*All the values are in eV for energy and eV/A for force. Please convert them to meV and meV/A for comparing against EgraFF-Bench (Xie, Y., et al. (2024))

Structured Comparative Analysis of NEquIP Models

1. MAPI1000K Dataset

1.1 Charge Layer Variation (Total Layers = 3)

n_charge	f_mae	f_rmse	e_mae	e_rmse	e/N_mae
0	0.072782	0.124360	0.901294	1.079445	0.009388
1	0.123662	0.197440	1.577349	1.930799	0.016431
2	0.061835	0.101860	0.562185	0.677054	0.005856
3	0.058681	0.099345	0.584568	0.701575	0.006089

1.2 Charge Layer Variation (Total Layers = 4)

n_charge	Model	f_mae	f_rmse	e_mae	e_rmse	e/N_mae
0	NEquIP	0.184149	0.299831	2.100765	2.622714	0.021883
1	NEquIP-LR	0.055685	0.096749	0.708633	0.819685	0.007382
2	NEquIP-LR	0.053880	0.092473	0.425607	0.525767	0.004233
3	NEquIP-LR	0.051466	0.091768	0.499241	0.579926	0.005200
4	NEquIP-LR	0.097778	0.157487	1.129627	1.345132	0.011767

1.2 Charge Layer Variation (Total Layers = 6)

1.2.1 NEquIP-LR (Charge Encoding)

n_charge	f_mae	f_rmse	e_mae	e_rmse	e/N_mae
0	0.043252	0.076170	0.393750	-	0.004102
1	0.036346	0.085771	0.335005	0.413108	0.003490
2	0.038373	0.075317	0.362729	0.458624	0.003778
3	0.053466	0.177785	0.519740	0.638799	0.005414
4	0.042153	0.079786	0.403392	0.518841	0.004202
5	0.070449	0.124761	0.859333	0.988547	0.008951
6	0.059281	0.099151	0.665777	0.780321	0.006935

1.2.2 NEquIP-noQeQ Branch

n_charge	f_mae	e_mae
0	0.043252	0.393750
1	0.092711	1.022670
2	0.033452	0.265367
3	0.048241	0.513812
4	0.058869	0.559674
5	0.203602	2.248575
6	0.075748	0.818591

1.3 Cutoff Radius (rmax) Variation (Total Layers = 6)

1.3.1 NEquIP-LR

rmax	f_mae	f_rmse	e_mae	e_rmse	e/N_mae
3.0	0.138675	0.226072	1.177262	1.660445	0.012263
4.0	0.053708	0.111494	0.547961	0.646453	-
5.0	0.038373	0.075317	0.362729	0.458624	-

1.3.2 NEquIP

rmax	f_mae	f_rmse	e_mae	e_rmse	e/N_mae
3.0	0.116975	0.182293	0.741719	-	0.007726
4.0	0.026748	0.040258	0.229922	-	0.002395
5.0	0.043252	0.076170	0.393750	-	0.004102

2. 3BPA Dataset

2.1 Charge Layer Variation (Total Layers = 3)

n_charge	Model	f_mae	f_rmse	e_mae	e/N_mae
0	NEquIP-LR	0.028580	0.044286	0.013588	0.000503
1	NEquIP-LR	0.045568	0.070022	0.026055	0.000965
2	NEquIP-LR	0.043190	0.063589	0.024439	0.000905
3	NEquIP-LR	0.025407	0.038495	0.011943	0.000442

2.2 Charge Layer Variation (Total Layers = 4)

n_charge	Model	f_mae	f_rmse	e_mae	e_rmse	e/N_mae
0	NEquIP-LR	0.024790	0.038558	0.010697	-	0.000396
1	NEquIP-LR	0.025707	0.039469	0.012319	-	0.000456
2	NEquIP-LR	0.041336	0.061439	0.021718	-	0.000804
3	NEquIP-LR	0.018950	0.030520	0.008835	0.013594	-
4	NEquIP-LR	0.022375	0.035024	0.009774	-	0.000362

2.3 Charge Layer Variation (Total Layers = 6)

2.3.1 NEquIP-LR (Charge Encoding)

n_charge	f_mae	f_rmse	e_mae	e/N_mae
0	0.025718	0.040186	0.013425	0.000497
1	0.028327	0.047643	0.013170	0.000488
2	0.022782	0.035857	0.010661	0.000395
3	0.029082	0.044118	0.013693	0.000507
4	0.021968	0.034052	0.009262	0.000343
5	0.020810	0.033271	0.010570	0.000391
6	0.022155	0.035610	0.009977	0.000370

2.3.2 NEquIP-noQeQ Branch

n_charge	f_mae	e_mae
0	0.025718	0.013425
1	0.021256	0.010126
2	0.020842	0.009747
3	0.025268	0.011797
4	0.022153	0.010048
5	0.022439	0.009883
6	0.024466	0.011530

2.4 Cutoff Radius (rmax) Variation

2.4.1 Total Layers = 3

NEquIP (Standard)

rmax	f_mae	e_mae
3	0.032146	0.019357
4	0.027585	0.012814
5	0.028580	0.013588

NEquIP-LR (Charge Encoding)

rmax	f_mae	e_mae
3	0.029923	0.018563
4	0.025919	0.014470
5	0.025407	0.011943

2.4.2 Total Layers = 4

NEquIP-LR (Charge Encoding)

rmax	f_mae	f_rmse	e_mae	e/N_mae
3	0.029563	0.046567	0.018828	0.000697
4	0.041104	0.061375	0.022087	0.000818
5	0.018950	0.030520	0.008835	-

NEquIP (Standard)

rmax	f_mae	e_mae
3	0.028188	0.017228
4	0.023353	0.010950
5	0.025718	0.013425

2.4.3 Total Layers = 6

NEquIP-LR (Charge Encoding)

rmax	f_mae	f_rmse	e_mae	e/N_mae
3	0.028833	0.047215	0.016317	0.000604
4	0.027763	0.045499	0.013127	0.000486
5	0.022782	0.035855	0.010661	0.000395

NEquIP (Standard)

rmax	f_mae	f_rmse	e_mae	e/N_mae
3	0.025323	0.042507	0.013933	0.000516
4	0.024370	0.040888	0.011776	0.000436
5	0.025718	0.040186	0.013425	0.000497

3. GeTe Dataset

3.1 Charge Layer Variation (Total Layers = 3)

n_charge	Model	f_mae	e_mae
0	NEquIP-LR	1.991741	3.379050
1	NEquIP-LR	2.647799	31.028854
2	NEquIP-LR	4.151660	10.792540
3	NEquIP-LR	11.910707	17.928699

3.2 Charge Layer Variation (Total Layers = 4)

n_charge	f_mae	e_mae
0	2.496615	2.167891
1	7.945761	89.264259
2	3.415764	5.060729
3	1.611934	2.276979
4	1.148685	0.842432

3.3 Charge Layer Variation (Total Layers = 6)

3.3.1 NEquIP-LR (Charge Encoding)

n_charge	f_mae	e_mae
0	0.874339	2.563542
1	4.601954	11.234857
2	0.377638	7.452135
3	4.460473	47.577240
4	0.519346	8.017422
5	0.418282	8.829323
6	12.024601	12.204453

3.3.2 NEquIP-noQeQ Branch (Most significant)

n_charge	f_mae	e_mae
0	0.874339	2.563542
1	0.242904	0.832826
2	0.241251	0.831849
3	0.239561	0.916237
4	0.241532	0.615117
5	0.234879	1.144414
6	0.238885	1.415169

Note that rmax variation experiments for x total layers are done with configurations that performed best in charge layers variation plot for x total layers . For ex. lets say for mapi 1000K total layers = 6, the configuration that performed best for 1 (charge layer) + 5 (standard nequip layers), then the experiments for rmax variation for total 6 layers in mapi-1000K is done with this configuration.

The table of comparision for GeTe : NequIP-NoQeQ and NequIP-charge-encoding is significant. It establishes SOTA performance with NequIP-NoQeQ for GeTe . It outperforms the sota performance in EGraFF-Bench (IITD) . Please find the results for both in their respective sections with which a comparision graph can be drawn.

In the EgraFF-Bench, Equiformer is reported as the best performing model for GeTe with e_mae - 0.66634 . For f_mae, vanilla Nequip gave the best performance in that paper. Nequip's metrics in the paper are shown as :
e_mae = 1.780951, f_mae = 0.24440
NequIP-NoQeQ outperforms them : e_mae = 0.615117. , f_mae = 0.234879

** highlight - best peformance with the present model and layers

** highlight - best performance in overall nequip-benchmark