

Model	F1 ↑	DAF ↑	Prec ↑	Acc ↑	TPR ↑	TNR ↑	MAE ↓	RMSE ↓	R <sup>2</sup> ↑
eqV2 M	0.896	5.24	0.9	0.965	0.893	0.979	0.02	0.071	0.842
DPA3-v1-OpenLAM	0.862	5.01	0.86	0.953	0.865	0.971	0.023	0.067	0.863
GRACE-2L-OAM	0.861	5.05	0.866	0.953	0.856	0.973	0.023	0.068	0.856
ORB	0.858	5.28	0.906	0.954	0.815	0.983	0.028	0.078	0.814
MatterSim v1 5M	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
GRACE-1L-OAM	0.808	4.62	0.792	0.933	0.824	0.955	0.03	0.073	0.836
eqV2 S DeNS	0.798	4.36	0.748	0.927	0.855	0.941	0.035	0.084	0.785
DPA3-v1-MPtrj	0.757	4.13	0.709	0.911	0.812	0.931	0.04	0.082	0.793
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