

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	MAE ↓	RMSE ↓	R <sup>2</sup> ↑
MatterSim	0.989	6.4	0.978	0.978	0.02	0.065	0.906
eqV2 M	0.988	6.38	0.976	0.976	0.015	0.066	0.904
ORB	0.985	6.35	0.97	0.97	0.019	0.068	0.897
eqV2 S DeNS	0.983	6.33	0.967	0.967	0.031	0.091	0.823
ORB MPtrj	0.971	6.17	0.944	0.944	0.037	0.098	0.801
GNoME	0.967	6.13	0.937	0.937	0.035	0.089	0.836
SevenNet	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
MACE	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
ALIGNNN	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