

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	TPR ↑	TNR ↑	MAE ↓	RMSE ↓	R <sup>2</sup> ↑	Training Set	Model Params	Targets	Date Added
eqV2 M	0.917	6.05	0.924	0.975	0.91	0.986	0.02	0.072	0.848	3M (102.4M) (OMat24+ <a href="#">MPtrj</a> )	86.6M	EFS <sub>D</sub>	2024-10-18
DPA3-v1-OpenLAM	0.883	5.75	0.88	0.963	0.885	0.978	0.023	0.067	0.869	7M (112.9M) (OMat24+ <a href="#">MPtrj</a> + <a href="#">sAlex</a> )	8.2M	EFS <sub>G</sub>	2025-01-10
GRACE-2L-OAM	0.88	5.77	0.883	0.963	0.878	0.979	0.023	0.068	0.862	7M (112.9M) (OMat24+ <a href="#">sAlex</a> + <a href="#">MPtrj</a> )	12.6M	EFS <sub>G</sub>	2025-02-06
ORB	0.88	6.04	0.924	0.965	0.841	0.987	0.028	0.077	0.824	3M (32.1M) ( <a href="#">MPtrj</a> + <a href="#">Alex</a> )	25.2M	EFS <sub>D</sub>	2024-10-11
MatterSim v1 5M	0.862	5.85	0.895	0.959	0.831	0.982	0.024	0.068	0.863	17M (MatterSim)	4.5M	EFS <sub>G</sub>	2024-12-16
MACE-MPA-0	0.852	5.58	0.853	0.954	0.851	0.973	0.028	0.073	0.842	3M (12.0M) ( <a href="#">MPtrj</a> + <a href="#">sAlex</a> )	9.1M	EFS <sub>G</sub>	2024-12-09
GNoME	0.829	5.52	0.844	0.955	0.814	0.972	0.035	0.085	0.785	6M (89.0M) (GNoME)	16.2M	EF <sub>G</sub>	2024-02-03
GRACE-1L-OAM	0.824	5.25	0.803	0.944	0.846	0.962	0.031	0.073	0.842	7M (112.9M) (OMat24+ <a href="#">sAlex</a> + <a href="#">MPtrj</a> )	3.4M	EFS <sub>G</sub>	2025-02-06
eqV2 S DeNS	0.815	5.04	0.771	0.941	0.864	0.953	0.036	0.085	0.788	146K (1.6M) ( <a href="#">MPtrj</a> )	31.2M	EFS <sub>D</sub>	2024-10-18
DPA3-v1-MPtrj	0.765	4.65	0.711	0.921	0.828	0.938	0.042	0.083	0.798	146K (1.6M) ( <a href="#">MPtrj</a> )	3.4M	EFS <sub>G</sub>	2025-01-10
ORB MPtrj	0.765	4.7	0.719	0.922	0.817	0.941	0.045	0.091	0.756	146K (1.6M) ( <a href="#">MPtrj</a> )	25.2M	EFS <sub>D</sub>	2024-10-14
SevenNet-l3i5	0.76	4.63	0.708	0.92	0.821	0.938	0.044	0.087	0.776	146K (1.6M) ( <a href="#">MPtrj</a> )	1.2M	EFS <sub>G</sub>	2024-12-10
SevenNet-0	0.724	4.25	0.65	0.904	0.818	0.919	0.048	0.092	0.75	146K (1.6M) ( <a href="#">MPtrj</a> )	842.4K	EFS <sub>G</sub>	2024-07-13
GRACE-2L (r6)	0.691	4.16	0.636	0.896	0.757	0.921	0.052	0.094	0.741	146K (1.6M) ( <a href="#">MPtrj</a> )	15.3M	EFS <sub>G</sub>	2024-11-21
MACE-MP-0	0.669	3.78	0.577	0.878	0.796	0.893	0.057	0.101	0.697	146K (1.6M) ( <a href="#">MPtrj</a> )	4.7M	EFS <sub>G</sub>	2023-07-14
CHGNet	0.613	3.36	0.514	0.851	0.758	0.868	0.063	0.103	0.689	146K (1.6M) ( <a href="#">MPtrj</a> )	412.5K	EFS <sub>G</sub> <sup>M</sup>	2023-03-03
M3GNet	0.569	2.88	0.441	0.813	0.803	0.813	0.075	0.118	0.585	63K (188.3K) ( <a href="#">MPF</a> )	227.5K	EFS <sub>G</sub>	2022-09-20
ALIGNNN	0.567	3.21	0.49	0.841	0.672	0.872	0.093	0.154	0.297	155K ( <a href="#">MP 2022</a> )	4.0M	Energy	2023-06-02
MEGNet	0.51	2.96	0.452	0.826	0.585	0.87	0.13	0.206	-0.248	133K ( <a href="#">MP Graphs</a> )	167.8K	Energy	2022-11-14
CGCNN	0.507	2.85	0.436	0.818	0.605	0.857	0.138	0.233	-0.603	155K ( <a href="#">MP 2022</a> )	128.4K (N=10)	Energy	2022-12-28
CGCNN+P	0.5	2.56	0.392	0.786	0.693	0.803	0.113	0.182	0.019	155K ( <a href="#">MP 2022</a> )	128.4K (N=10)	Energy	2023-02-03
Wrenformer	0.466	2.26	0.345	0.745	0.719	0.75	0.11	0.186	-0.018	155K ( <a href="#">MP 2022</a> )	5.2M (N=10)	Energy	2022-11-26
BOWSR	0.423	1.96	0.3	0.712	0.718	0.693	0.118	0.167	0.151	133K ( <a href="#">MP Graphs</a> )	167.8K	Energy	2022-11-17
Voronoi RF	0.333	1.58	0.241	0.668	0.535	0.692	0.148	0.212	-0.329	155K ( <a href="#">MP 2022</a> )	26.2M	Energy	2022-11-26
Dummy	0.185	1	0.154	0.687	0.232	0.769	0.124	0.184	0				