Model

eqV2 S DeNS

ORB MPtri

AlphaNet-MPTri

DPA3-v1-MPtrj

SevenNet-I3i5

GRACE-2L-MPtri

SevenNet-0

MACE-MP-0

CHGNet

M3GNet

ALIGNN

MEGNet

CGCNN

BOWSR

Dummy

CGCNN+P

Wrenformer

Voronoi RF

0.815 5.042

0.567 3.206 0.490

0.466 2.256 0.345

0.743

DAF \uparrow Prec \uparrow Acc \uparrow TPR \uparrow TNR \uparrow MAE \downarrow RMSE \downarrow R² \uparrow

0.941 0.864 0.953

0.933 0.864 0.945

0.765 4.702 0.719 0.922 0.817 0.941 0.045

0.760 4.629 0.708 0.920 0.821 0.938 0.044

0.724 4.252 0.650 0.904 0.818 0.919 0.048

0.691 4.163 0.636 0.896 0.757 0.921 0.052

0.669 3.777 0.577 0.878 0.796 0.893 0.057

0.613 3.361 0.514 0.851 0.758 0.868 0.063

0.500 2.563 0.392 0.786 0.693 0.803 0.113

0.423 1.964 0.300 0.712 0.718 0.693 0.118

0.185 1.000 0.154 0.687 0.232 0.769 0.124

0.510 2.959 0.452 0.826 0.585 0.870

0.507 2.855 0.436 0.818 0.605 0.857

0.241

0.569 2.882 0.441 0.813 0.803 0.813 0.075 0.118

0.841 0.672 0.872 0.093

0.745 0.719 0.750 0.110

0.668 0.535 0.692 0.148

0.765 4.654 0.711 0.921 0.828 0.938 0.042 0.083

K_{SRME} ↓ Training Set

146k (1.6M) (MPtrj)

146k (1.6M) (MPtrj) 16.2M

146k (1.6M) (MPtri) 25.2M

146k (1.6M) (MPtrj) 3.4M

146k (1.6M) (MPtrj) 1.2M

146k (1.6M) (MPtrj) 842.4k

146k (1.6M) (MPtrj) 15.3M

146k (1.6M) (MPtrj) 4.7M

63k (188.3k) (MPF)

155k (MP 2022)

133k (MP Graphs)

133k (MP Graphs)

146k (1.6M) (MPtrj) 412.5k

31.2M

227.5k

167.8k

167.8k

26.2M

128.4k (N=10)

128.4k (N=10)

5.2M (N=10)

4.0M

0.788

0.745

0.756

0.798

0.776

0.750

0.697

0.689

0.585

0.297

-0.248

-0.603

0.019

-0.018

0.151

-0.329

0.000

0.087

0.092

0.094

0.101

0.103

0.206

0.186

0.212

0.130

0.138 0.233

1.676

1.310

1.725

0.964

0.550

0.767

0.647

1.717

1.412

0.741 0.525

Model Params Targets Date Added

EFS_D

EFS_G

EFS_D

EFS_G

EFS_G

EFS_G

EFS_G

EFS_G

EFS_CM

EFS_G

Energy

Energy

Energy

Energy

Energy

Energy

Energy

2024-10-18

2025-03-05

2024-10-14

2025-01-10

2024-12-10

2024-07-13

2024-11-21

2023-07-14

2023-03-03

2022-09-20

2023-06-02

2022-11-14

2022-12-28

2023-02-03

2022-11-26

2022-11-17

2022-11-26