Supplementary material for Enhancing extrapolation in Materials Science through Contrastive Learning of Chemical Compositions

Anonymous Author(s)
Affiliation
Address
email

A Datasets

In table 1 we report a summary of different datasets of chemical properties examined in this study. The stated dataset sizes correspond to the application of the preprocessing steps outlined in the main paper.

Table 1: Utilized datasets to benchmark the proposed approach.

Dataset name	Property	units	size	original source
seebeck	Seebeck coefficient	μV/K	403	UCSB
kappa	Thermal conductivity	W/mK (log10)	319	UCSB
tcongrmelt	Temperature for congruent melting	K	3674	MPDS
elecmass	Effective mass of electrons	m_0 (log10)	320	MPDS
bmodulus	Bulk modulus	GPa	1432	MPDS
smodulus	Shear modulus	GPa	317	MPDS
bandgap	Band gap	eV	2728	MPDS

B Implementation details

All neural network-based models have been implemented utilizing PyTorch [1] and PyTorch Geometric [2]. CombNet's encoder module is configured with 128 input channels, 256 hidden channels, and 256 output channels, employing 3 message-passing layers. The projection head MLP_{proj} is designed as a single-layer MLP with a hidden dimension set to 512. The separate MLP_{pred} model, emloyed both as baseline and for fine-tuning contrastive-learned representations, adopts hidden dimensions [512, 256, 128, 64]. All neural networks utilize ReLU as activation function. CrabNet model is utilized with its default settings, while Ridge and SVR are implemented using the sci-kit learn package [3], also with default settings.

References

[1] Pytorch: An imperative style, high-performance deep learning library, 2019.

[2] Matthias Fey and Jan E. Lenssen. Fast graph representation learning with PyTorch Geometric. In *ICLR Workshop on Representation Learning on Graphs and Manifolds*, 2019.

Submitted to 37th Conference on Neural Information Processing Systems (NeurIPS 2023). Do not distribute.

[3] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 2011.