

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	TPR ↑	TNR ↑	MAE ↓	RMSE ↓	R ² ↑	K _{SRME} ↓	Training Set	Model Params	Targets	Date Added
eqV2 M	0.917	6.047	0.924	0.975	0.910	0.986	0.020	0.072	0.848	1.771	3M (102.4M) (OMat24+ MPtrj)	86.6M	EFS _D	2024-10-18
DPA3-v1-OpenLAM	0.883	5.754	0.880	0.963	0.885	0.978	0.023	0.067	0.869	0.741	7M (112.9M) (OMat24+ MPtrj + sAlex)	8.2M	EFS _G	2025-01-10
GRACE-2L-OAM	0.880	5.774	0.883	0.963	0.878	0.979	0.023	0.068	0.862	0.294	7M (112.9M) (OMat24+ sAlex + MPtrj)	12.6M	EFS _G	2025-02-06
ORB	0.880	6.041	0.924	0.965	0.841	0.987	0.028	0.077	0.824	1.732	3M (32.1M) (MPtrj + Alex)	25.2M	EFS _D	2024-10-11
MatterSim v1 5M	0.862	5.852	0.895	0.959	0.831	0.982	0.024	0.068	0.863	0.574	17M (MatterSim)	4.5M	EFS _G	2024-12-16
MACE-MPA-0	0.852	5.582	0.853	0.954	0.851	0.973	0.028	0.073	0.842	0.412	3M (12.0M) (MPtrj + sAlex)	9.1M	EFS _G	2024-12-09
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 _G	2024-02-03
GRACE-1L-OAM	0.824	5.255	0.803	0.944	0.846	0.962	0.031	0.073	0.842	0.516	7M (112.9M) (OMat24+ sAlex + MPtrj)	3.4M	EFS _G	2025-02-06
eqV2 S DeNS	0.815	5.042	0.771	0.941	0.864	0.953	0.036	0.085	0.788	1.676	146k (1.6M) (MPtrj)	31.2M	EFS _D	2024-10-18
AlphaNet-MPTrj	0.799	4.863	0.743	0.933	0.864	0.945	0.041	0.093	0.745	1.310	146k (1.6M) (MPtrj)	16.2M	EFS _G	2025-03-05
ORB MPtrj	0.765	4.702	0.719	0.922	0.817	0.941	0.045	0.091	0.756	1.725	146k (1.6M) (MPtrj)	25.2M	EFS _D	2024-10-14
DPA3-v1-MPtrj	0.765	4.654	0.711	0.921	0.828	0.938	0.042	0.083	0.798	0.964	146k (1.6M) (MPtrj)	3.4M	EFS _G	2025-01-10
SevenNet-l3i5	0.760	4.629	0.708	0.920	0.821	0.938	0.044	0.087	0.776	0.550	146k (1.6M) (MPtrj)	1.2M	EFS _G	2024-12-10
SevenNet-0	0.724	4.252	0.650	0.904	0.818	0.919	0.048	0.092	0.750	0.767	146k (1.6M) (MPtrj)	842.4k	EFS _G	2024-07-13
GRACE-2L-MPtrj	0.691	4.163	0.636	0.896	0.757	0.921	0.052	0.094	0.741	0.525	146k (1.6M) (MPtrj)	15.3M	EFS _G	2024-11-21
MACE-MP-0	0.669	3.777	0.577	0.878	0.796	0.893	0.057	0.101	0.697	0.647	146k (1.6M) (MPtrj)	4.7M	EFS _G	2023-07-14
CHGNet	0.613	3.361	0.514	0.851	0.758	0.868	0.063	0.103	0.689	1.717	146k (1.6M) (MPtrj)	412.5k	EFS _G ^M	2023-03-03
M3GNet	0.569	2.882	0.441	0.813	0.803	0.813	0.075	0.118	0.585	1.412	63k (188.3k) (MPF)	227.5k	EFS _G	2022-09-20
ALIGNNN	0.567	3.206	0.490	0.841	0.672	0.872	0.093	0.154	0.297		155k (MP 2022)	4.0M	Energy	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	Energy	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)	Energy	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)	Energy	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)	Energy	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	Energy	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)	26.2M	Energy	2022-11-26
Dummy	0.185	1.000	0.154	0.687	0.232	0.769	0.124	0.184	0.000					