

	F1 ↑	DAF ↑	Prec ↑	Acc ↑	MAE ↓	RMSE ↓	R <sup>2</sup> ↑
MatterSim	0.989	6.401	0.978	0.978	0.020	0.065	0.906
ORB	0.988	6.390	0.977	0.977	0.019	0.064	0.908
GNoME	0.967	6.127	0.937	0.937	0.035	0.089	0.836
ORB MPtrj	0.963	6.079	0.929	0.929	0.041	0.103	0.781
SevenNet	0.945	5.857	0.895	0.895	0.054	0.124	0.700
CHGNet	0.920	5.567	0.851	0.851	0.063	0.095	0.816
MACE	0.888	5.221	0.798	0.798	0.087	0.165	0.508
M3GNet	0.868	5.020	0.767	0.767	0.101	0.158	0.551
ALIGNN	0.748	3.905	0.597	0.597	0.176	0.247	0.081
CGCNN	0.745	3.880	0.593	0.593	0.165	0.230	0.181
CGCNN+P	0.736	3.813	0.583	0.583	0.200	0.275	-0.076
Wrenformer	0.721	3.691	0.564	0.564	0.182	0.239	0.138
BOWSR	0.664	3.252	0.497	0.497	0.259	0.320	-1.172
MEGNet	0.632	3.022	0.462	0.462	0.304	0.336	-0.908
Voronoi RF	0.551	2.487	0.380	0.380	0.349	0.417	-1.012
Dummy	0.194	1	0.168	0.680	0.120	0.181	0