Supporting Information for

High-Throughput Computational Discovery of 3,218 Ultralow Thermal Conductivity and Dynamically Stable Materials by Dual Machine Learning Models

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Figure S1: Overview of the workflow. After training classification model and predicting stable structures (Step 1), step 2 is to train and screen the stable structures for low LTC. Step 3 and step 4 are recommendation and verification of low LTC structures, respectively.
Figure S2: (a) Outliers within the independent variables for the machine learning classification models. Panel (b) explains the boxplot, showing the outliers.
Figure S3: Phonon dispersions of selected structures (a) Br$_5$Cs$_3$Zn, (b) Cl$_6$PtRb$_2$, (c) AuBr$_5$ClCs, and (d) Br$_6$Cs$_2$Pt along high symmetry paths. The non-negative phonon dispersions prove the thermodynamic stability of the structures. The low-lying acoustic phonon frequencies are also clearly seen, which is partially responsible for their ultralow lattice thermal conductivity.
Figure S4: Testing results of $P_3$ parameter for the three GNN predictive models for 808 structures: (a) OGCNN, (b) deeperGATGNN, and (c) ALIGNN.
Figure S5: Testing results of mean squared displacement (MSD) of three GNN predictive models for 808 structures: (a) OGCNN, (b) DeeperGATGNN, and (c) ALIGNN.
Figure S6: (a) DFT calculated $P_3$ parameter versus LTC, (b) ALIGNN model predicted $P_3$ parameter versus LTC, (c) DFT calculated MSD versus LTC, (d) ALIGNN model predicted MSD versus LTC.