

Model	F1 \uparrow	DAF \uparrow	Prec \uparrow	Acc \uparrow	MAE \downarrow	RMSE \downarrow	R ² \uparrow
eqV2 M	0.988	6.38	0.976	0.976	0.015	0.066	0.904
DPA3-1-OpenLAM	0.987	6.37	0.974	0.974	0.019	0.065	0.904
ORB	0.985	6.35	0.97	0.97	0.019	0.068	0.897
MatterSim-v1	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
DPA3-1-MPtrj	0.971	6.17	0.944	0.944	0.039	0.128	0.649
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-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