

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	TPR ↑	TNR ↑	MAE ↓	RMSE ↓	R <sup>2</sup> ↑
eqV2 S DeNS	0.798	4.36	0.748	0.927	0.855	0.941	0.035	0.084	0.785
DPA3-1-MPtrj	0.757	4.13	0.708	0.911	0.812	0.931	0.04	0.085	0.776
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
ALIGNN	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