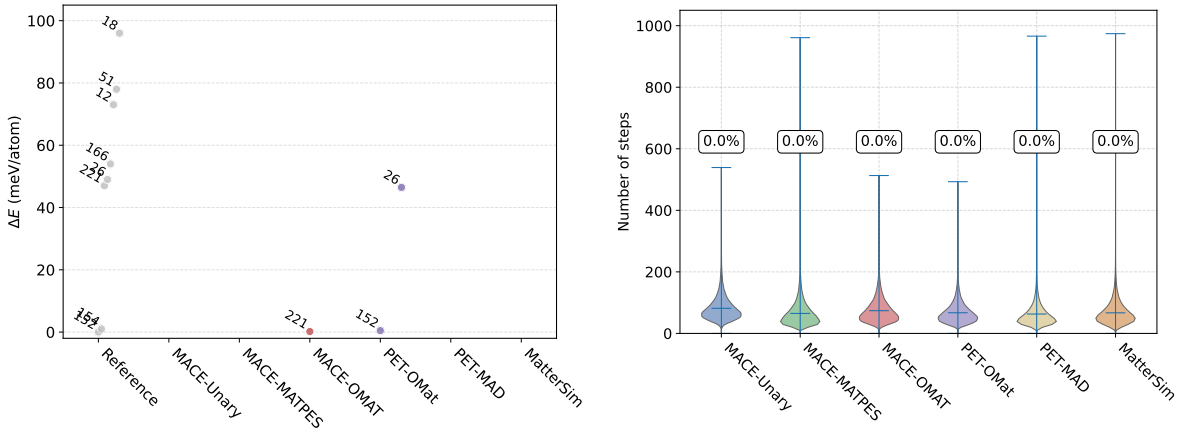

Fig. S11 Same as Fig. S1 for Te.

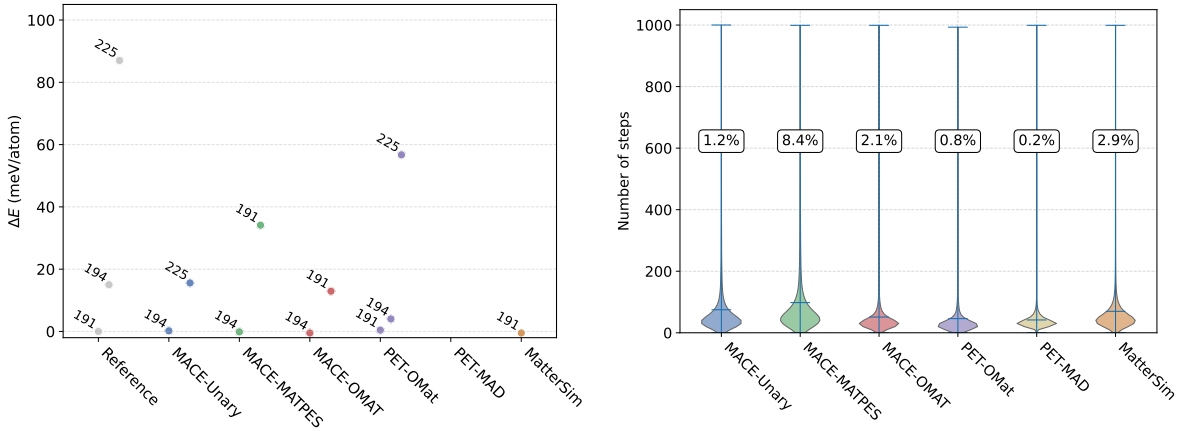

Fig. S12 Same as Fig. S1 for Ti.

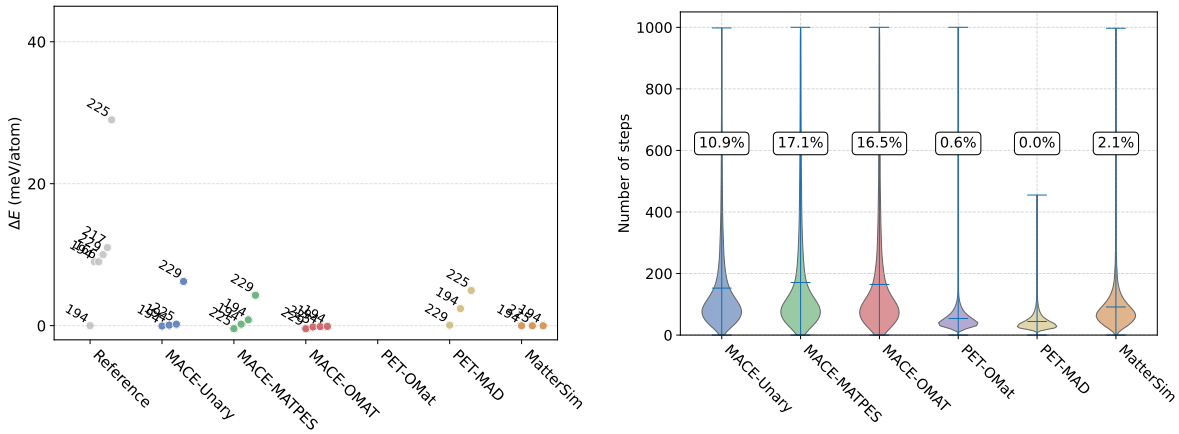

Fig. S13 Same as Fig. S1 for Tl.

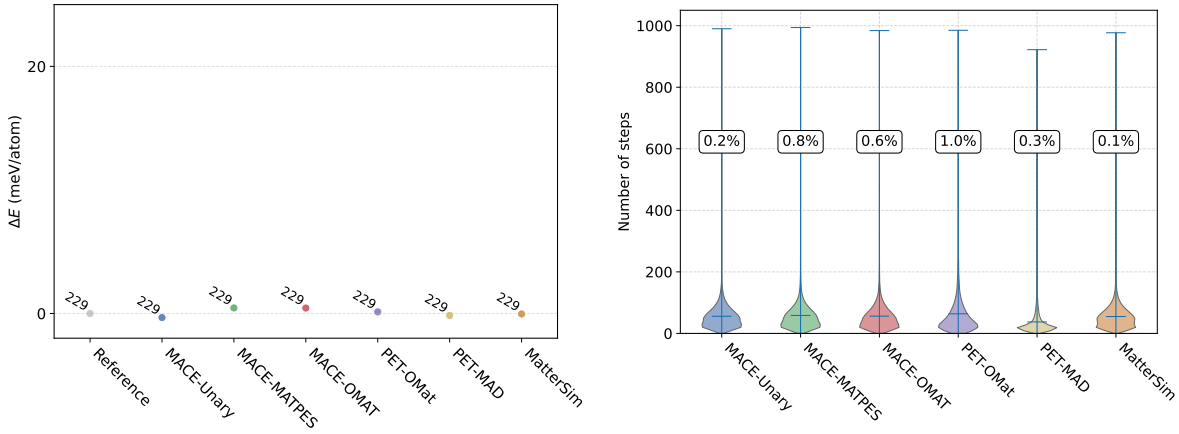

Fig. S14 Same as Fig. S1 for W.

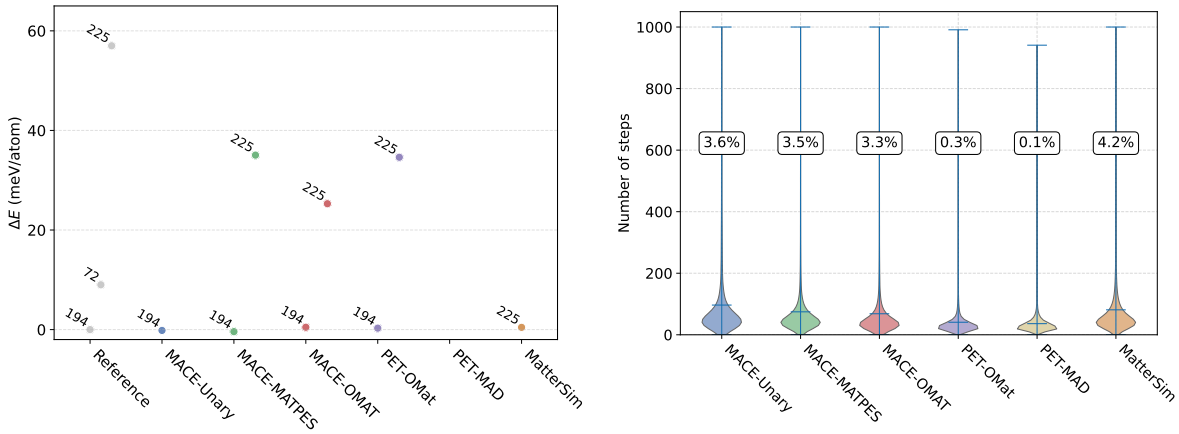

Fig. S15 Same as Fig. S1 for Zr.