–Electronic Supporting Information–
Optimal pre-train/fine-tune strategies for accurate material property predictions

Reshma Devi[1], **Keith T. Butler**[2,*], **and Gopalakrishnan Sai Gautam**[1,*]

[1]Department of Materials Engineering, Indian Institute of Science, Bengaluru 560012, Karnataka, India
[2]Department of Chemistry, University College London, London WC1E 6BT, United Kingdom
[*]k.t.butler@ucl.ac.uk; saigautamg@iisc.ac.in

S1 Default ALIGNN configuration

The default atomistic line graph neural network (ALIGNN) configuration utilized in this study is depicted in Table S1. Across all experiments, we maintained the number of epochs at 500, as we consistently observed the validation loss converging around this epoch count in all instances. In fine-tune (FT) experiments involving 10 datapoints, we set the batch size to 1. For pre-training (PT) with larger datasets of 50K and 100K, we used a batch size of 64.

Parameter	Value
ALIGNN layers	4
Graph Convolutional Network(GCN) layers	4
Atom input features	92
Edge input features	80
Bond angle input features	40
Embedding features	64
Hidden features	256
Normalization	Batch
Batch size	16 (or 1 or 64 depending on the dataset size)
PT learning rate	0.0001
FT learning rate	0.001
Optimizer	Adaptive Moment Estimation with weight decay (Adamw)
Weight decay	0.00001
Random seed	123
Epochs	500

Table S1. Configuration of the ALIGNN model used in this work.

S2 Statistics within each dataset considered

Table S2 presents dataset size, mean, range (minimum and maximum), standard deviation (σ) of the training dataset, and the specified units of each dataset considered in this work. GV, PH, FE, BG, PZ, DC, and EBG stand for average shear modulus, frequency of the highest optical phonon mode peak, formation energy, computed band gap, piezoelectric modulus, dielectric constant, and experimental band gap, respectively. EBG dataset contains fewer datapoints than the original available in the Matminer library, as we considered only those datapoints that were tagged with a valid materials project (MP) ID.

Name	Dataset size	Units	Minimum	Maximum	Mean	σ
GV	10987	$\log_{10}$(GV in GPa)	0.0	2.719	1.551	0.373
PH	1265	cm^{-1}	59.586	3643.743	568.354	464.218
FE	132752	eV/atom	-4.612	2.500	-1.410	1.623
BG	106113	eV	0.0	9.721	1.216	1.599
PZ	941	$C\ m^{-2}$	6^{-06}	46.193	0.740	1.845
DC	1056	-	2.080	277.780	15.107	20.262
EBG	2481	eV	0.0	11.7	1.044	1.614

Table S2. Compilation of training data statistics within all datasets considered.

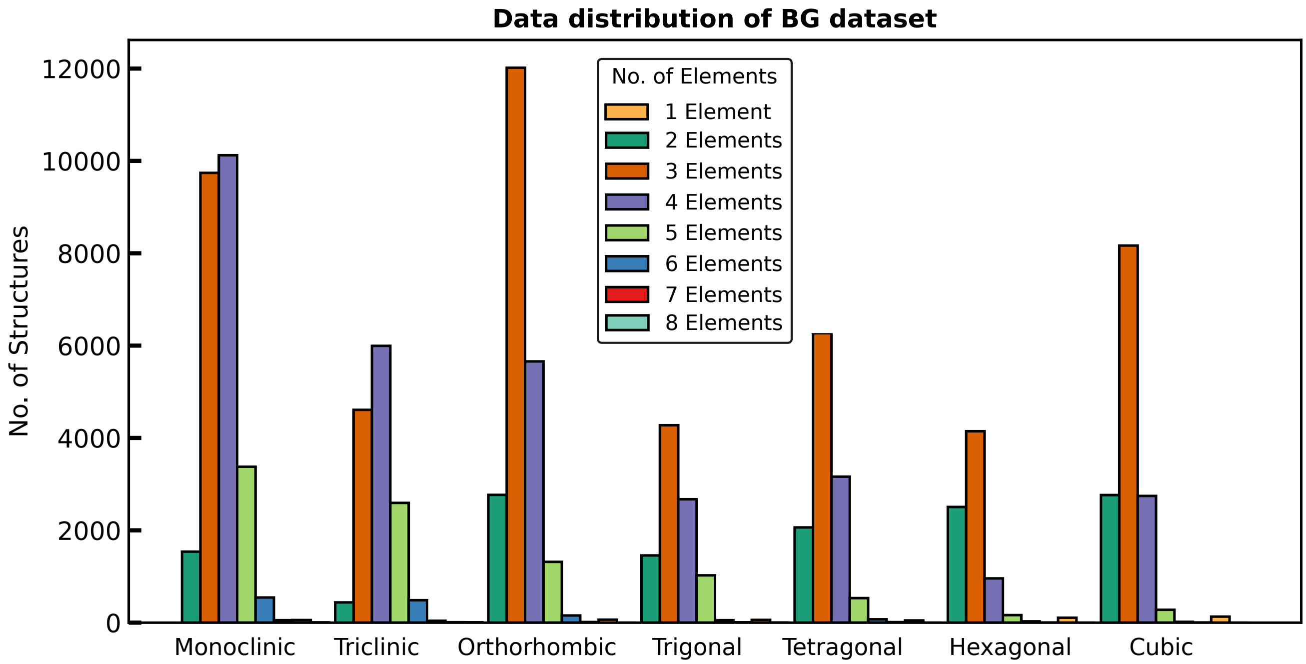

Figure S1. Data distribution within BG dataset. Histogram illustrating the distribution of different crystal systems within the BG dataset. Different colors of the bars differentiate the number of elements present in each structure that falls under a given crystal system.

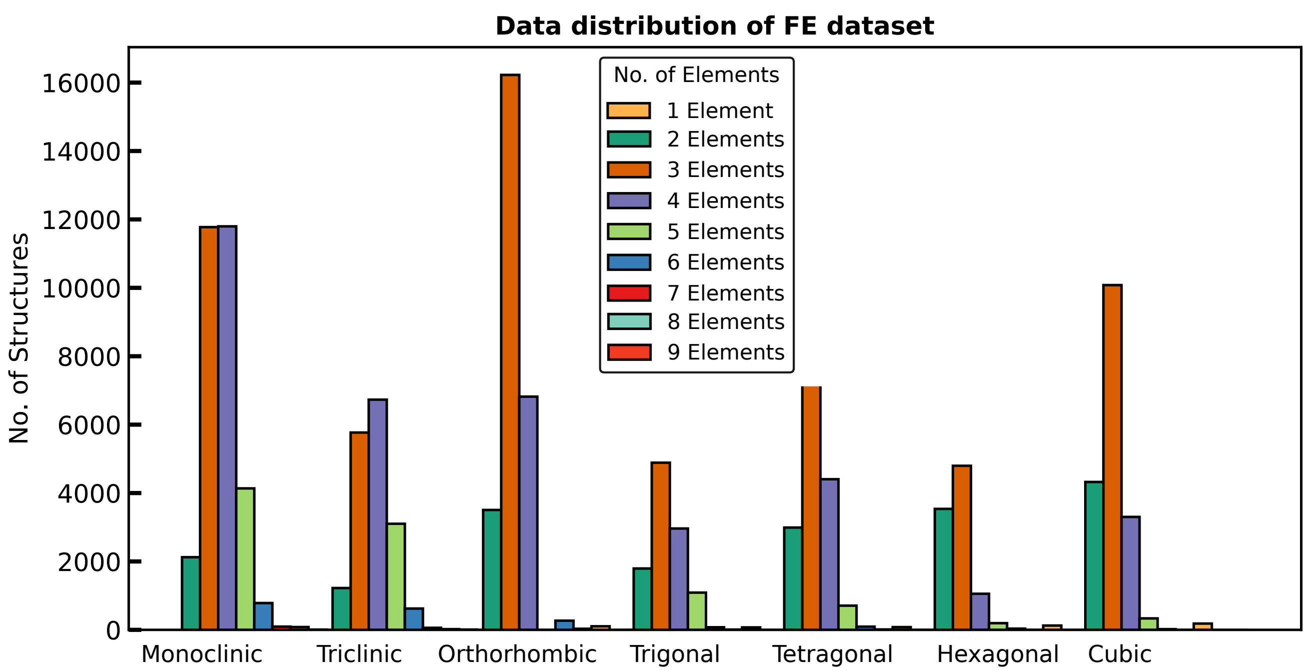

Figure S2. Data distribution within FE dataset. Histogram illustrating the distribution of different crystal systems within the FE dataset. Notations used are identical to Figure S1.

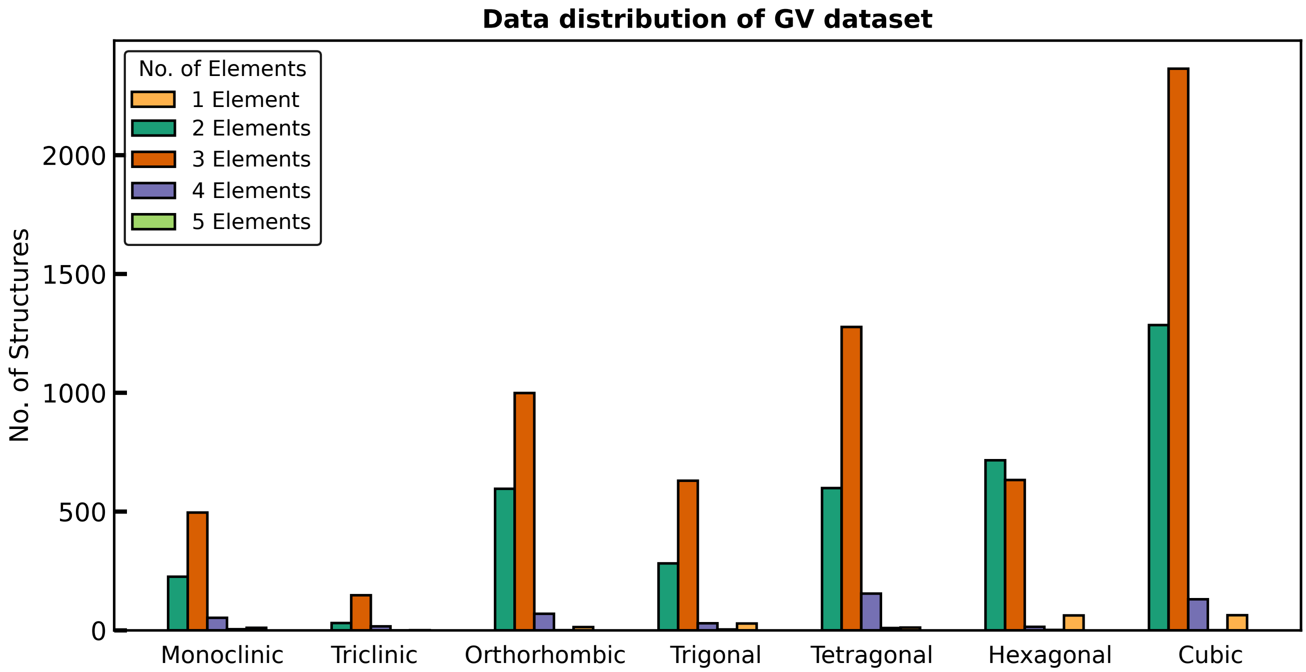

Figure S3. Data distribution within GV dataset. Histogram illustrating the distribution of different crystal systems within the GV dataset. Notations used are identical to Figure S1.

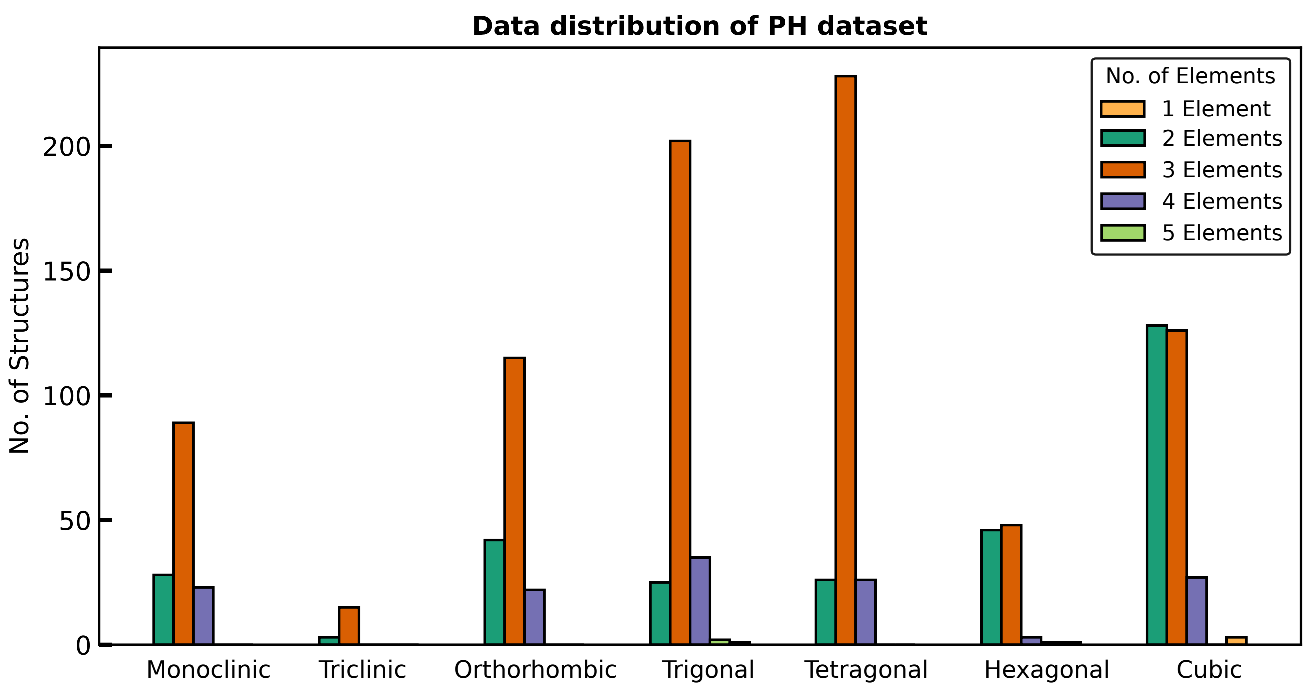

Figure S4. Data distribution within PH dataset. Histogram illustrating the distribution of different crystal systems within the PH dataset. Notations used are identical to Figure S1.

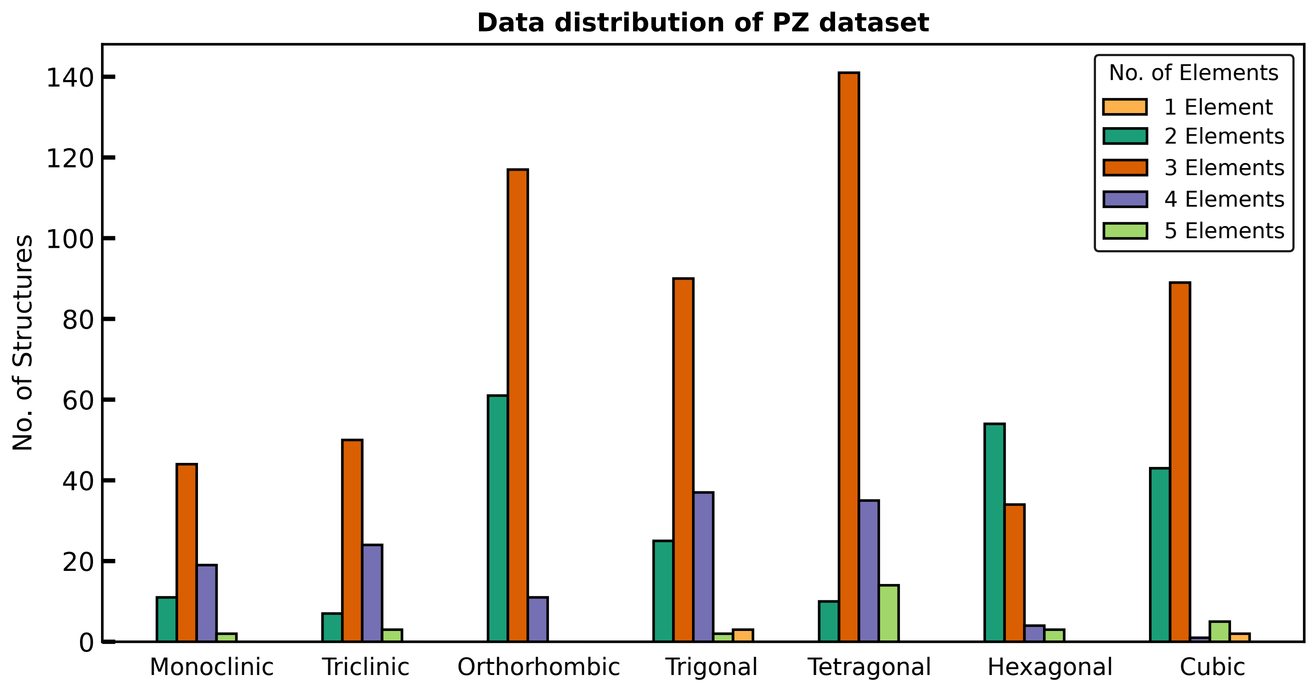

Figure S5. Data distribution within PZ dataset. Histogram illustrating the distribution of different crystal systems within the PZ dataset. Notations used are identical to Figure S1.

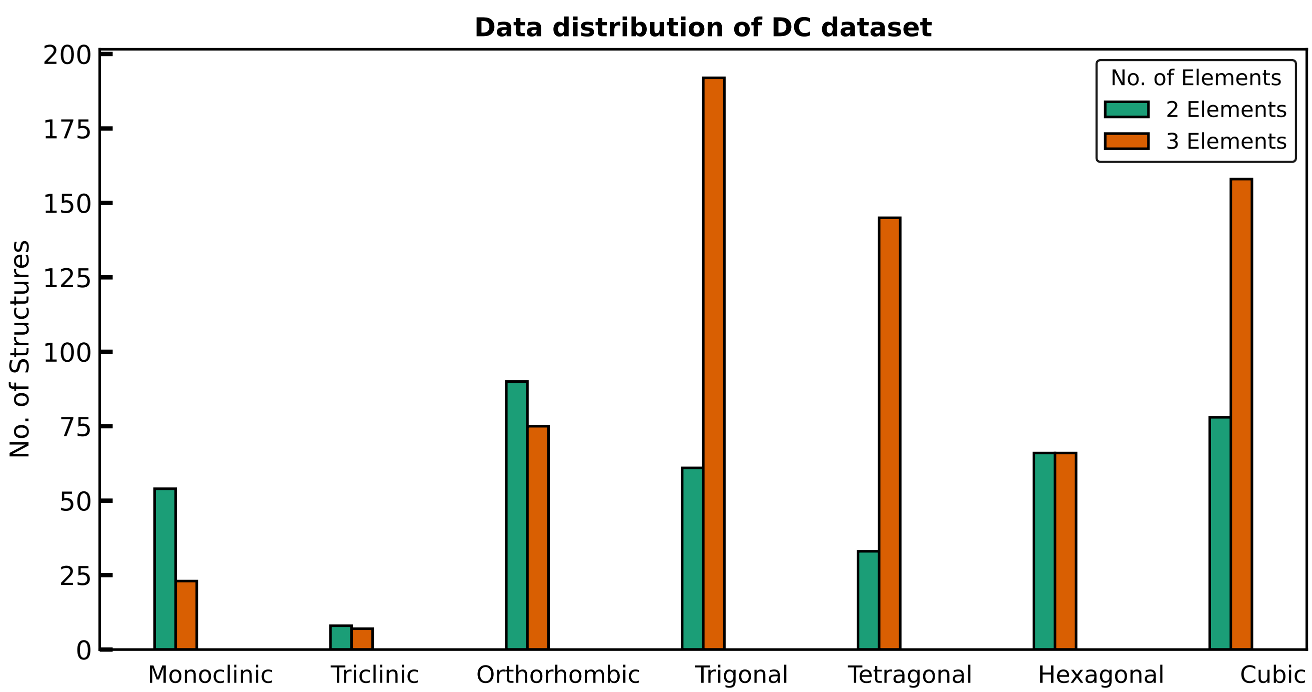

Figure S6. Data distribution within DC dataset. Histogram illustrating the distribution of different crystal systems within the DC dataset. Notations used are identical to Figure S1.

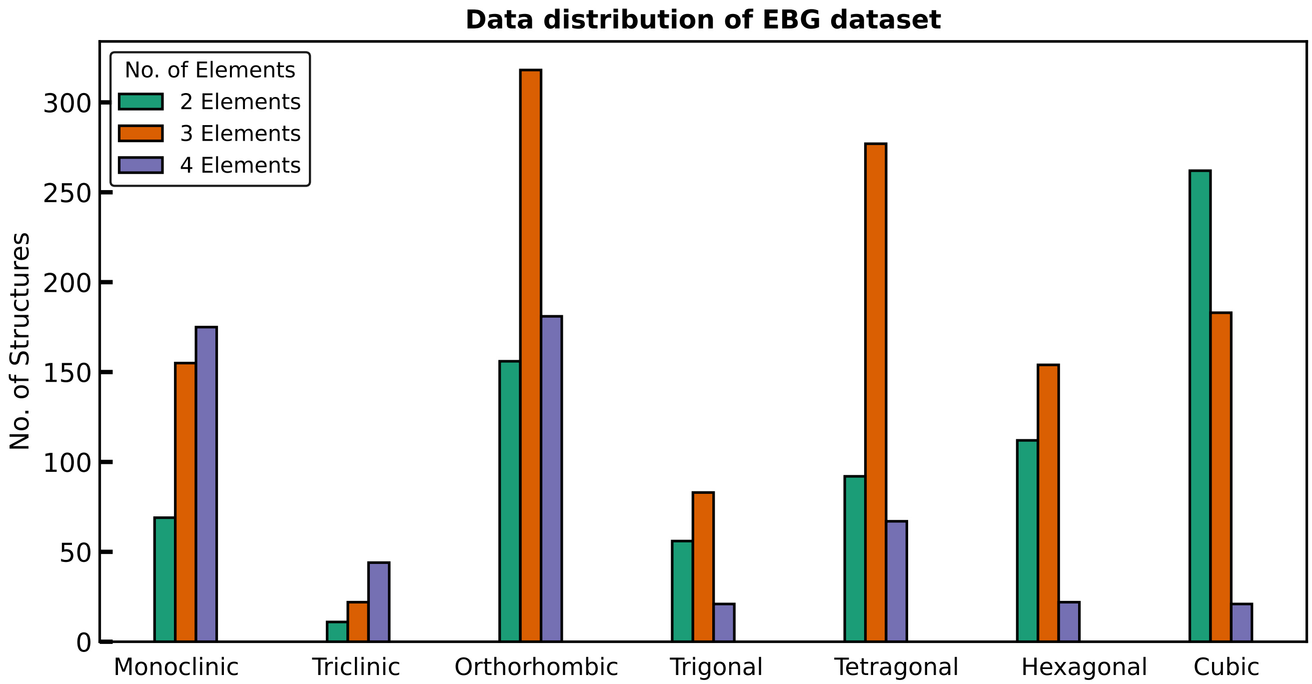

Figure S7. Data distribution within EBG dataset. Histogram illustrating the distribution of different crystal systems within the EBG dataset. Notations used are identical to Figure S1.

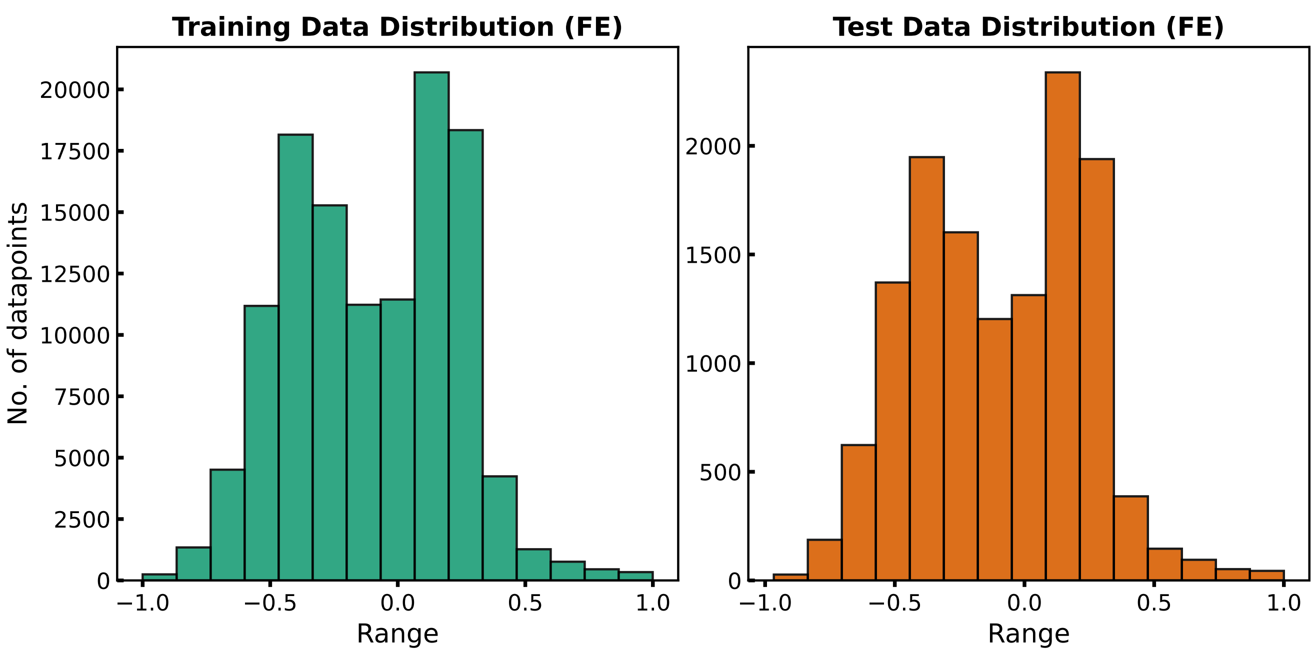

Figure S8. Comparison of train and test data distribution within FE. Distribution of the train and test data (90% and 10% of the total data, respectively) after standardization and normalization of the FE dataset.

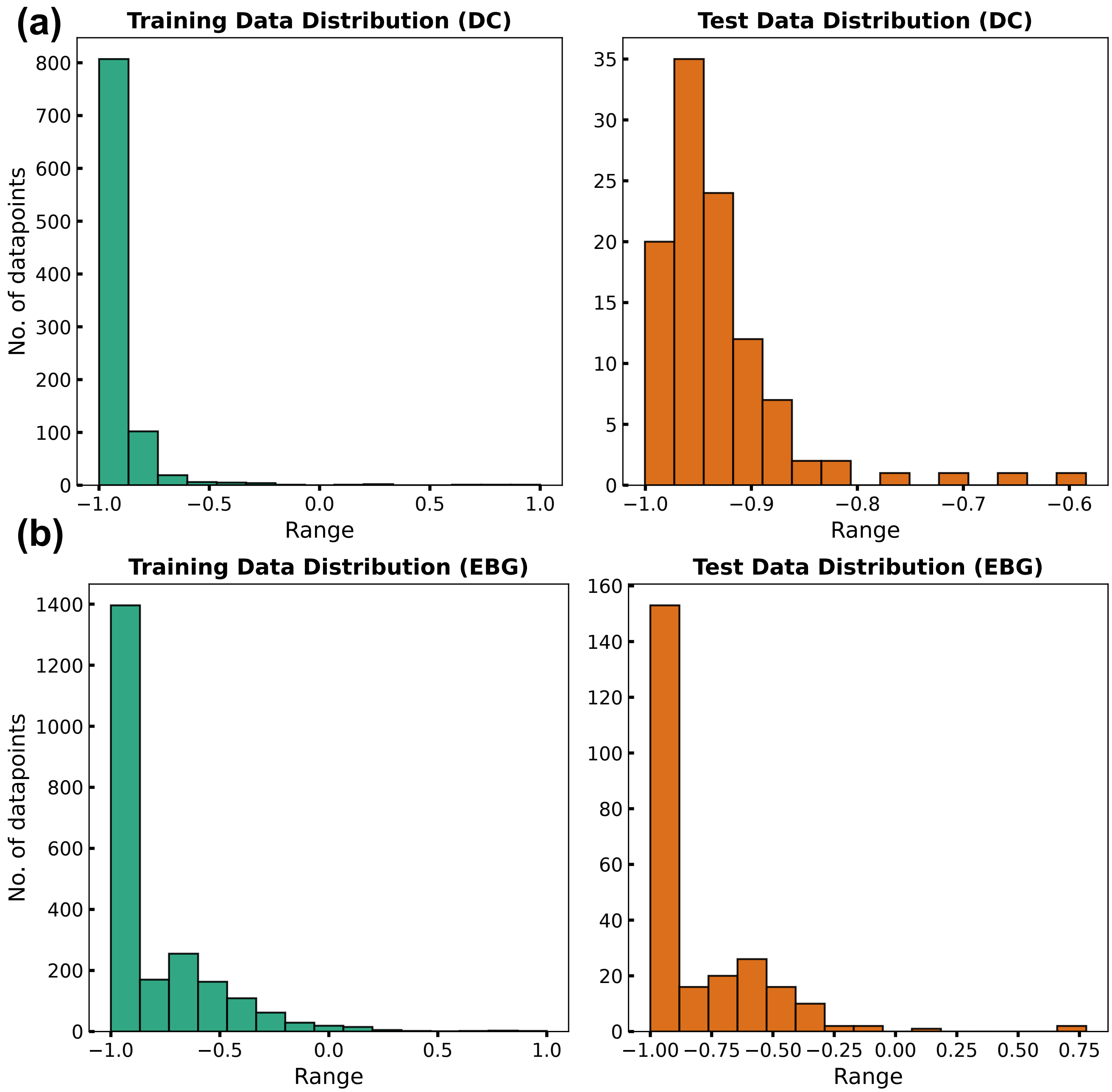

Figure S9. **Comparison of train and test data distribution within EBG and DC**. Distribution of the train and test data (90% and 10% of the total data, respectively) after standardization and normalization for (a) EBG, and (b) DC.

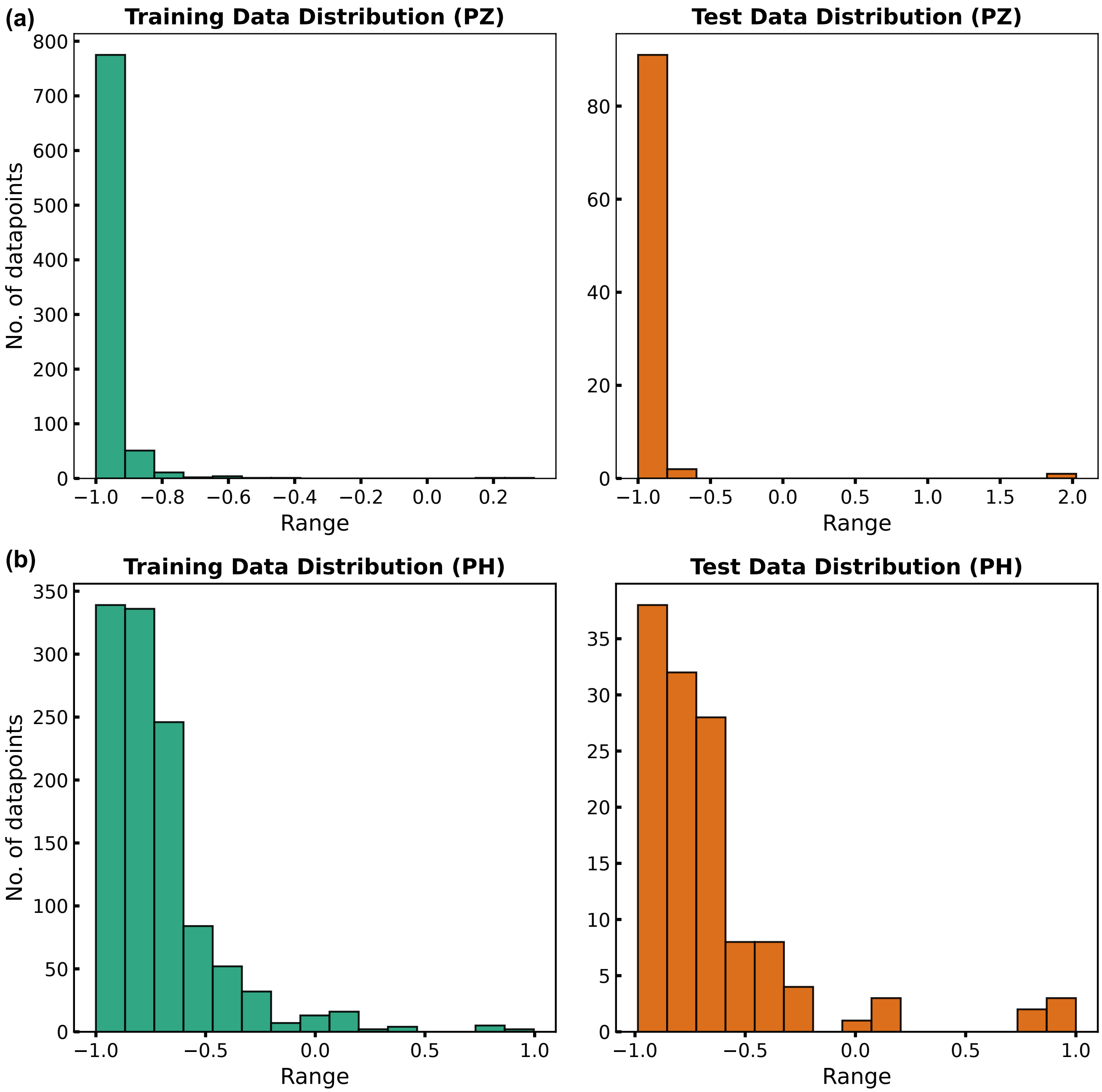

Figure S10. Comparison of train and test data distribution within PZ and PH. Distribution of the train and test data (90% and 10% of the total data, respectively) after standardization and normalization for (a) PZ, and (b) PH.

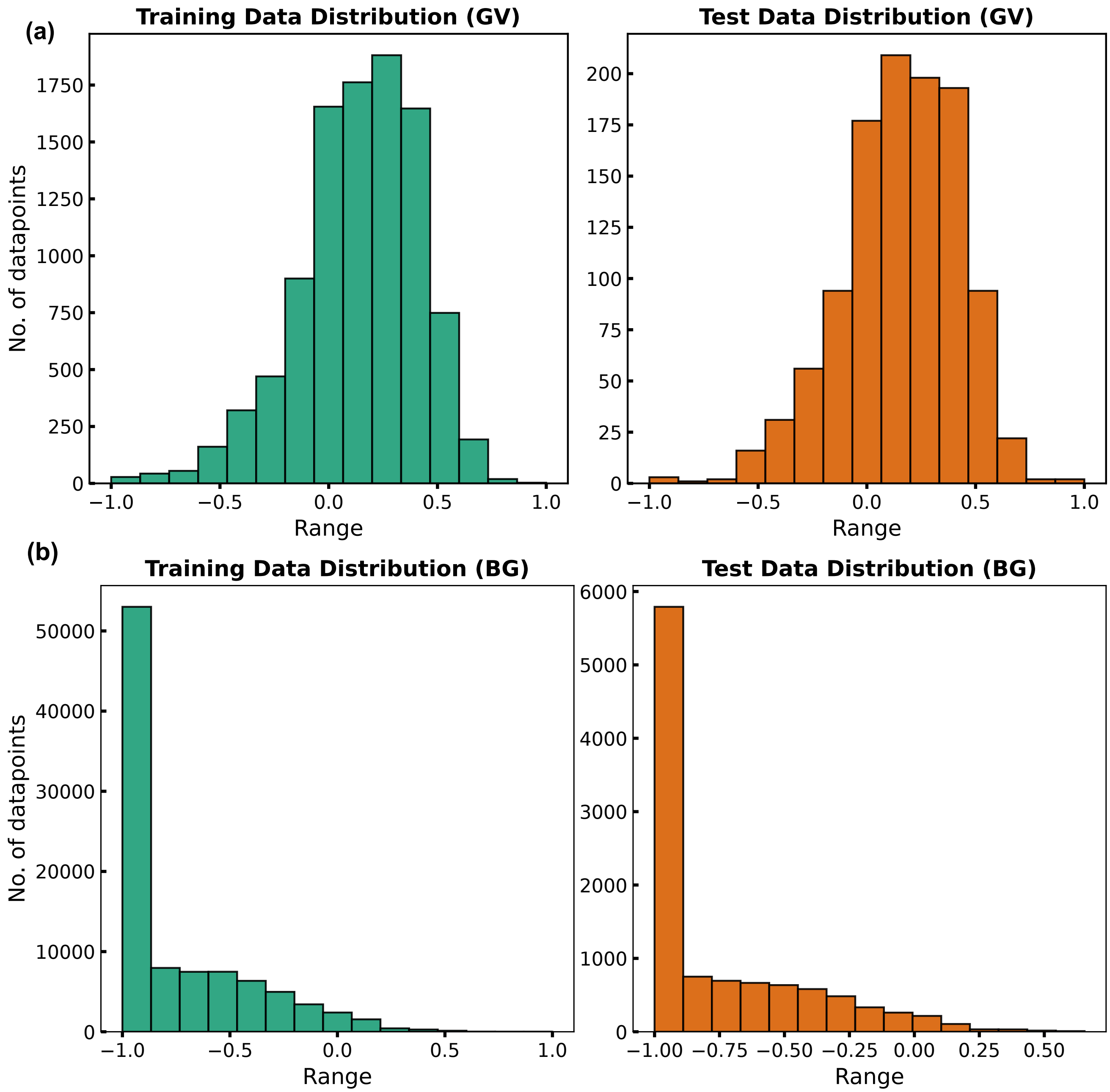

Figure S11. Comparison of train and test data distribution within GV and BG. Distribution of the train and test data (90% and 10% of the total data, respectively) after standardization and normalization for (a) GV, and (b) BG.

S3 Hyper-parameter optimization

S3.1 Data sampling technique

There are three different ways in which one can sample a data distribution: random, uniform, and weighted. We obtained samples of 500 datapoints corresponding to each sampling technique, as described below. Other model parameters that were kept fixed while optimizing the sampling technique are tabulated in Table S3.

Random Sampling

Five hundred datapoints were randomly sampled from the 90% training dataset (i.e., 500 datapoints from the overall dataset split of 90% training-validation and 10% for testing).

Uniform Sampling

The data distribution was split into ten equally-spaced bins, each spanning different target value ranges (i.e., -1 to -0.8, -0.8 to -0.6, etc.). We randomly sampled an exact number of datapoints (i.e., 50 randomly sampled points) from each bin to select 500 datapoints. If the number of datapoints in a bin was less than or equal to 50, we chose all the datapoints corresponding to that bin, with additional datapoints taken equally from the other bins (each bin sampled at random) to balance the deficit.

Weighted Sampling

The data distribution was split into ten equally-spaced bins, each spanning different target value ranges. The number of datapoints chosen, at random, from each bin is weighted by the number of datapoints contributed by each bin to the total distribution (i.e., Number of datapoints in each bin/ Number of datapoints in total distribution). Hence, the weighted sampling favors sampling more datapoints from bins that contain more datapoints, and eventually aims to mimic the overall dataset distribution.

Parameter	Value
ALIGNN layers	4
Number of datapoints	500
Epochs	500
Batch size	16
Learning rate	0.0001

Table S3. ALIGNN configuration used while optimizing data sampling technique.

S3.2 Learning rate and number of unfrozen layers

Random sampling was used to sample 500 datapoints from the data distribution for the select PT-FT pairs. Other model parameters kept fixed while optimizing the learning rate are tabulated in Table S4. We used the FT strategy of unfreezing only the last layer (strategy 3) to obtain the results of Table S5. The results in Figure S12b were obtained by adding a new prediction head, as discussed in Section 2.5 of the main text, and keeping the number of frozen layers to either 1 or 6, for three different learning rates. It can be seen that as the learning rate increases, the model performance improves in both the FT strategies. Note that R^2 scores also increase when the number of unfrozen layers is higher, as illustrated by higher R^2 scores for cases with 1 unfrozen layer compared to 6 in Figure S12b.

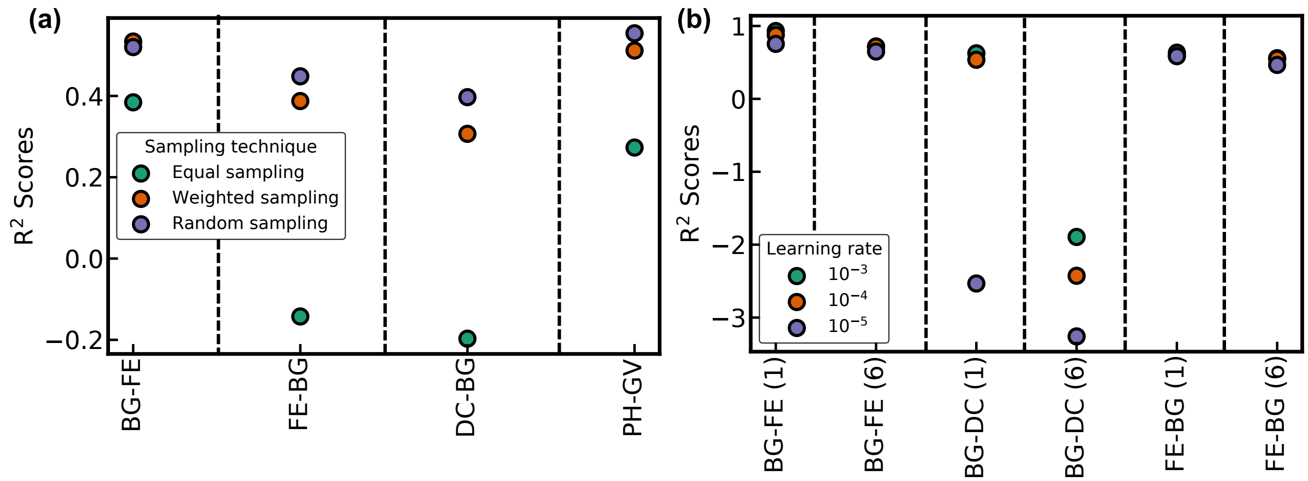

Figure S12. Optimization of sampling technique, learning rate and number of unfrozen layers. The test R^2 scores for the different PT-FT pairs considered for optimizing (a) data sampling, and (b) learning rate and number of unfrozen layers. Purple, orange, and green circles correspond to R^2 scores for random, weighted, and equal sampling in panel a. In panel b, learning rates of 10^{-3}, 10^{-4}, and 10^{-5} are represented by green, orange and purple circles, respectively. The number in parenthesis next to the PT-FT pair in panel b corresponds to the number of frozen layers in the model configuration.

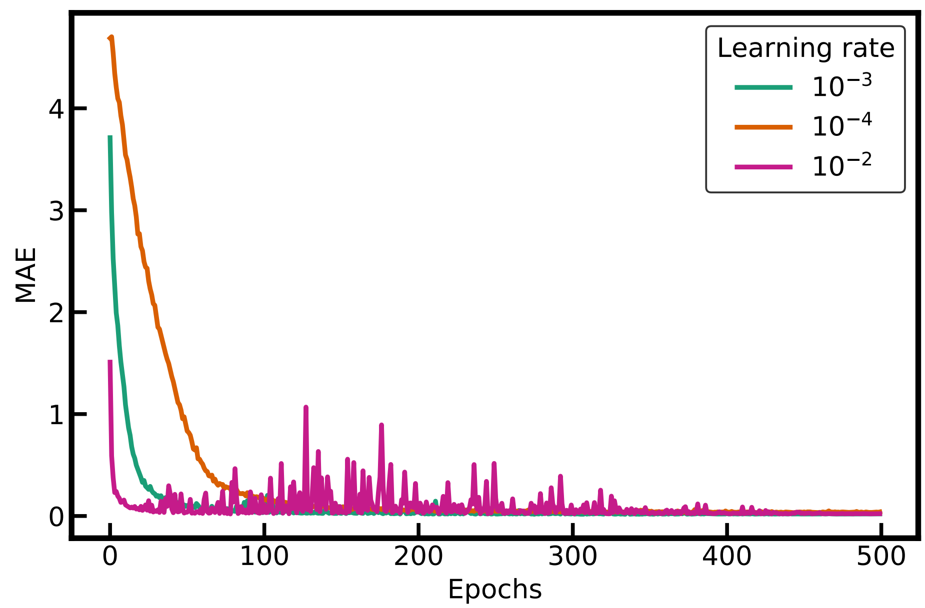

Figure S13. Variation of MAEs with increasing epochs during FT. Mean absolute error (MAE) versus the number of epochs for BG-FE with 500 datapoints for different learning rates. FT strategy 3 was used to construct the plot. It can be seen that the losses tend to converge better for the learning rate 10^{-3} compared to 10^{-2}.

S3.3 Number of datapoints

To observe the trend on increasing the number of datapoints for FT, we performed the same set of experiments but increased the randomly selected datapoints from 500 to 1000. Other model parameters, as listed in Table S3 are kept constant. The results are tabulated in Table S6.

Parameter	Value
ALIGNN layers	4
number of datapoints	500
Epochs	500
Batch size	16
Data sampling	Random

Table S4. ALIGNN configuration used while optimizing learning rate and the number of unfrozen layers.

PT-FT pairs	Test R^2 score	Test R^2 score	Test R^2 score	Test R^2 score
Learning rate	10^{-5}	10^{-4}	10^{-3}	10^{-2}
FE-BG	-0.184	0.448	0.557	0.540
BG-FE	-0.962	0.520	0.709	0.700
PH-GV	0.335	0.554	0.607	0.633
DC-BG	0.332	0.397	0.402	0.404

Table S5. Model performance for four different learning rates. In general, higher learning rates offer better R^2 scores than lower rates.

PT-FT pairs	Test R^2 score	Test R^2 score
Learning rate	500	1000
FE-BG	0.448	0.585
BG-FE	0.520	0.687
PH-GV	0.554	0.602
DC-BG	0.397	0.458

Table S6. Model performance for two different sizes of FT dataset. The R^2 scores improve as the number of datapoints for FT increases.

S4 PT and FT loss for MPT model training

We compare the absolute PT and FT losses of as a function of the number of properties available to each structure in Figure S14. The PT loss is obtained from a multi-property PT (MPT) model trained on all properties except PH and tested on FE500 (i.e., FE with a dataset size of 500). The FT loss is obtained from a model PT on all but FE and FT on FE500. The FT model was subsequently tested on the same FE500 dataset again to obtain the FT loss. Since the PT and FT loss were obtained from completely different PT models, they should not be compared with each other. We observe the PT and FT loss to decrease as the number of properties available for simultaneous training increases.

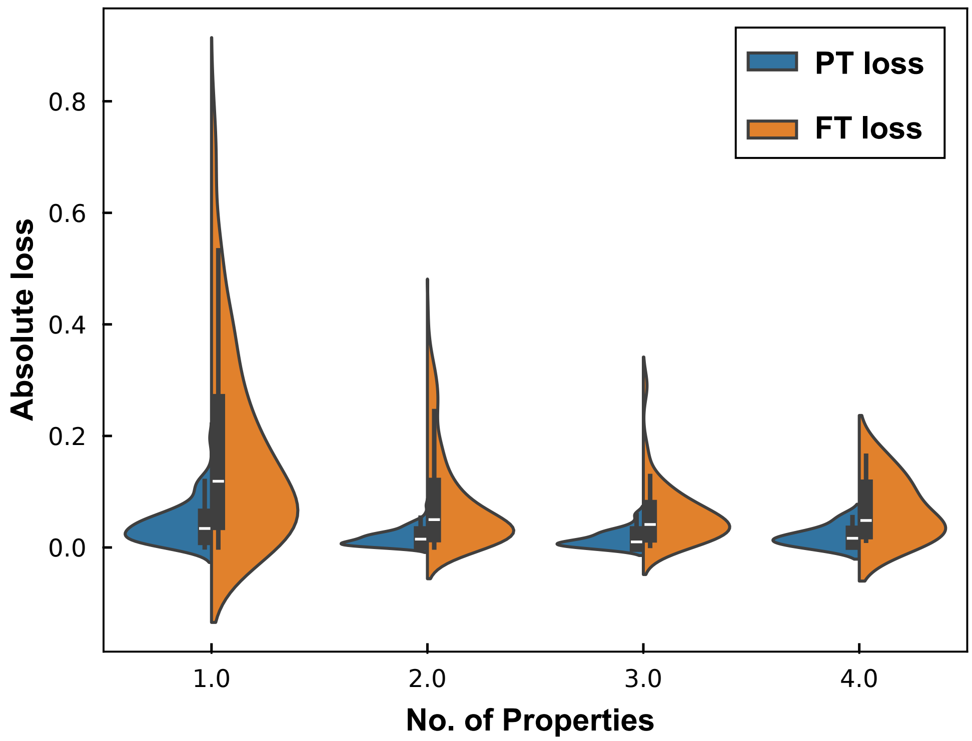

Figure S14. **Absolute PT and FT losses for different number of properties during training**. Violin plots illustrating the absolute loss for PT and FT during MPT training as a function of the number of properties available for each structure. The length of the box plot inside the violin summarizes the interquartile range of the data. The white lines within the box indicate the median.

Parameter	Value
ALIGNN layers	4
GCN layers	4
Atom input features	92
Edge input features	80
Bond angle input features	40
Embedding features	64
Hidden features	256
Normalization	Batch normalization
Batch size	4
PT learning rate	0.001
Output dimension of the PT model	6
FT learning rate	0.001
No. of hidden layers in the head	2
Optimizer	Adamw
Weight decay	0.00001
Random seed	123
Epochs	500

Table S7. ALIGNN configuration used for MPT.

S5 Scratch model scores

Table S8. Test R^2 scores for the scratch models with varying dataset sizes.

Dataset	10	100	200	500	800
GV	-267.986 ± 356.666	0.408 ± 0.061	0.502 ± 0.027	0.674 ± 0.034	0.742 ± 0.035
PH	-18.543 ± 21.54	0.534 ± 0.123	0.613 ± 0.101	0.796 ± 0.051	0.904 ± 0.047
FE	-85.457 ± 88.808	0.721 ± 0.032	0.773 ± 0.011	0.883 ± 0.008	0.913 ± 0.01
BG	-83.378 ± 105.411	0.327 ± 0.027	0.359 ± 0.035	0.515 ± 0.02	0.572 ± 0.023
PZ	-47.045 ± 25.391	0.006 ± 0.018	-0.116 ± 0.207	0.004 ± 0.047	-0.039 ± 0.083
DC	-1003.089 ± 1595.166	-1.123 ± 2.143	-0.154 ± 0.217	0.273 ± 0.34	0.653 ± 0.086
EBG	-165.202 ± 123.229	-0.052 ± 0.566	0.1 ± 0.065	0.325 ± 0.041	0.415 ± 0.046

Table S9. Test MAEs for the scratch models with varying dataset sizes.

Dataset	10	100	200	500	800
GV	3.357 ± 2.54	0.155 ± 0.008	0.142 ± 0.005	0.109 ± 0.006	0.096 ± 0.007
PH	1.257 ± 0.721	0.128 ± 0.01	0.11 ± 0.011	0.068 ± 0.006	0.043 ± 0.005
FE	2.516 ± 1.506	0.127 ± 0.009	0.109 ± 0.004	0.071 ± 0.002	0.057 ± 0.003
BG	2.045 ± 1.051	0.196 ± 0.008	0.193 ± 0.009	0.157 ± 0.002	0.142 ± 0.002
PZ	1.567 ± 0.411	0.067 ± 0.006	0.093 ± 0.01	0.058 ± 0.005	0.056 ± 0.007
DC	1.238 ± 1.143	0.06 ± 0.035	0.047 ± 0.01	0.031 ± 0.008	0.022 ± 0.003
EBG	2.733 ± 1.255	0.166 ± 0.051	0.157 ± 0.005	0.121 ± 0.006	0.104 ± 0.002

S6 Performance of models on the PZ dataset

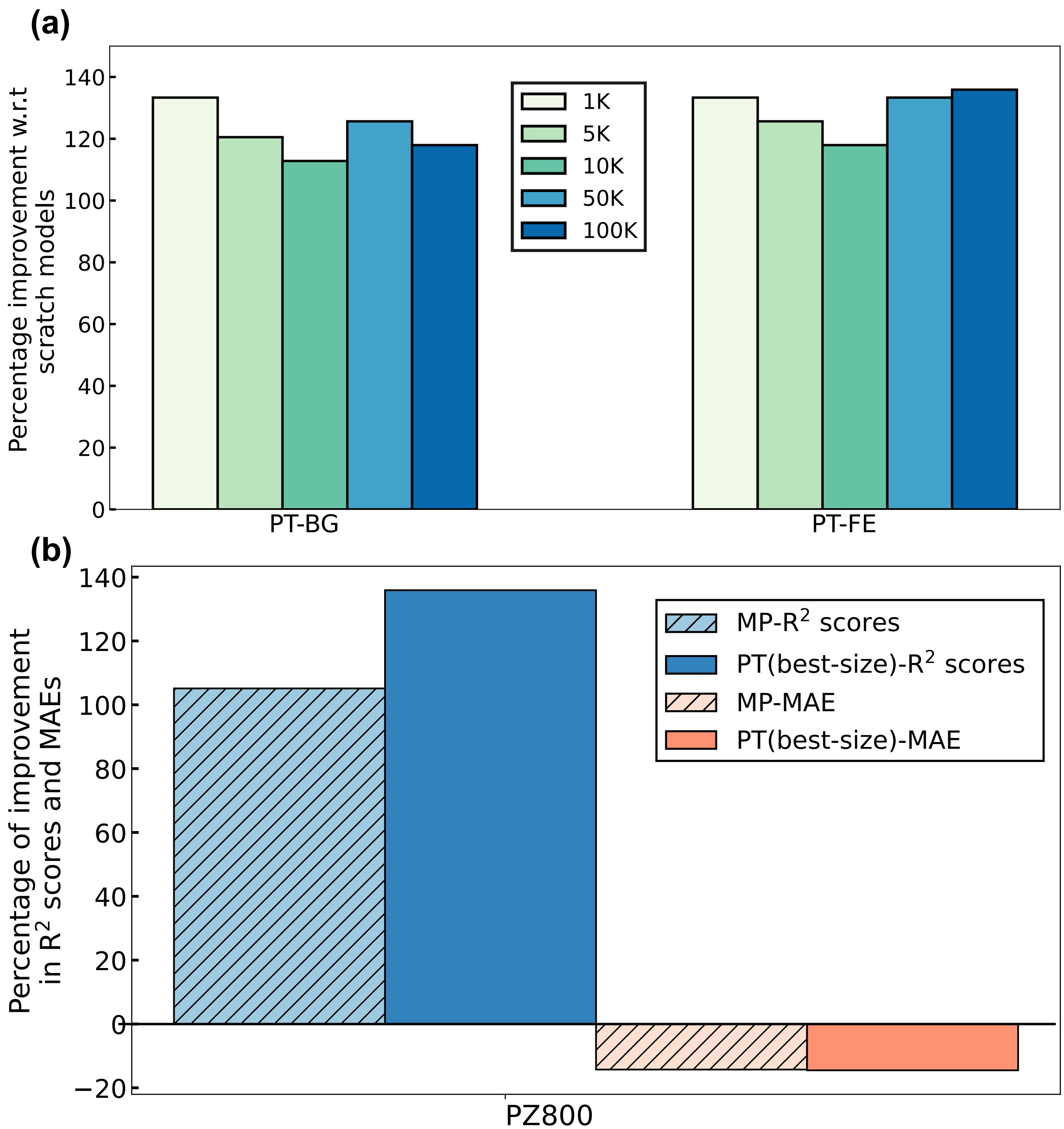

Figure S15. Pair-wise TL and MPT model performance on PZ dataset. Bar plots illustrating the percentage of improvement in R^2 scores and MAEs with respect to the scratch models for the PZ dataset using (a) larger PT size and (b) MPT and FT(best-size) models for PT.

S7 Influence of varying PT dataset size

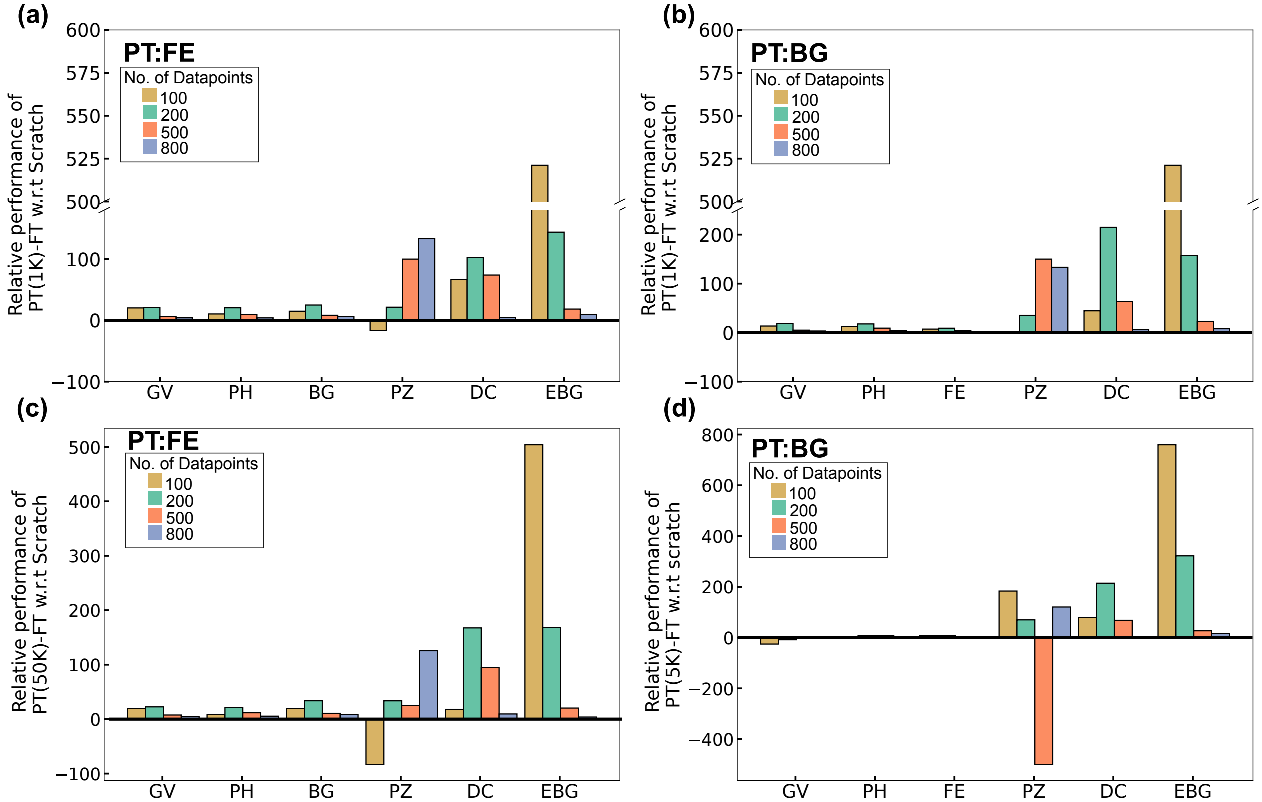

Figure S16. Performance with respect to scratch for different PT sizes (1K and 5K). Bar plots illustrating the percentage change in R^2 scores relative to scratch for the PT(1K)-FT (top row) and PT(5K)-FT (bottom row) models, where PT is done on the FE (panels a, c) and BG (b, d) datasets. The *x* tick marks in all panels indicate the FT dataset.

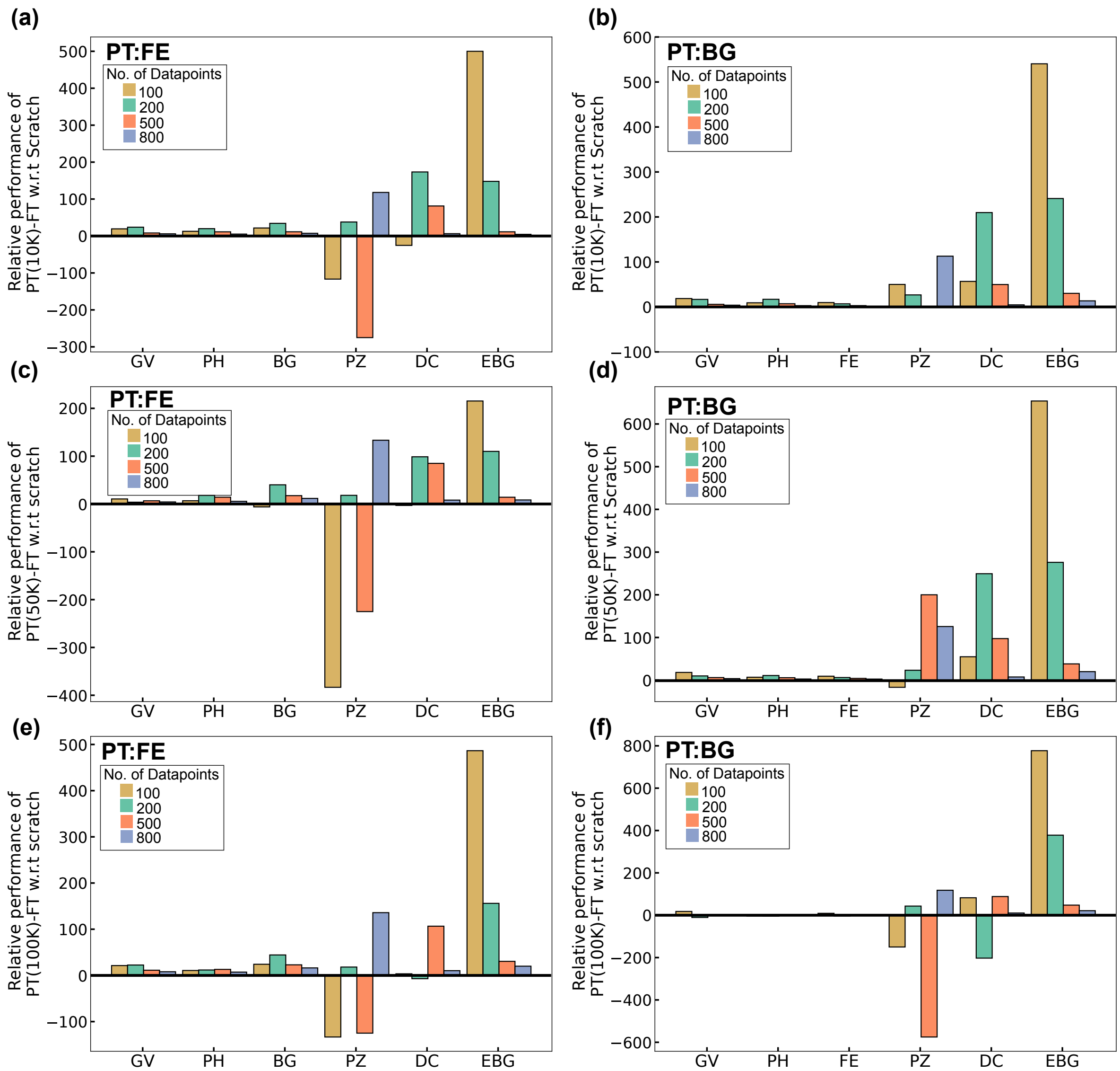

Figure S17. Performance with respect to scratch for different PT sizes (10K,50K and 100K). Bar plots illustrating the percentage change in R^2 scores relative to scratch for the PT(10K)-FT (top row), PT(50K)-FT (middle row), and PT(100K)-FT (bottom row) models, where PT is done on the FE (panels a, c, and e) and BG (b, d, and f) datasets. The *x* tick marks in all panels indicate the FT dataset.

Table S10. Test R^2 scores upon FT with margins of errors for varying PT (FE) sizes.

FT Size	1K	5K	10K	50K	100K
GV10	-2.166 ± 1.657	-3.426 ± 3.443	-12.438 ± 19.483	-2.74 ± 4.147	-1311.727 ± 3597.145
GV100	0.491 ± 0.037	0.488 ± 0.036	0.487 ± 0.047	0.451 ± 0.114	0.495 ± 0.032
GV200	0.607 ± 0.038	0.615 ± 0.039	0.622 ± 0.041	0.521 ± 0.17	0.615 ± 0.046
GV500	0.717 ± 0.029	0.725 ± 0.026	0.729 ± 0.019	0.719 ± 0.037	0.75 ± 0.021
GV800	0.773 ± 0.019	0.78 ± 0.019	0.786 ± 0.015	0.774 ± 0.024	0.801 ± 0.018
PH10	-0.755 ± 0.697	-0.867 ± 0.911	-1.507 ± 1.773	-1.244 ± 0.518	-1.256 ± 0.561
PH100	0.59 ± 0.129	0.58 ± 0.138	0.602 ± 0.129	0.57 ± 0.101	0.591 ± 0.076
PH200	0.739 ± 0.128	0.742 ± 0.146	0.735 ± 0.154	0.723 ± 0.185	0.685 ± 0.192
PH500	0.874 ± 0.066	0.889 ± 0.063	0.886 ± 0.068	0.909 ± 0.057	0.9 ± 0.07
PH800	0.941 ± 0.045	0.953 ± 0.033	0.951 ± 0.038	0.954 ± 0.021	0.969 ± 0.025
BG10	-2.165 ± 1.604	-3.176 ± 1.817	-2.927 ± 2.486	-2.781 ± 1.448	-3.187 ± 0.603
BG100	0.376 ± 0.053	0.391 ± 0.035	0.398 ± 0.043	0.307 ± 0.141	0.406 ± 0.054
BG200	0.449 ± 0.056	0.48 ± 0.056	0.482 ± 0.05	0.503 ± 0.037	0.518 ± 0.057
BG500	0.558 ± 0.027	0.57 ± 0.027	0.574 ± 0.03	0.605 ± 0.041	0.633 ± 0.026
BG800	0.608 ± 0.017	0.619 ± 0.015	0.614 ± 0.02	0.639 ± 0.026	0.665 ± 0.021
PZ10	-1.646 ± 0.864	-1.149 ± 0.516	-1.281 ± 0.621	-3.517 ± 1.441	-251.293 ± 510.261
PZ100	0.005 ± 0.016	0.001 ± 0.018	-0.001 ± 0.019	-0.017 ± 0.043	-0.002 ± 0.023
PZ200	-0.091 ± 0.219	-0.077 ± 0.212	-0.072 ± 0.206	-0.095 ± 0.151	-0.095 ± 0.182
PZ500	0.013 ± 0.022	0.01 ± 0.015	-0.007 ± 0.044	-0.005 ± 0.02	-0.001 ± 0.019
PZ800	0.008 ± 0.006	0.005 ± 0.006	0.007 ± 0.013	0.013 ± 0.029	0.014 ± 0.005
DC10	-45.038 ± 51.375	-27.456 ± 19.06	-33.747 ± 26.198	-33.425 ± 24.965	-768.657 ± 1898.335
DC100	-0.375 ± 0.775	-0.921 ± 1.945	-1.408 ± 2.841	-1.157 ± 1.839	-1.084 ± 1.531
DC200	0.004 ± 0.765	0.104 ± 0.559	0.113 ± 0.507	-0.002 ± 0.512	-0.165 ± 0.637
DC500	0.475 ± 0.141	0.532 ± 0.096	0.495 ± 0.159	0.505 ± 0.146	0.564 ± 0.101
DC800	0.682 ± 0.058	0.715 ± 0.032	0.694 ± 0.032	0.706 ± 0.047	0.72 ± 0.027
EBG10	-4.213 ± 4.492	-2.68 ± 2.306	-2.857 ± 2.901	-10.857 ± 14.784	-46.128 ± 79.977
EBG100	0.219 ± 0.139	0.21 ± 0.093	0.208 ± 0.117	0.06 ± 0.114	0.201 ± 0.11
EBG200	0.244 ± 0.114	0.268 ± 0.109	0.248 ± 0.097	0.21 ± 0.083	0.256 ± 0.15
EBG500	0.385 ± 0.059	0.391 ± 0.031	0.362 ± 0.054	0.371 ± 0.05	0.424 ± 0.047
EBG800	0.456 ± 0.064	0.431 ± 0.064	0.434 ± 0.054	0.45 ± 0.068	0.498 ± 0.044

Table S11. Test MAEs upon FT with margins of errors for varying PT (FE) sizes.

FT Size	1K	5K	10K	50K	100K
GV10	0.372 ± 0.092	0.436 ± 0.204	0.681 ± 0.387	0.397 ± 0.246	2.521 ± 5.472
GV100	0.14 ± 0.006	0.141 ± 0.007	0.141 ± 0.008	0.146 ± 0.015	0.138 ± 0.007
GV200	0.122 ± 0.007	0.121 ± 0.007	0.119 ± 0.007	0.133 ± 0.026	0.121 ± 0.007
GV500	0.1 ± 0.005	0.098 ± 0.005	0.097 ± 0.003	0.099 ± 0.007	0.092 ± 0.003
GV800	0.089 ± 0.004	0.088 ± 0.005	0.086 ± 0.004	0.089 ± 0.007	0.083 ± 0.004
PH10	0.405 ± 0.088	0.418 ± 0.157	0.484 ± 0.189	0.467 ± 0.099	0.474 ± 0.063
PH100	0.106 ± 0.014	0.109 ± 0.015	0.106 ± 0.017	0.118 ± 0.011	0.114 ± 0.013
PH200	0.073 ± 0.013	0.072 ± 0.016	0.072 ± 0.016	0.076 ± 0.022	0.08 ± 0.021
PH500	0.047 ± 0.004	0.044 ± 0.003	0.044 ± 0.006	0.04 ± 0.005	0.041 ± 0.007
PH800	0.031 ± 0.006	0.029 ± 0.006	0.029 ± 0.006	0.034 ± 0.004	0.025 ± 0.006
BG10	0.485 ± 0.127	0.565 ± 0.109	0.537 ± 0.156	0.544 ± 0.102	0.571 ± 0.044
BG100	0.182 ± 0.005	0.178 ± 0.007	0.176 ± 0.003	0.192 ± 0.023	0.173 ± 0.005
BG200	0.167 ± 0.013	0.158 ± 0.01	0.156 ± 0.009	0.158 ± 0.007	0.154 ± 0.011
BG500	0.142 ± 0.003	0.137 ± 0.003	0.134 ± 0.003	0.134 ± 0.006	0.125 ± 0.004
BG800	0.129 ± 0.003	0.123 ± 0.003	0.123 ± 0.003	0.123 ± 0.005	0.114 ± 0.003
PZ10	0.377 ± 0.106	0.314 ± 0.088	0.335 ± 0.087	0.526 ± 0.105	1.777 ± 2.123
PZ100	0.056 ± 0.002	0.057 ± 0.003	0.057 ± 0.003	0.065 ± 0.012	0.055 ± 0.002
PZ200	0.064 ± 0.016	0.06 ± 0.015	0.06 ± 0.015	0.069 ± 0.02	0.064 ± 0.014
PZ500	0.051 ± 0.004	0.05 ± 0.003	0.051 ± 0.005	0.055 ± 0.006	0.05 ± 0.004
PZ800	0.049 ± 0.001	0.048 ± 0.0	0.048 ± 0.001	0.051 ± 0.004	0.048 ± 0.001
DC10	0.331 ± 0.181	0.276 ± 0.112	0.307 ± 0.152	0.311 ± 0.119	0.813 ± 0.916
DC100	0.049 ± 0.014	0.055 ± 0.022	0.059 ± 0.028	0.057 ± 0.023	0.058 ± 0.023
DC200	0.034 ± 0.009	0.033 ± 0.007	0.034 ± 0.007	0.038 ± 0.008	0.041 ± 0.009
DC500	0.025 ± 0.003	0.024 ± 0.002	0.024 ± 0.003	0.023 ± 0.003	0.023 ± 0.002
DC800	0.019 ± 0.001	0.018 ± 0.001	0.018 ± 0.002	0.017 ± 0.002	0.016 ± 0.001
EBG10	0.495 ± 0.195	0.422 ± 0.153	0.421 ± 0.142	0.677 ± 0.277	0.924 ± 0.709
EBG100	0.138 ± 0.019	0.137 ± 0.02	0.135 ± 0.021	0.156 ± 0.019	0.13 ± 0.019
EBG200	0.127 ± 0.007	0.121 ± 0.006	0.121 ± 0.004	0.134 ± 0.012	0.123 ± 0.006
EBG500	0.107 ± 0.006	0.102 ± 0.006	0.102 ± 0.008	0.108 ± 0.01	0.1 ± 0.005
EBG800	0.092 ± 0.005	0.092 ± 0.004	0.091 ± 0.004	0.097 ± 0.009	0.088 ± 0.005

Table S12. Test R^2 scores upon FT with margins of errors for varying PT (BG) sizes.

FT Size	1K	5K	10K	50K	100K
GV10	-13.414 ± 22.253	-5.106 ± 4.491	-9.623 ± 14.541	-29.646 ± 65.36	-226.863 ± 252.806
GV100	0.463 ± 0.078	0.304 ± 0.262	0.484 ± 0.071	0.482 ± 0.041	0.481 ± 0.051
GV200	0.594 ± 0.032	0.459 ± 0.229	0.586 ± 0.039	0.552 ± 0.046	0.449 ± 0.054
GV500	0.708 ± 0.029	0.661 ± 0.067	0.713 ± 0.026	0.715 ± 0.027	0.688 ± 0.028
GV800	0.767 ± 0.023	0.731 ± 0.039	0.771 ± 0.017	0.769 ± 0.017	0.77 ± 0.015
PH10	-0.093 ± 0.155	-0.02 ± 0.152	-0.151 ± 0.354	-0.217 ± 0.25	-0.542 ± 0.441
PH100	0.602 ± 0.133	0.548 ± 0.125	0.583 ± 0.17	0.571 ± 0.162	0.512 ± 0.177
PH200	0.722 ± 0.103	0.665 ± 0.236	0.717 ± 0.122	0.68 ± 0.112	0.585 ± 0.171
PH500	0.869 ± 0.07	0.853 ± 0.06	0.852 ± 0.064	0.842 ± 0.077	0.824 ± 0.091
PH800	0.941 ± 0.032	0.942 ± 0.026	0.93 ± 0.042	0.929 ± 0.042	0.909 ± 0.059
FE10	-3.086 ± 3.092	-0.511 ± 0.272	-1.177 ± 1.033	-1.519 ± 0.946	-213.632 ± 575.766
FE100	0.773 ± 0.018	0.773 ± 0.015	0.791 ± 0.009	0.788 ± 0.015	0.786 ± 0.013
FE200	0.843 ± 0.013	0.834 ± 0.015	0.826 ± 0.016	0.821 ± 0.021	0.745 ± 0.035
FE500	0.917 ± 0.017	0.914 ± 0.02	0.909 ± 0.02	0.92 ± 0.02	0.909 ± 0.017
FE800	0.934 ± 0.017	0.93 ± 0.017	0.927 ± 0.016	0.937 ± 0.013	0.933 ± 0.013
PZ10	-0.736 ± 0.534	-0.299 ± 0.236	-0.203 ± 0.277	-0.115 ± 0.119	-2.709 ± 3.837
PZ100	0.006 ± 0.02	0.017 ± 0.044	0.009 ± 0.022	0.005 ± 0.023	-0.003 ± 0.023
PZ200	-0.075 ± 0.215	-0.035 ± 0.087	-0.085 ± 0.188	-0.089 ± 0.246	-0.066 ± 0.104
PZ500	0.01 ± 0.011	-0.016 ± 0.089	0.004 ± 0.014	0.012 ± 0.011	-0.019 ± 0.063
PZ800	0.013 ± 0.009	0.008 ± 0.015	0.005 ± 0.002	0.01 ± 0.009	0.007 ± 0.006
DC10	-17.605 ± 11.295	-16.392 ± 8.947	-20.364 ± 10.925	-17.088 ± 5.465	-49.852 ± 30.538
DC100	-0.623 ± 1.097	-0.234 ± 0.556	-0.486 ± 1.092	-0.507 ± 1.009	-0.198 ± 0.432
DC200	0.177 ± 0.473	0.176 ± 0.461	0.169 ± 0.415	0.23 ± 0.428	-0.466 ± 0.342
DC500	0.446 ± 0.17	0.459 ± 0.141	0.409 ± 0.35	0.539 ± 0.173	0.514 ± 0.168
DC800	0.692 ± 0.069	0.668 ± 0.058	0.683 ± 0.031	0.702 ± 0.054	0.721 ± 0.029
EBG10	-1.479 ± 1.058	0.17 ± 0.32	-0.735 ± 1.535	-1.231 ± 2.749	-0.828 ± 1.75
EBG100	0.219 ± 0.108	0.343 ± 0.141	0.229 ± 0.107	0.288 ± 0.068	0.352 ± 0.059
EBG200	0.257 ± 0.081	0.422 ± 0.049	0.341 ± 0.094	0.376 ± 0.077	0.478 ± 0.061
EBG500	0.4 ± 0.036	0.412 ± 0.083	0.423 ± 0.029	0.449 ± 0.035	0.49 ± 0.04
EBG800	0.448 ± 0.091	0.484 ± 0.055	0.471 ± 0.068	0.498 ± 0.055	0.504 ± 0.048

Table S13. Test MAEs upon FT with margins of errors for varying PT (BG) sizes.

FT Size	1K	5K	10K	50K	100K
GV10	0.718 ± 0.481	0.546 ± 0.231	0.664 ± 0.391	0.887 ± 0.864	2.252 ± 1.887
GV100	0.145 ± 0.01	0.165 ± 0.027	0.141 ± 0.012	0.141 ± 0.008	0.145 ± 0.009
GV200	0.125 ± 0.006	0.144 ± 0.034	0.124 ± 0.007	0.13 ± 0.007	0.143 ± 0.006
GV500	0.101 ± 0.006	0.11 ± 0.014	0.099 ± 0.005	0.099 ± 0.004	0.104 ± 0.004
GV800	0.09 ± 0.005	0.098 ± 0.008	0.089 ± 0.003	0.089 ± 0.003	0.089 ± 0.003
PH10	0.277 ± 0.044	0.273 ± 0.014	0.283 ± 0.046	0.307 ± 0.065	0.333 ± 0.068
PH100	0.104 ± 0.015	0.135 ± 0.036	0.098 ± 0.019	0.1 ± 0.018	0.107 ± 0.024
PH200	0.076 ± 0.011	0.093 ± 0.044	0.077 ± 0.011	0.08 ± 0.012	0.118 ± 0.013
PH500	0.05 ± 0.005	0.055 ± 0.005	0.051 ± 0.004	0.051 ± 0.008	0.055 ± 0.008
PH800	0.033 ± 0.004	0.033 ± 0.004	0.034 ± 0.006	0.034 ± 0.006	0.036 ± 0.007
FE10	0.49 ± 0.199	0.332 ± 0.039	0.389 ± 0.091	0.436 ± 0.081	1.536 ± 2.423
FE100	0.112 ± 0.006	0.113 ± 0.006	0.108 ± 0.005	0.108 ± 0.005	0.108 ± 0.002
FE200	0.086 ± 0.005	0.089 ± 0.005	0.091 ± 0.005	0.094 ± 0.006	0.115 ± 0.008
FE500	0.058 ± 0.005	0.06 ± 0.005	0.061 ± 0.005	0.058 ± 0.006	0.062 ± 0.005
FE800	0.049 ± 0.004	0.05 ± 0.004	0.051 ± 0.003	0.048 ± 0.004	0.049 ± 0.003
PZ10	0.278 ± 0.073	0.213 ± 0.063	0.2 ± 0.078	0.158 ± 0.048	0.334 ± 0.089
PZ100	0.056 ± 0.003	0.075 ± 0.029	0.055 ± 0.002	0.054 ± 0.002	0.054 ± 0.002
PZ200	0.06 ± 0.012	0.072 ± 0.021	0.063 ± 0.014	0.06 ± 0.016	0.075 ± 0.013
PZ500	0.05 ± 0.003	0.059 ± 0.011	0.051 ± 0.004	0.05 ± 0.003	0.053 ± 0.007
PZ800	0.049 ± 0.001	0.053 ± 0.004	0.048 ± 0.001	0.049 ± 0.001	0.049 ± 0.001
DC10	0.223 ± 0.078	0.209 ± 0.052	0.238 ± 0.065	0.221 ± 0.042	0.338 ± 0.101
DC100	0.051 ± 0.017	0.045 ± 0.015	0.046 ± 0.013	0.047 ± 0.018	0.044 ± 0.011
DC200	0.033 ± 0.007	0.032 ± 0.007	0.033 ± 0.006	0.033 ± 0.006	0.051 ± 0.006
DC500	0.026 ± 0.004	0.026 ± 0.003	0.026 ± 0.006	0.024 ± 0.004	0.024 ± 0.003
DC800	0.019 ± 0.002	0.019 ± 0.002	0.019 ± 0.001	0.018 ± 0.001	0.018 ± 0.001
EBG10	0.328 ± 0.085	0.161 ± 0.055	0.244 ± 0.086	0.292 ± 0.206	0.212 ± 0.171
EBG100	0.137 ± 0.019	0.125 ± 0.02	0.134 ± 0.016	0.131 ± 0.013	0.116 ± 0.011
EBG200	0.126 ± 0.009	0.11 ± 0.007	0.11 ± 0.006	0.105 ± 0.005	0.092 ± 0.008
EBG500	0.103 ± 0.007	0.107 ± 0.017	0.098 ± 0.005	0.094 ± 0.006	0.088 ± 0.006
EBG800	0.094 ± 0.005	0.096 ± 0.008	0.089 ± 0.004	0.085 ± 0.003	0.081 ± 0.004

Table S14. % change in test MAE and test R^2 scores with respect to scratch models for varying PT (FE) dataset size.

1K										
DATASET	% change in MAE					% change in R^2 scores				
	10	100	200	500	800	10	100	200	500	800
GV	-88.919	-9.677	-14.085	-8.257	-7.292	99.192	20.343	20.916	6.380	4.178
PH	-67.780	-17.188	-33.636	-30.882	-27.907	95.928	10.487	20.555	9.799	4.093
BG	-76.284	-7.143	-13.472	-9.554	-9.155	97.403	14.985	25.070	8.350	6.294
PZ	-75.941	-16.418	-31.183	-12.069	-12.500	96.501	-16.667	21.552	100.000	133.333
DC	-73.263	-18.333	-27.660	-19.355	-13.636	95.510	66.607	102.597	73.993	4.441
EBG	-81.888	-16.867	-19.108	-11.570	-11.538	97.450	521.154	144.000	18.462	9.880

5K										
DATASET	% change in MAE					% change in R^2 scores				
	10	100	200	500	800	10	100	200	500	800
GV	-87.012	-9.032	-14.789	-10.092	-8.333	98.722	19.608	22.510	7.567	5.121
PH	-66.746	-14.844	-34.545	-35.294	-32.558	95.324	8.614	21.044	11.683	5.420
BG	-72.372	-9.184	-18.135	-12.739	-13.380	96.191	19.572	33.705	10.680	8.217
PZ	-79.962	-14.925	-35.484	-13.793	-14.286	97.558	-83.333	33.621	25.000	125.641
DC	-77.706	-8.333	-29.787	-22.581	-18.182	97.263	17.988	167.532	94.872	9.495
EBG	-84.559	-17.470	-22.930	-15.702	-11.538	98.378	503.846	168.000	20.308	3.855

10K										
DATASET	% change in MAE					% change in R^2 scores				
	10	100	200	500	800	10	100	200	500	800
GV	-79.714	-9.032	-16.197	-11.009	-10.417	95.359	19.363	23.904	8.160	5.930
PH	-61.496	-17.188	-34.545	-35.294	-32.558	91.873	12.734	19.902	11.307	5.199
BG	-73.741	-10.204	-19.171	-14.650	-13.380	96.489	21.713	34.262	11.456	7.343
PZ	-78.622	-14.925	-35.484	-12.069	-14.286	97.277	-116.667	37.931	-275.000	117.949
DC	-75.202	-1.667	-27.660	-22.581	-18.182	96.636	-25.378	173.377	81.319	6.279
EBG	-84.596	-18.675	-22.930	-15.702	-12.500	98.271	500.000	148.000	11.385	4.578

50K										
DATASET	% change in MAE					% change in R^2 scores				
	10	100	200	500	800	10	100	200	500	800
GV	-88.174	-5.806	-6.338	-9.174	-7.292	98.978	10.539	3.785	6.677	4.313
PH	-62.848	-7.812	-30.909	-41.176	-20.930	93.291	6.742	17.945	14.196	5.531
BG	-73.399	-2.041	-18.135	-14.650	-13.380	96.665	-6.116	40.111	17.476	11.713
PZ	-66.433	-2.985	-25.806	-5.172	-8.929	92.524	-383.333	18.103	-225.000	133.333
DC	-74.879	-5.000	-19.149	-25.806	-22.727	96.668	-3.028	98.701	84.982	8.116
EBG	-75.229	-6.024	-14.650	-10.744	-6.731	93.428	215.385	110.000	14.154	8.434

100K										
DATASET	% change in MAE					% change in R^2 scores				
	10	100	200	500	800	10	100	200	500	800
GV	-24.903	-10.968	-14.789	-15.596	-13.542	-389.476	21.324	22.510	11.276	7.951
PH	-62.291	-10.938	-27.273	-39.706	-41.860	93.227	10.674	11.746	13.065	7.190
BG	-72.078	-11.735	-20.207	-20.382	-19.718	96.178	24.159	44.290	22.913	16.259
PZ	13.401	-17.910	-31.183	-13.793	-14.286	-434.155	-133.333	18.103	-125.000	135.897
DC	-34.330	-3.333	-12.766	-25.806	-27.273	23.371	3.473	-7.143	106.593	10.260
EBG	-66.191	-21.687	-21.656	-17.355	-15.385	72.078	486.538	156.000	30.462	20.000

Table S15. % change in test MAE and test R^2 scores with respect to scratch models for varying PT (BG) dataset size.

DATASET	% change in MAE					% change in R^2 scores				
	10	100	200	500	800	10	100	200	500	800
1K										
GV	-78.612	-6.452	-11.972	-7.339	-6.250	94.995	13.480	18.327	5.045	3.369
PH	-77.963	-18.750	-30.909	-26.471	-23.256	99.498	12.734	17.781	9.171	4.093
FE	-80.525	-11.811	-21.101	-18.310	-14.035	96.389	7.212	9.056	3.851	2.300
PZ	-82.259	-16.418	-35.484	-13.793	-12.500	98.436	0.000	35.345	150.000	133.333
DC	-81.987	-15.000	-29.787	-16.129	-13.636	98.245	44.524	214.935	63.370	5.972
EBG	-87.999	-17.470	-19.745	-14.876	-9.615	99.105	521.154	157.000	23.077	7.952
5K										
GV	-83.735	6.452	1.408	0.917	2.083	98.095	-25.490	-8.566	-1.929	-1.482
PH	-78.282	5.469	-15.455	-19.118	-23.256	99.892	2.622	8.483	7.161	4.204
FE	-86.804	-11.024	-18.349	-15.493	-12.281	99.402	7.212	7.891	3.511	1.862
PZ	-86.407	11.940	-22.581	1.724	-5.357	99.364	183.333	69.828	-500.000	120.513
DC	-83.118	-25.000	-31.915	-16.129	-13.636	98.366	79.163	214.286	68.132	2.297
EBG	-94.109	-24.699	-29.936	-11.570	-7.692	100.103	759.615	322.000	26.769	16.627
10K										
GV	-80.220	-9.032	-12.676	-9.174	-7.292	96.409	18.627	16.733	5.786	3.908
PH	-77.486	-23.438	-30.000	-25.000	-20.930	99.186	9.176	16.966	7.035	2.876
FE	-84.539	-14.961	-16.514	-14.085	-10.526	98.623	9.709	6.856	2.945	1.533
PZ	-87.237	-17.910	-32.258	-12.069	-14.286	99.568	50.000	26.724	0.000	112.821
DC	-80.775	-23.333	-29.787	-16.129	-13.636	97.970	56.723	209.740	49.817	4.594
EBG	-91.072	-19.277	-29.936	-19.008	-14.423	99.555	540.385	241.000	30.154	13.494
50K										
GV	-73.578	-9.032	-8.451	-9.174	-7.292	88.937	18.137	9.960	6.083	3.639
PH	-75.577	-21.875	-27.273	-25.000	-20.930	98.830	6.929	10.930	5.779	2.765
FE	-82.671	-14.961	-13.761	-18.310	-15.789	98.222	9.293	6.210	4.190	2.629
PZ	-89.917	-19.403	-35.484	-13.793	-12.500	99.756	-16.667	23.276	200.000	125.641
DC	-82.149	-21.667	-29.787	-22.581	-18.182	98.296	54.853	249.351	97.436	7.504
EBG	-89.316	-21.084	-33.121	-22.314	-18.269	99.255	653.846	276.000	38.154	20.000
100K										
GV	-32.916	-7.742	2.113	-4.587	-7.292	15.345	17.892	-10.558	2.077	3.774
PH	-73.508	-16.406	7.273	-19.118	-16.279	97.077	-4.120	-4.568	3.518	0.553
FE	-38.951	-14.961	5.505	-12.676	-14.035	-149.988	9.015	-3.622	2.945	2.191
PZ	-78.685	-19.403	-19.355	-8.621	-12.500	94.242	-150.000	43.103	-575.000	117.949
DC	-72.698	-26.667	8.511	-22.581	-18.182	95.030	82.369	-202.597	88.278	10.413
EBG	-92.243	-30.120	-41.401	-27.273	-22.115	99.499	776.923	378.000	47.692	21.446

S8 Pair-wise PT-FT models

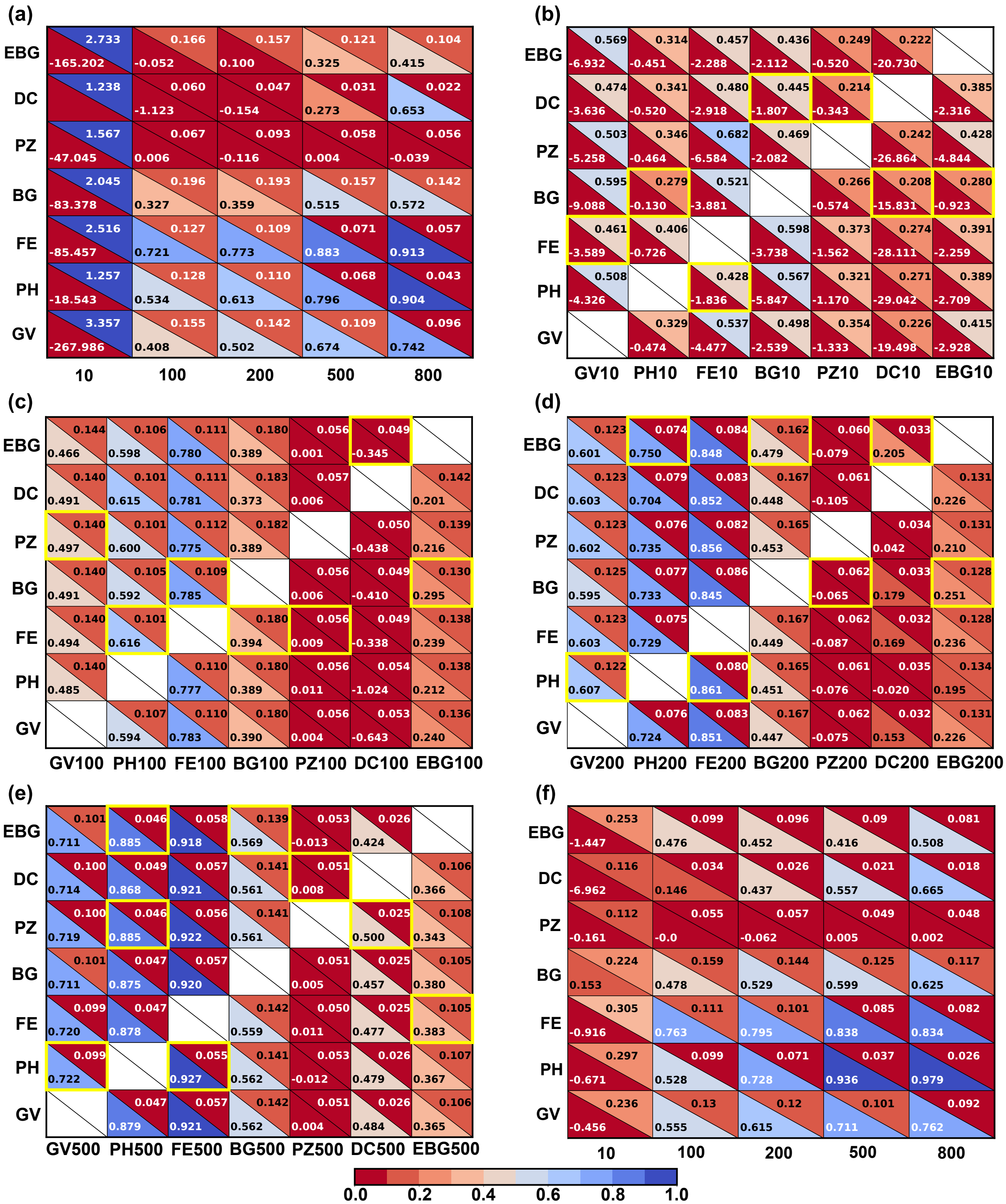

Figure S18. Performance of pair-wise TL and MPT models for different datasets sizes. Heatmap illustrating the test R^2 scores (lower triangles) and test MAEs (upper triangles) for the scratch (panel a), the 7×6 PT-FT (b-e), and MPT (f) models for different dataset sizes. Notations used are similar to those used in Figure 6 of the main text.

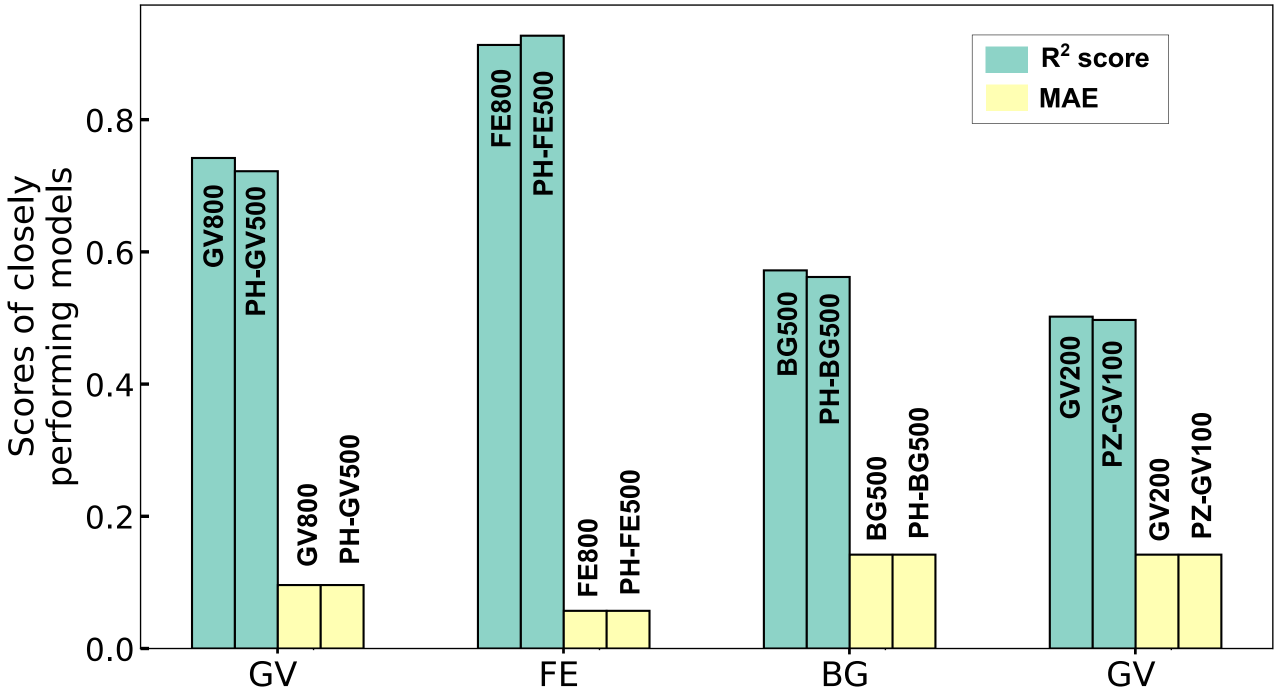

Figure S19. Illustration of closely performing models. Bar plots illustrating the R^2 scores and MAEs for the closely performing models in pair-wise transfer learning.

Table S16. R^2 scores with margins of errors for all PT-FT combinations.

FT size	GV	PH	FE	BG	PZ	DC	EBG
GV10	*	-4.326 ± 1.146	-3.589 ± 2.063	-9.088 ± 15.387	-5.258 ± 8.11	-3.636 ± 1.395	-6.932 ± 6.629
GV100	*	0.485 ± 0.049	0.494 ± 0.049	0.491 ± 0.043	0.497 ± 0.032	0.491 ± 0.049	0.466 ± 0.048
GV200	*	0.607 ± 0.043	0.603 ± 0.036	0.595 ± 0.047	0.602 ± 0.051	0.603 ± 0.043	0.601 ± 0.04
GV500	*	0.722 ± 0.031	0.72 ± 0.026	0.711 ± 0.03	0.719 ± 0.029	0.714 ± 0.028	0.711 ± 0.031
GV800	*	0.774 ± 0.021	0.774 ± 0.02	0.768 ± 0.023	0.772 ± 0.027	0.768 ± 0.022	0.766 ± 0.022
PH10	-0.474 ± 0.214	*	-0.726 ± 0.559	-0.13 ± 0.226	-0.464 ± 0.321	-0.52 ± 0.337	-0.451 ± 0.214
PH100	0.594 ± 0.098	*	0.616 ± 0.102	0.592 ± 0.123	0.6 ± 0.121	0.615 ± 0.089	0.598 ± 0.145
PH200	0.724 ± 0.124	*	0.729 ± 0.102	0.733 ± 0.102	0.735 ± 0.135	0.704 ± 0.122	0.75 ± 0.131
PH500	0.879 ± 0.066	*	0.878 ± 0.065	0.875 ± 0.078	0.885 ± 0.06	0.868 ± 0.075	0.885 ± 0.067
PH800	0.947 ± 0.032	*	0.946 ± 0.034	0.946 ± 0.039	0.947 ± 0.036	0.94 ± 0.025	0.94 ± 0.038
FE10	-4.477 ± 8.267	-1.836 ± 1.623	*	-3.881 ± 5.233	-6.584 ± 9.016	-2.918 ± 4.181	-2.288 ± 2.555
FE100	0.783 ± 0.012	0.777 ± 0.031	*	0.785 ± 0.015	0.775 ± 0.027	0.781 ± 0.01	0.78 ± 0.02
FE200	0.851 ± 0.014	0.861 ± 0.012	*	0.845 ± 0.018	0.856 ± 0.01	0.852 ± 0.015	0.848 ± 0.015
FE500	0.921 ± 0.017	0.927 ± 0.019	*	0.92 ± 0.018	0.922 ± 0.016	0.921 ± 0.018	0.918 ± 0.019
FE800	0.936 ± 0.016	0.938 ± 0.016	*	0.936 ± 0.016	0.938 ± 0.014	0.936 ± 0.017	0.934 ± 0.017
BG10	-2.539 ± 1.733	-5.847 ± 9.849	-3.738 ± 2.3	*	-2.082 ± 1.674	-1.807 ± 1.036	-2.112 ± 2.693
BG100	0.39 ± 0.022	0.389 ± 0.027	0.394 ± 0.03	*	0.389 ± 0.011	0.373 ± 0.037	0.389 ± 0.032
BG200	0.447 ± 0.054	0.451 ± 0.052	0.449 ± 0.051	*	0.453 ± 0.038	0.448 ± 0.048	0.479 ± 0.038
BG500	0.562 ± 0.03	0.562 ± 0.034	0.559 ± 0.024	*	0.561 ± 0.03	0.561 ± 0.031	0.569 ± 0.027
BG800	0.609 ± 0.016	0.611 ± 0.012	0.609 ± 0.014	*	0.607 ± 0.018	0.598 ± 0.016	0.619 ± 0.013
PZ10	-1.333 ± 0.88	-1.17 ± 0.906	-1.562 ± 1.217	-0.574 ± 0.302	*	-0.343 ± 0.21	-0.52 ± 0.444
PZ100	0.004 ± 0.02	0.011 ± 0.024	0.009 ± 0.01	0.006 ± 0.025	*	0.006 ± 0.011	0.001 ± 0.017
PZ200	-0.075 ± 0.228	-0.076 ± 0.204	-0.087 ± 0.254	0.006 ± 0.178	*	-0.105 ± 0.309	0.079 ± 0.209
PZ500	0.004 ± 0.037	-0.012 ± 0.064	0.011 ± 0.015	0.005 ± 0.01	*	0.008 ± 0.021	-0.013 ± 0.078
PZ800	0.009 ± 0.005	0.012 ± 0.006	0.014 ± 0.01	0.007 ± 0.008	*	0.001 ± 0.019	0.012 ± 0.005
DC10	-19.498 ± 12.135	-29.042 ± 23.261	-28.111 ± 28.429	-15.831 ± 7.339	-26.864 ± 43.935	*	-20.73 ± 21.417
DC100	-0.643 ± 1.155	-1.024 ± 2.024	-0.338 ± 0.666	-0.41 ± 0.871	-0.438 ± 0.639	*	-0.345 ± 0.679
DC200	0.153 ± 0.587	-0.02 ± 0.743	0.169 ± 0.631	-0.179 ± 0.459	0.042 ± 0.666	*	0.205 ± 0.441
DC500	0.484 ± 0.108	0.479 ± 0.19	0.477 ± 0.117	0.457 ± 0.177	0.5 ± 0.101	*	0.424 ± 0.235
DC800	0.687 ± 0.031	0.661 ± 0.049	0.677 ± 0.066	0.697 ± 0.054	0.681 ± 0.047	*	0.68 ± 0.035
EBG10	-2.928 ± 1.991	-2.709 ± 1.533	-2.259 ± 1.648	-0.923 ± 0.544	-4.844 ± 9.271	-2.316 ± 1.942	*
EBG100	0.24 ± 0.09	0.212 ± 1.125	0.239 ± 0.095	0.295 ± 0.068	0.216 ± 0.179	0.201 ± 0.182	*
EBG200	0.226 ± 0.085	0.195 ± 0.054	0.236 ± 0.084	0.251 ± 0.067	0.21 ± 0.079	0.226 ± 0.082	*
EBG500	0.365 ± 0.048	0.367 ± 0.073	0.383 ± 0.055	0.38 ± 0.039	0.343 ± 0.053	0.366 ± 0.069	*
EBG800	0.461 ± 0.083	0.442 ± 0.075	0.459 ± 0.072	0.452 ± 0.092	0.436 ± 0.08	0.449 ± 0.076	*

Table S17. MAEs with margins of errors for all PT-FT combinations.

FT size	GV	PH	FE	BG	PZ	DC	EBG
GV10	*	0.508 ± 0.06	0.461 ± 0.13	0.595 ± 0.368	0.503 ± 0.285	0.474 ± 0.084	0.569 ± 0.227
GV100	*	0.14 ± 0.01	0.14 ± 0.009	0.14 ± 0.008	0.14 ± 0.008	0.14 ± 0.007	0.144 ± 0.009
GV200	*	0.122 ± 0.008	0.123 ± 0.006	0.125 ± 0.008	0.123 ± 0.009	0.123 ± 0.008	0.123 ± 0.007
GV500	*	0.099 ± 0.005	0.099 ± 0.005	0.101 ± 0.005	0.01 ± 0.006	0.1 ± 0.005	0.101 ± 0.006
GV800	*	0.089 ± 0.005	0.089 ± 0.004	0.09 ± 0.005	0.089 ± 0.006	0.09 ± 0.004	0.09 ± 0.005
PH10	0.329 ± 0.053	*	0.406 ± 0.102	0.279 ± 0.046	0.346 ± 0.089	0.341 ± 0.085	0.314 ± 0.069
PH100	0.107 ± 0.01	*	0.101 ± 0.01	0.105 ± 0.009	0.101 ± 0.014	0.101 ± 0.011	0.106 ± 0.014
PH200	0.076 ± 0.013	*	0.075 ± 0.01	0.077 ± 0.014	0.076 ± 0.014	0.079 ± 0.012	0.074 ± 0.014
PH500	0.047 ± 0.005	*	0.047 ± 0.003	0.047 ± 0.004	0.046 ± 0.004	0.049 ± 0.006	0.046 ± 0.003
PH800	0.031 ± 0.004	*	0.031 ± 0.006	0.03 ± 0.006	0.03 ± 0.004	0.032 ± 0.004	0.032 ± 0.007
FE10	0.537 ± 0.385	0.428 ± 0.104	*	0.521 ± 0.294	0.682 ± 0.442	0.48 ± 0.22	0.457 ± 0.183
FE100	0.11 ± 0.004	0.11 ± 0.01	*	0.109 ± 0.006	0.112 ± 0.01	0.111 ± 0.004	0.111 ± 0.006
FE200	0.083 ± 0.004	0.08 ± 0.005	*	0.086 ± 0.006	0.082 ± 0.003	0.083 ± 0.005	0.084 ± 0.006
FE500	0.057 ± 0.004	0.055 ± 0.006	*	0.057 ± 0.005	0.056 ± 0.005	0.057 ± 0.005	0.058 ± 0.006
FE800	0.048 ± 0.004	0.047 ± 0.004	*	0.048 ± 0.004	0.048 ± 0.003	0.048 ± 0.004	0.049 ± 0.004
BG10	0.498 ± 0.145	0.567 ± 0.308	0.598 ± 0.161	*	0.469 ± 0.139	0.445 ± 0.072	0.436 ± 0.174
BG100	0.18 ± 0.006	0.18 ± 0.006	0.18 ± 0.006	*	0.182 ± 0.005	0.183 ± 0.008	0.18 ± 0.005
BG200	0.167 ± 0.013	0.165 ± 0.011	0.167 ± 0.012	*	0.165 ± 0.011	0.167 ± 0.012	0.162 ± 0.011
BG500	0.142 ± 0.004	0.141 ± 0.005	0.142 ± 0.003	*	0.141 ± 0.003	0.141 ± 0.003	0.139 ± 0.004
BG800	0.129 ± 0.002	0.128 ± 0.001	0.128 ± 0.002	*	0.128 ± 0.002	0.13 ± 0.002	0.126 ± 0.002
PZ10	0.354 ± 0.133	0.321 ± 0.111	0.373 ± 0.163	0.266 ± 0.065	*	0.214 ± 0.038	0.249 ± 0.081
PZ100	0.056 ± 0.002	0.056 ± 0.002	0.056 ± 0.002	0.056 ± 0.003	*	0.057 ± 0.002	0.056 ± 0.002
PZ200	0.062 ± 0.018	0.061 ± 0.011	0.062 ± 0.014	0.062 ± 0.016	*	0.061 ± 0.016	0.06 ± 0.012
PZ500	0.051 ± 0.005	0.053 ± 0.006	0.05 ± 0.003	0.051 ± 0.003	*	0.051 ± 0.005	0.053 ± 0.008
PZ800	0.049 ± 0.001	0.049 ± 0.001	0.049 ± 0.001	0.049 ± 0.003	*	0.05 ± 0.004	0.049 ± 0.001
DC10	0.226 ± 0.077	0.271 ± 0.107	0.274 ± 0.137	0.208 ± 0.041	0.242 ± 0.18	*	0.222 ± 0.085
DC100	0.053 ± 0.019	0.054 ± 0.021	0.049 ± 0.014	0.049 ± 0.017	0.05 ± 0.015	*	0.049 ± 0.015
DC200	0.032 ± 0.005	0.035 ± 0.008	0.032 ± 0.006	0.033 ± 0.006	0.034 ± 0.006	*	0.033 ± 0.005
DC500	0.026 ± 0.004	0.026 ± 0.005	0.025 ± 0.003	0.025 ± 0.004	0.025 ± 0.003	*	0.026 ± 0.004
DC800	0.019 ± 0.001	0.02 ± 0.001	0.019 ± 0.001	0.019 ± 0.001	0.019 ± 0.001	*	0.02 ± 0.001
EBG10	0.415 ± 0.072	0.389 ± 0.104	0.391 ± 0.12	0.28 ± 0.034	0.428 ± 0.28	0.385 ± 0.12	*
EBG100	0.136 ± 0.017	0.138 ± 0.019	0.138 ± 0.02	0.13 ± 0.007	0.139 ± 0.021	0.142 ± 0.024	*
EBG200	0.131 ± 0.009	0.134 ± 0.011	0.128 ± 0.007	0.128 ± 0.008	0.131 ± 0.008	0.131 ± 0.011	*
EBG500	0.106 ± 0.006	0.107 ± 0.007	0.105 ± 0.007	0.105 ± 0.007	0.108 ± 0.008	0.106 ± 0.009	*
EBG800	0.091 ± 0.004	0.093 ± 0.005	0.092 ± 0.003	0.093 ± 0.005	0.093 ± 0.005	0.092 ± 0.003	*

Table S18. Percentage change in the evaluation metrics of PT-FT models with respect to scratch.

PT-FTsize	% Increase in R^2 scores	% Decrease in MAEs
FE-GV10	98.66	86.268
BG-PH10	99.3	77.804
PH-FE10	97.85	82.99
EBG-BG10	97.83	78.68
DC-PZ10	99.27	86.34
BG-DC10	98.42	83.20
BG-EBG10	99.44	89.755
PZ-GV100	21.814	9.677
FE-PH100	15.356	21.094
BG-FE100	8.877	14.173
FE-BG100	20.49	8.163
PH-PZ100	83.33	16.42
FE-DC100	69.90	18.33
BG-EBG100	667.31	21.687
PH-GV200	20.916	14.085
EBG-PH200	22.349	32.727
PH-FE200	11.384	26.606
EBG-BG200	33.426	16.062
BG-PZ200	43.97	33.33
EBG-DC200	233.10	31.91
BG-EBG200	151	18.471
PH-GV500	7.122	9.174
EBG/PZ-PH500	11.181	32.353
PH-FE500	4.983	22.535
EBG-BG500	10.49	11.46
FE-PZ500	175	13.79
PZ-DC500	83.15	19.355
FE-EBG500	17.850	13.223
FE/PH-GV800	4.313	7.292
PZ-PH800	4.757	30.233
PH-FE800	2.738	17.544
EBG-BG800	8.216	11.268
FE-PZ800	135.90	12.5
GV-DC800	6.738	13.636
GV-EBG800	11.084	12.500

S9 Scores of MPT models

Table S19. Test R^2 scores with margins of errors for MPT models corresponding to each property.

Models	10	100	200	500	800
GV	-0.456 $\pm$ 1.45	0.555 $\pm$ 0.048	0.615 $\pm$ 0.069	0.711 $\pm$ 0.032	0.762 $\pm$ 0.031
PH	-0.671 $\pm$ 2.149	0.528 $\pm$ 0.141	0.728 $\pm$ 0.193	0.936 $\pm$ 0.033	0.979 $\pm$ 0.012
FE	-0.916 $\pm$ 3.737	0.763 $\pm$ 0.09	0.795 $\pm$ 0.11	0.838 $\pm$ 0.132	0.834 $\pm$ 0.174
BG	0.153 $\pm$ 0.425	0.478 $\pm$ 0.083	0.529 $\pm$ 0.018	0.599 $\pm$ 0.028	0.625 $\pm$ 0.039
PZ	-0.161 $\pm$ 0.456	-0.0 $\pm$ 0.02	-0.062 $\pm$ 0.175	0.005 $\pm$ 0.019	0.002 $\pm$ 0.007
DC	-6.962 $\pm$ 14.75	0.146 $\pm$ 0.297	0.437 $\pm$ 0.22	0.557 $\pm$ 0.152	0.665 $\pm$ 0.144
EBG	-1.447 $\pm$ 4.912	0.476 $\pm$ 0.041	0.452 $\pm$ 0.039	0.416 $\pm$ 0.029	0.508 $\pm$ 0.04

Table S20. Test MAEs with margins of errors for MPT models corresponding to each property.

Models	10	100	200	500	800
GV	0.236 $\pm$ 0.109	0.13 $\pm$ 0.007	0.12 $\pm$ 0.007	0.101 $\pm$ 0.003	0.092 $\pm$ 0.006
PH	0.297 $\pm$ 0.275	0.099 $\pm$ 0.018	0.071 $\pm$ 0.024	0.037 $\pm$ 0.005	0.026 $\pm$ 0.003
FE	0.305 $\pm$ 0.321	0.111 $\pm$ 0.025	0.101 $\pm$ 0.033	0.085 $\pm$ 0.04	0.082 $\pm$ 0.052
BG	0.224 $\pm$ 0.06	0.159 $\pm$ 0.02	0.144 $\pm$ 0.01	0.125 $\pm$ 0.005	0.117 $\pm$ 0.005
PZ	0.112 $\pm$ 0.074	0.055 $\pm$ 0.002	0.057 $\pm$ 0.016	0.049 $\pm$ 0.003	0.048 $\pm$ 0.001
DC	0.116 $\pm$ 0.128	0.034 $\pm$ 0.006	0.026 $\pm$ 0.003	0.021 $\pm$ 0.002	0.018 $\pm$ 0.002
EBG	0.253 $\pm$ 0.324	0.099 $\pm$ 0.005	0.096 $\pm$ 0.004	0.09 $\pm$ 0.005	0.081 $\pm$ 0.003

S10 Comparison with literature models

It is important to undo the standardization and normalization operations of the target values before model evaluation for a fair comparison with the values reported in the literature. Thus, the operations should be undone sequentially in reverse, i.e., removing normalization ('unnormalize') followed by removing the standardization ('unscale'). The following are the formulae for unnormalizing and unscaling the reported values.

$$\text{Unnormalized\_value} = \frac{(\text{Normalized\_value} + 1)}{2} \times (\text{Original\_scaled\_max} - \text{Original\_scaled\_min}) + \text{Original\_scaled\_min}$$

$$\text{Original\_value} = (\text{Unnormalized\_value} \times \text{Original\_stddev}) + \text{Original\_mean}$$

Here, the Original_stddev and Original_mean correspond to the mean and standard deviation, respectively, of the unscaled and unnormalized training dataset. The scaled maxima and minima of the training dataset should be correspondingly substituted for Original_scaled_max and Original_scaled_min variables.

Reference	PT dataset and size	FT dataset and size	MAE reported	Our model	Our MAE
[1]	FE(MP) and 113,000	BG(MP) and 500	0.866	FE(941)-BG500	0.688
[1]	BG(MP) and 54,000	FE(MP) and 500	0.149	BG(941)-FE500	0.204
[2]	FE(OQMD) and 341,000	FE(MP) and 23,641	0.108	GV(941)-FE(800)	0.170
[3]	FE(MP) and 69,239	FE(Jarvis 3D) and 55,711	0.032	GV(941)-FE(800)	0.170

Table S21. Comparison between MAEs reported in previous work and this work. MP and OQMD stand for Materials Project and Open Quantum Materials Database, respectively.

References

1. Lee, J. & Asahi, R. Transfer learning for materials informatics using crystal graph convolutional neural network. *Comput. Mater. Sci.* **190**, 110314 (2021).

2. Jha, D. *et al.* Enhancing materials property prediction by leveraging computational and experimental data using deep transfer learning. *Nat. communications* **10**, 5316 (2019).

3. Gupta, V. *et al.* Structure-aware graph neural network based deep transfer learning framework for enhanced predictive analytics on diverse materials datasets. *npj Comput. Mater.* **10**, 1 (2024).