

| Model | F1 ↑ | DAF ↑ | Prec ↑ | Acc ↑ | MAE ↓ | RMSE ↓ | R ² ↑ |
|------------|-------|-------|--------|-------|-------|--------|------------------|
| eqV2 DeNS | 0.983 | 6.326 | 0.967 | 0.967 | 0.031 | 0.091 | 0.823 |
| ORB MPtrj | 0.971 | 6.173 | 0.944 | 0.944 | 0.037 | 0.098 | 0.801 |
| SevenNet | 0.945 | 5.857 | 0.895 | 0.895 | 0.054 | 0.124 | 0.700 |
| CHGNet | 0.920 | 5.567 | 0.851 | 0.851 | 0.063 | 0.095 | 0.816 |
| MACE | 0.888 | 5.221 | 0.798 | 0.798 | 0.087 | 0.165 | 0.508 |
| M3GNet | 0.868 | 5.020 | 0.767 | 0.767 | 0.101 | 0.158 | 0.551 |
| ALIGNN | 0.748 | 3.905 | 0.597 | 0.597 | 0.176 | 0.247 | 0.081 |
| CGCNN | 0.745 | 3.880 | 0.593 | 0.593 | 0.165 | 0.230 | 0.181 |
| CGCNN+P | 0.736 | 3.813 | 0.583 | 0.583 | 0.200 | 0.275 | -0.076 |
| Wrenformer | 0.721 | 3.691 | 0.564 | 0.564 | 0.182 | 0.239 | 0.138 |
| BOWSR | 0.664 | 3.252 | 0.497 | 0.497 | 0.259 | 0.320 | -1.172 |
| MEGNet | 0.632 | 3.022 | 0.462 | 0.462 | 0.304 | 0.336 | -0.908 |
| Voronoi RF | 0.551 | 2.487 | 0.380 | 0.380 | 0.349 | 0.417 | -1.012 |
| Dummy | 0.194 | 1 | 0.168 | 0.680 | 0.120 | 0.181 | 0 |