

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	TPR ↑	TNR ↑	MAE ↓	RMSE ↓	R ² ↑
eqV2 M	0.896	5.24	0.9	0.965	0.893	0.979	0.02	0.071	0.842
ORB	0.858	5.28	0.906	0.954	0.815	0.983	0.028	0.078	0.814
MatterSim-v1	0.838	5.12	0.879	0.947	0.801	0.977	0.024	0.069	0.854
MACE-MPA-0	0.836	4.87	0.836	0.944	0.836	0.966	0.028	0.073	0.837
GNoME	0.81	4.81	0.825	0.942	0.796	0.965	0.034	0.083	0.786
eqV2 S DeNS	0.798	4.36	0.748	0.927	0.855	0.941	0.035	0.084	0.785
ORB MPtrj	0.755	4.19	0.719	0.911	0.795	0.936	0.043	0.09	0.752
SevenNet-l3i5	0.751	4.11	0.706	0.909	0.803	0.931	0.042	0.086	0.773
SevenNet-0	0.719	3.8	0.653	0.893	0.8	0.912	0.046	0.09	0.75
GRACE-2L (r6)	0.687	3.71	0.637	0.884	0.746	0.912	0.05	0.092	0.74
MACE-MP-0	0.668	3.4	0.583	0.867	0.781	0.885	0.055	0.099	0.698
CHGNet	0.612	3.04	0.521	0.839	0.74	0.859	0.061	0.1	0.69
M3GNet	0.576	2.65	0.454	0.802	0.788	0.804	0.072	0.115	0.588
ALIGNNN	0.565	2.92	0.501	0.829	0.649	0.866	0.092	0.154	0.274
MEGNet	0.513	2.7	0.463	0.813	0.574	0.862	0.128	0.204	-0.277
CGCNN+P	0.51	2.4	0.411	0.779	0.67	0.801	0.108	0.178	0.027
CGCNN	0.51	2.63	0.451	0.807	0.587	0.852	0.135	0.229	-0.624
Wrenformer	0.479	2.13	0.365	0.741	0.693	0.751	0.105	0.182	-0.02
BOWSR	0.437	1.84	0.315	0.702	0.711	0.68	0.114	0.164	0.142
Voronoi RF	0.344	1.51	0.259	0.665	0.511	0.697	0.141	0.206	-0.316
Dummy	0.194	1	0.168	0.68	0.231	0.77	0.12	0.181	0