

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	MAE ↓	RMSE ↓	R ² ↑
eqV2 M	0.988	6.38	0.976	0.976	0.015	0.066	0.904
DPA3-v1-OpenLAM	0.987	6.37	0.974	0.974	0.019	0.066	0.905
GRACE-2L-OAM	0.985	6.35	0.971	0.971	0.022	0.081	0.861
ORB	0.985	6.35	0.97	0.97	0.019	0.068	0.897
MatterSim v1 5M	0.984	6.34	0.969	0.969	0.022	0.078	0.869
eqV2 S DeNS	0.983	6.33	0.967	0.967	0.031	0.091	0.823
MACE-MPA-0	0.978	6.26	0.957	0.957	0.032	0.105	0.776
ORB MPtrj	0.971	6.17	0.944	0.944	0.037	0.098	0.801
DPA3-v1-MPtrj	0.971	6.17	0.944	0.944	0.038	0.084	0.849
GNoME	0.967	6.13	0.937	0.937	0.035	0.089	0.836
GRACE-1L-OAM	0.962	6.06	0.927	0.927	0.035	0.087	0.843
SevenNet-l3i5	0.952	5.95	0.909	0.909	0.05	0.114	0.745
SevenNet-0	0.945	5.86	0.895	0.895	0.054	0.124	0.7
CHGNet	0.92	5.57	0.851	0.851	0.063	0.095	0.816
GRACE-2L (r6)	0.914	5.5	0.841	0.841	0.065	0.133	0.641
MACE-MP-0	0.888	5.22	0.798	0.798	0.087	0.165	0.508
M3GNet	0.868	5.02	0.767	0.767	0.101	0.158	0.551
ALIGNN	0.748	3.9	0.597	0.597	0.176	0.247	0.081
CGCNN	0.745	3.88	0.593	0.593	0.165	0.23	0.181
CGCNN+P	0.736	3.81	0.583	0.583	0.2	0.275	-0.076
Wrenformer	0.721	3.69	0.564	0.564	0.182	0.239	0.138
BOWSR	0.664	3.25	0.497	0.497	0.259	0.32	-1.17
MEGNet	0.632	3.02	0.462	0.462	0.304	0.336	-0.908
Voronoi RF	0.551	2.49	0.38	0.38	0.349	0.417	-1.01
Dummy	0.194	1	0.168	0.68	0.12	0.181	0