

| Model | F1 ↑ | DAF ↑ | Prec ↑ | Acc ↑ | TPR ↑ | TNR ↑ | MAE ↓ | RMSE ↓ | R ² ↑ | Training Set | Model Params | Targets | Date Added |
|------------|-------|-------|--------|-------|-------|-------|-------|--------|------------------|--|---------------|-------------------------------|------------|
| eqV2 | 0.917 | 6.047 | 0.924 | 0.975 | 0.910 | 0.986 | 0.020 | 0.072 | 0.848 | 3M (102.4M) (OMat24 + MPtrj) | 86.6M | EFS _D | 2024-10-18 |
| ORB | 0.880 | 6.041 | 0.924 | 0.965 | 0.841 | 0.987 | 0.028 | 0.077 | 0.824 | 3M (32.1M) (MPtrj + Alex) | 25.2M | EFS _D | 2024-10-11 |
| MatterSim | 0.859 | 5.646 | 0.863 | 0.957 | 0.856 | 0.975 | 0.026 | 0.080 | 0.812 | 17M (MatterSim) | 182.0M | EFS _D | 2024-06-16 |
| GNoME | 0.829 | 5.523 | 0.844 | 0.955 | 0.814 | 0.972 | 0.035 | 0.085 | 0.785 | 6M (89.0M) (GNoME) | 16.2M | EF _C | 2024-02-03 |
| eqV2 DeNS | 0.815 | 5.042 | 0.771 | 0.941 | 0.864 | 0.953 | 0.036 | 0.085 | 0.788 | 146K (1.6M) (MPtrj) | 31.2M | EFS _D | 2024-10-18 |
| ORB MPtrj | 0.765 | 4.702 | 0.719 | 0.922 | 0.817 | 0.941 | 0.045 | 0.091 | 0.756 | 146K (1.6M) (MPtrj) | 25.2M | EFS _D | 2024-10-14 |
| SevenNet | 0.724 | 4.252 | 0.650 | 0.904 | 0.818 | 0.919 | 0.048 | 0.092 | 0.750 | 146K (1.6M) (MPtrj) | 842.4K | EFS _C | 2024-07-13 |
| MACE | 0.669 | 3.777 | 0.577 | 0.878 | 0.796 | 0.893 | 0.057 | 0.101 | 0.697 | 146K (1.6M) (MPtrj) | 4.7M | EFS _C | 2023-07-14 |
| CHGNet | 0.613 | 3.361 | 0.514 | 0.851 | 0.758 | 0.868 | 0.063 | 0.103 | 0.689 | 146K (1.6M) (MPtrj) | 412.5K | EFS _C ^M | 2023-03-03 |
| M3GNet | 0.569 | 2.882 | 0.441 | 0.813 | 0.803 | 0.813 | 0.075 | 0.118 | 0.585 | 63K (188.3K) (MPF) | 227.5K | EFS _C | 2022-09-20 |
| ALIGNN | 0.567 | 3.206 | 0.490 | 0.841 | 0.672 | 0.872 | 0.093 | 0.154 | 0.297 | 155K (MP 2022) | 4.0M | E | 2023-06-02 |
| MEGNet | 0.510 | 2.959 | 0.452 | 0.826 | 0.585 | 0.870 | 0.130 | 0.206 | -0.248 | 133K (MP Graphs) | 167.8K | E | 2022-11-14 |
| CGCNN | 0.507 | 2.855 | 0.436 | 0.818 | 0.605 | 0.857 | 0.138 | 0.233 | -0.603 | 155K (MP 2022) | 128.4K (N=10) | E | 2022-12-28 |
| CGCNN+P | 0.500 | 2.563 | 0.392 | 0.786 | 0.693 | 0.803 | 0.113 | 0.182 | 0.019 | 155K (MP 2022) | 128.4K (N=10) | E | 2023-02-03 |
| Wrenformer | 0.466 | 2.256 | 0.345 | 0.745 | 0.719 | 0.750 | 0.110 | 0.186 | -0.018 | 155K (MP 2022) | 5.2M (N=10) | E | 2022-11-26 |
| BOWSR | 0.423 | 1.964 | 0.300 | 0.712 | 0.718 | 0.693 | 0.118 | 0.167 | 0.151 | 133K (MP Graphs) | 167.8K | E | 2022-11-17 |
| Voronoi RF | 0.333 | 1.579 | 0.241 | 0.668 | 0.535 | 0.692 | 0.148 | 0.212 | -0.329 | 155K (MP 2022) | 26.2M | E | 2022-11-26 |
| Dummy | 0.185 | 1 | 0.154 | 0.687 | 0.232 | 0.769 | 0.124 | 0.184 | 0 | | | | |