GNN Leaderboard - Formation Energy

Stability Threshold: 0.01 eV/atom

Dataset: convex_hull

GNN	MAE	R²	N	Precision	Recall	Accuracy	TP	FP	FN	TN
DPA31	0.038	1.00	295	0.969	0.969	0.986	63	2	2	228
ESEN_30M_OAM	0.042	1.00	295	0.970	0.985	0.990	64	2	1	228
SEVENNET	0.042	1.00	295	0.985	1.000	0.997	65	1	0	229
NEQUIP	0.044	1.00	295	1.000	1.000	1.000	65	0	0	230
ALLEGRO	0.045	1.00	295	0.985	0.985	0.993	64	1	1	229
GRACE_2L_OAM_L	0.071	0.99	295	1.000	0.985	0.997	64	0	1	230
MACE_MPA_0	0.071	0.99	295	0.985	0.985	0.993	64	1	1	229
ORBV3	0.111	0.97	295	0.985	0.985	0.993	64	1	1	229

Dataset: binary_alloys

GNN	MAE	R²	N	Precision	Recall	Accuracy	TP	FP	FN	TN
ALLEGRO	0.077	0.97	4840	0.917	0.957	0.962	1364	123	62	3291
SEVENNET	0.078	0.97	4840	0.912	0.955	0.960	1362	131	64	3283
NEQUIP	0.080	0.97	4840	0.900	0.959	0.957	1368	152	58	3262
MACE_MPA_0	0.081	0.97	4840	0.890	0.950	0.951	1354	167	72	3247
DPA31	0.086	0.97	4840	0.904	0.954	0.957	1361	145	65	3269
ORBV3	0.092	0.96	4840	0.903	0.950	0.955	1355	145	71	3269
GRACE_2L_OAM_L	0.108	0.94	4840	0.910	0.952	0.958	1357	134	69	3280
ESEN_30M_OAM	0.247	0.39	4840	0.866	0.959	0.944	1368	212	58	3202

Dataset: liquid_alloys

GNN	MAE	R²	N	Precision	Recall	Accuracy	TP	FP	FN	TN
GRACE_2L_OAM_L	0.005	0.98	4184	0.000	0.000	1.000	0	0	0	4184
ESEN_30M_OAM	0.006	0.97	4184	0.000	0.000	1.000	0	0	0	4184
MACE_MPA_0	0.006	0.96	4184	0.000	0.000	1.000	0	0	0	4184
DPA31	0.007	0.94	4184	0.000	0.000	1.000	0	0	0	4184
NEQUIP	0.007	0.95	4184	0.000	0.000	1.000	0	0	0	4184
ALLEGRO	0.008	0.94	4184	0.000	0.000	1.000	0	0	0	4184
SEVENNET	0.008	0.94	4184	0.000	0.000	1.000	0	0	0	4184
ORBV3	0.012	0.87	4184	0.000	0.000	1.000	0	0	0	4184

Dataset: random_alloys

GNN	MAE	R²	N	Precision	Recall	Accuracy	TP	FP	FN	TN
GRACE_2L_OAM_L	0.602	-9.23	4740	0.010	0.639	0.500	23	2358	13	2346
ESEN_30M_OAM	0.603	-9.25	4740	0.010	0.639	0.500	23	2356	13	2348
ALLEGRO	0.603	-9.25	4740	0.010	0.639	0.499	23	2361	13	2343
NEQUIP	0.604	-9.27	4740	0.010	0.639	0.498	23	2368	13	2336
ORBV3	0.604	-9.32	4740	0.010	0.639	0.502	23	2348	13	2356
SEVENNET	0.605	-9.31	4740	0.010	0.639	0.497	23	2372	13	2332
DPA31	0.609	-9.42	4740	0.009	0.639	0.491	23	2400	13	2304
MACE_MPA_0	0.624	-9.85	4740	0.010	0.694	0.478	25	2465	11	2239