

| 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            |
| DPA3-1-OpenLAM | 0.862 | 5.01  | 0.86   | 0.953 | 0.865 | 0.971 | 0.023 | 0.068  | 0.857            |
| ORB            | 0.858 | 5.28  | 0.906  | 0.954 | 0.815 | 0.983 | 0.028 | 0.078  | 0.814            |
| MatterSim-v1   | 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            |
| eqV2 S DeNS    | 0.798 | 4.36  | 0.748  | 0.927 | 0.855 | 0.941 | 0.035 | 0.084  | 0.785            |
| DPA3-1-MPtrj   | 0.757 | 4.13  | 0.708  | 0.911 | 0.812 | 0.931 | 0.04  | 0.085  | 0.776            |
| 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                |