DAF \uparrow **Prec** \uparrow **Acc** \uparrow **TPR** \uparrow **TNR** \uparrow **MAE** \downarrow **RMSE** \downarrow **R**² \uparrow

0.922 0.817 0.941 0.045

0.441 0.813 0.803 0.813 0.075 0.118

0.904 0.818 0.919 0.048 0.092

0.841 0.672 0.872 0.093 0.154

0.712 0.718 0.693 0.118 0.167

0.668 0.535 0.692 0.148

0.036

0.13

0.138

0.113

0.124

0.11

0.091

0.101

0.103

0.206

0.186

0.212

0.941 0.864 0.953

0.577 0.878 0.796 0.893 0.057

0.514 0.851 0.758 0.868 0.063

0.452 0.826 0.585 0.87

0.436 0.818 0.605 0.857

0.392 0.786 0.693 0.803

0.745 0.719 0.75

0.687 0.232 0.769

K_{SRME} ↓ Training Set

146K (1.6M) (MPtrj) 31.2M

146K (1.6M) (MPtrj) 25.2M

146K (1.6M) (MPtri) 842.4K

146K (1.6M) (MPtri) 412.5K

227.5K

167.8K

167.8K

26.2M

128.4K (N=10)

128.4K (N=10)

5.2M (N=10)

4.0M

146K (1.6M) (MPtrj) 4.7M

63K (188.3K) (MPF)

133K (MP Graphs)

155K (MP 2022)

133K (MP Graphs)

1.67

1.73

0.767

0.647

1.72

1.41

0.788

0.756

0.75

0.697

0.689

0.585

0.297

-0.248

-0.603

0.019

0.151

-0.329

-0.018

Model Params Targets Date Added

EFS_D

EFS_D

EFS_C

EFS_C

EFS_CM

EFS_C

Е

Ε

Е

2024-10-18

2024-10-14

2024-07-13

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

Model

eqV2 S DeNS

ORB MPtri

SevenNet

MACE

CHGNet

M3GNet

ALIGNN

MEGNet

CGCNN

BOWSR

Dummy

CGCNN+P

Wrenformer

Voronoi RF

0.815 5.04

0.765 4.7

0.724 4.25

0.613 3.36

0.567 3.21

0.507 2.85

0.466 2.26

0.423 1.96

0.333 1.58

0.185 1

2.56

0.771

0.719

0.65

0.49

0.345

0.241

0.154