Supplementary Information

Predicting melting temperature of inorganic crystals via crystal graph neural network enhanced by transfer learning

Jaesun Kim[1], *Jisu Jung*[1], *Sookyung Kim*[2], *Seungwu Han*[1,3*]

[1] Department of Material Science and Engineering, Seoul National University, Seoul 08826, Korea

[2] Palo Alto Research Center (PARC), Palo Alto, CA, USA

[3] Korea Institute for Advanced Study, Seoul 02455, Korea

* Corresponding author

E-mail: hansw@snu.ac.kr

Correlation with pre-training properties

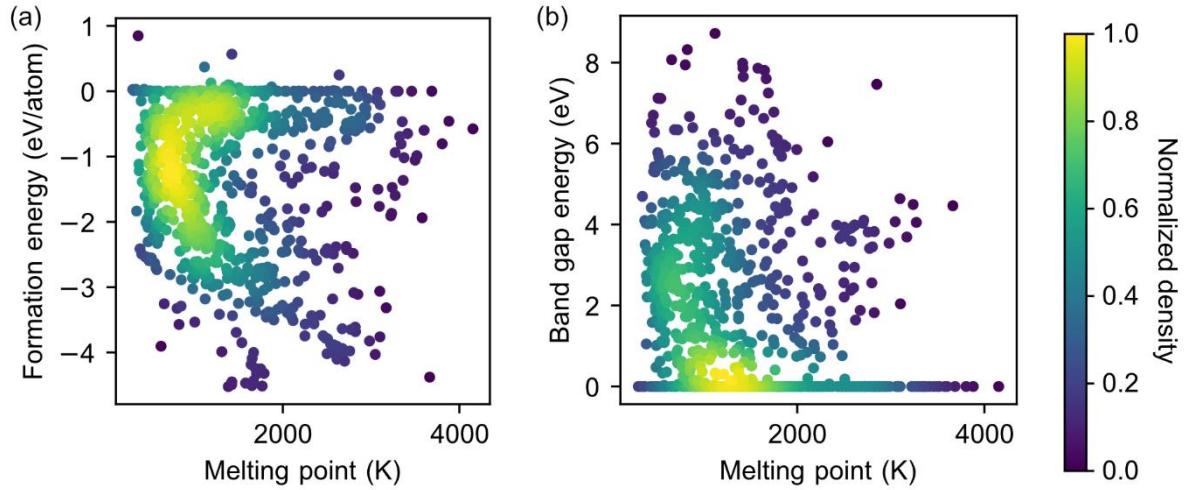

Fig. S1. The correlation between melting points and pre-training features. Pre-training features are (a) formation energy and (b) band gap energy.

Correlation of ternary compounds with pre-training properties

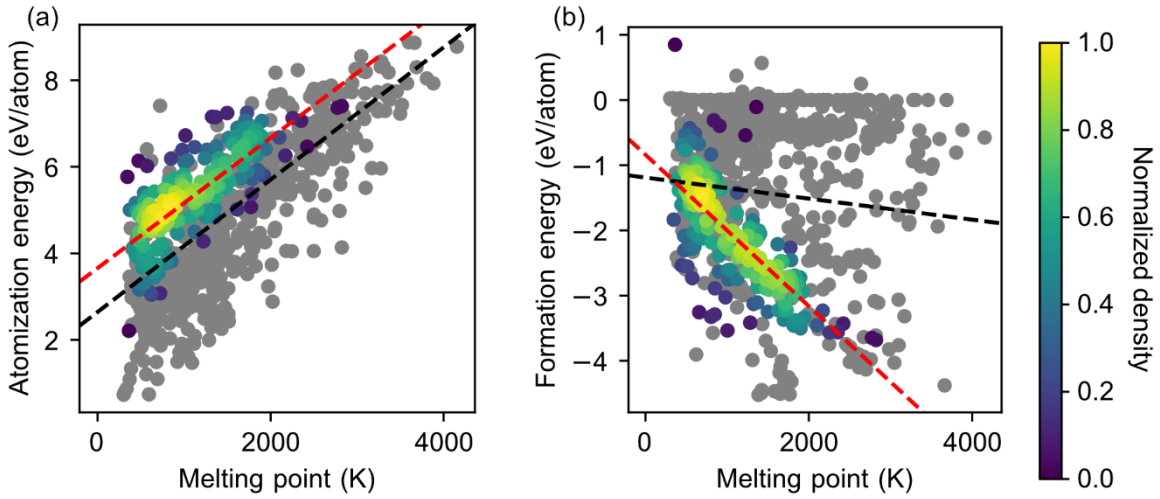

Fig. S2. The correlation between melting points and pre-training features. Pre-training features are (a) atomization energy and (b) formation energy. While ternary compounds are colored by their densities, others are filled with gray. The black and red dashed lines denote the linear regression lines of total and ternary compounds, respectively.

Effect of TL by the choice of training set

We perform an experiment utilizing training sets that exclusively consist of crystals without transition metals (called Model-TL-w/o TM hereafter) and those with transition metals (called Model-TL-w/ TM hereafter). The outcomes are depicted in Fig. S3. In Fig. S3(a), Model-TL-w/o TM consistently exhibits higher RMSE values than the other models. This can be attributed to the limitation of Model-TL-w/o TM in capturing information about transition metals, resulting in a diminished overall accuracy in the test set. Model-TL-w/ TM demonstrates lower RMSE in the test set, but its accuracy does not improve with an increase in the size of the training set. While the training sets of Model-TL-w/ TM include both transition and non-transition metals, providing a clear advantage at a smaller training set size compared to Model-TL-w/o TM, there is a limitation. The absence of information pertaining to interactions between non-transition metals within Model-TL-w/ TM may contribute to the observed plateau trend in RMSE. This plateau trend bears an analogy to the pattern identified in Model-TL-binary.

In Fig. S3(b), we present the RMSE values for each model and crystal category within the test set, considering an equal size of the training set. For the evaluation, we selected 125 data points, corresponding to the dashed line in Fig. S3(a). Despite Model-TL-w/o TM and Model-TL-w/ TM exhibiting higher overall RMSE in the total test set compared to Model-TL, they demonstrate lower RMSE values when focusing on specific crystal groups. Specifically, Model-TL-w/o TM displays a 19 K lower RMSE for the w/o TM category, while Model-TL-w/ TM exhibits a 26 K lower RMSE for the w/ TM crystal group. It is noteworthy that both models are not transferable to an untrained domain, resulting in higher RMSEs. These findings underscore the advantages of concentrating on specific crystal classes of interest when constructing a database.

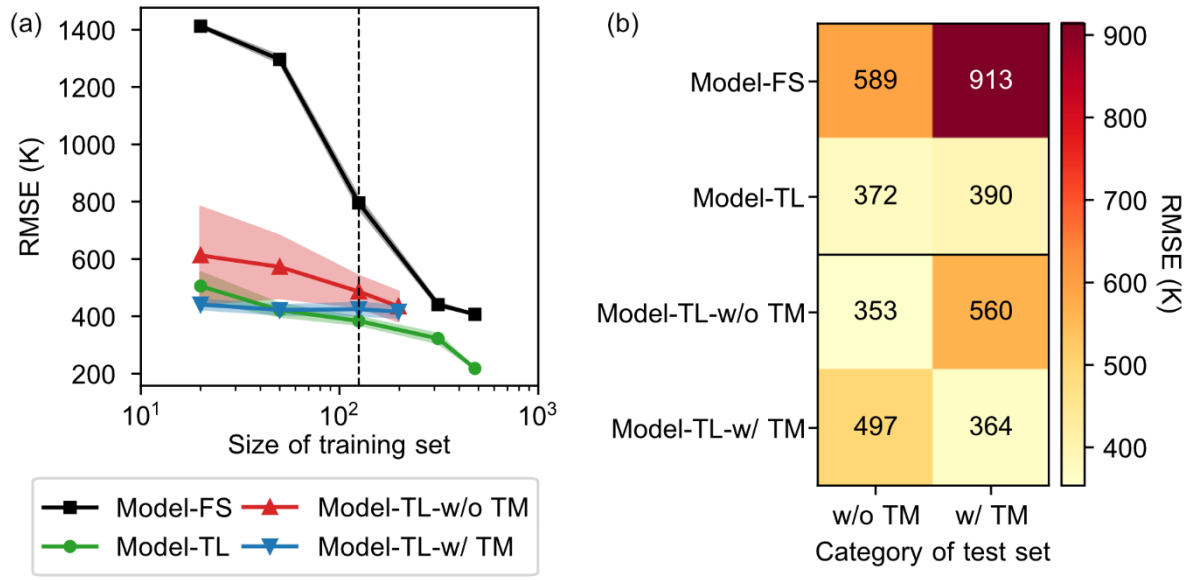

Fig. S3. Test set RMSEs of Model-FS, Model-TL, and its variations. (a) RMSEs illustrating variations with changes in the size of the training set. (b) RMSEs for subsets within the test set with 125 training points. Model-TL-w/o TM and -w/ TM denote the TL model exclusively trained on melting points of crystals without transition metal elements (w/o TM) and crystals containing transition metal elements (w/ TM), respectively. The shadings in (a) represent the standard deviation across 5 models.