

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	MAE ↓	RMSE ↓	R ² ↑
eqV2 S DeNS	0.983	6.326	0.967	0.967	0.031	0.091	0.823
ORB MPtrj	0.971	6.173	0.944	0.944	0.037	0.098	0.801
DPA3-v1-MPtrj	0.971	6.174	0.944	0.944	0.038	0.084	0.849
AlphaNet-MPTrj	0.960	6.042	0.924	0.924	0.045	0.115	0.746
SevenNet-l3i5	0.952	5.945	0.909	0.909	0.050	0.114	0.745
SevenNet-0	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
GRACE-2L-MPtrj	0.914	5.503	0.841	0.841	0.065	0.133	0.641
MACE-MP-0	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	1.000	0.168	0.680	0.120	0.181	0.000