Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information for

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

Joshua Ojih,[1] Chen Shen,[2] Alejandro Rodriguez,[1] Uche Onyekpe,[3] Hongbin Zhang,[2,*] Kamal Choudhary,[4] and Ming Hu[1,*]

[1]Department of Mechanical Engineering, University of South Carolina, SC 29208, USA

[2]Institute of Materials Science, Technical University of Darmstadt, Darmstadt 64287, Germany

[3]Centre for Computational Sciences and Mathematical Modelling, Coventry University, Priory Road, Coventry, CV1 5FB, UK

[4]Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

[*] Authors to whom all correspondence should be addressed. E-Mail: hzhang@tmm.tu-darmstadt.de (H.Z.); hu@sc.edu (M.H.)

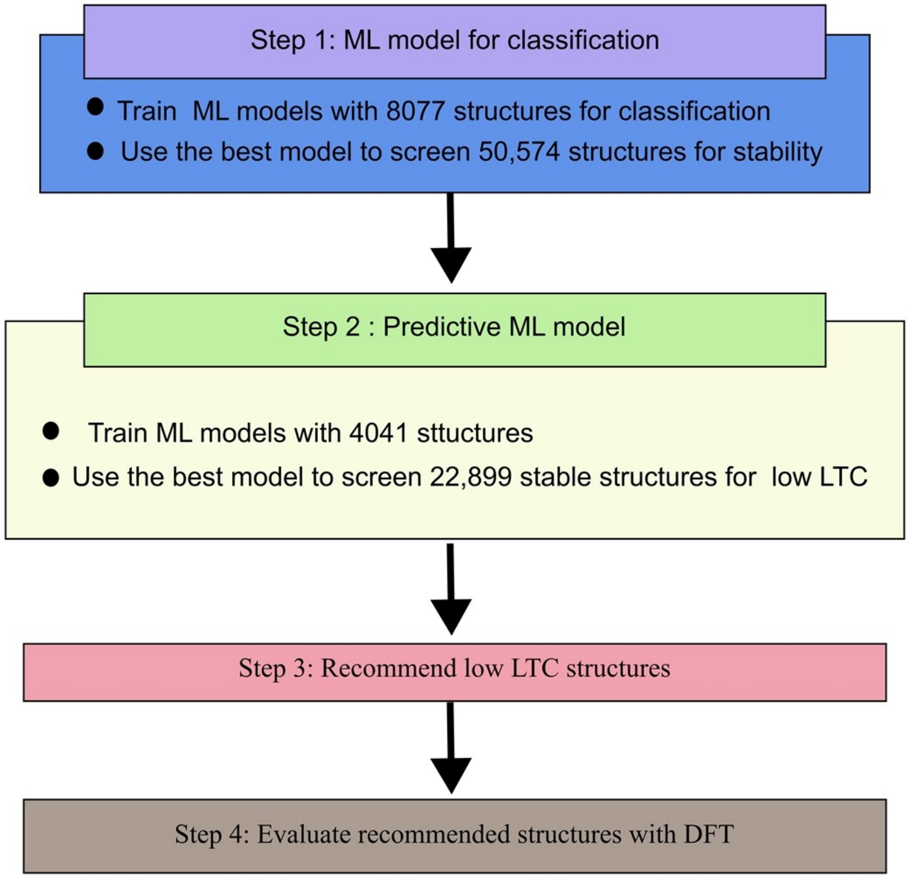

Figure S1: Overview of the workflow. After training classification model and predicting stable structures (Step 1), step 2 is to train and screen the stable structures for low LTC. Step 3 and step 4 are recommendation and verification of low LTC structures, respectively.

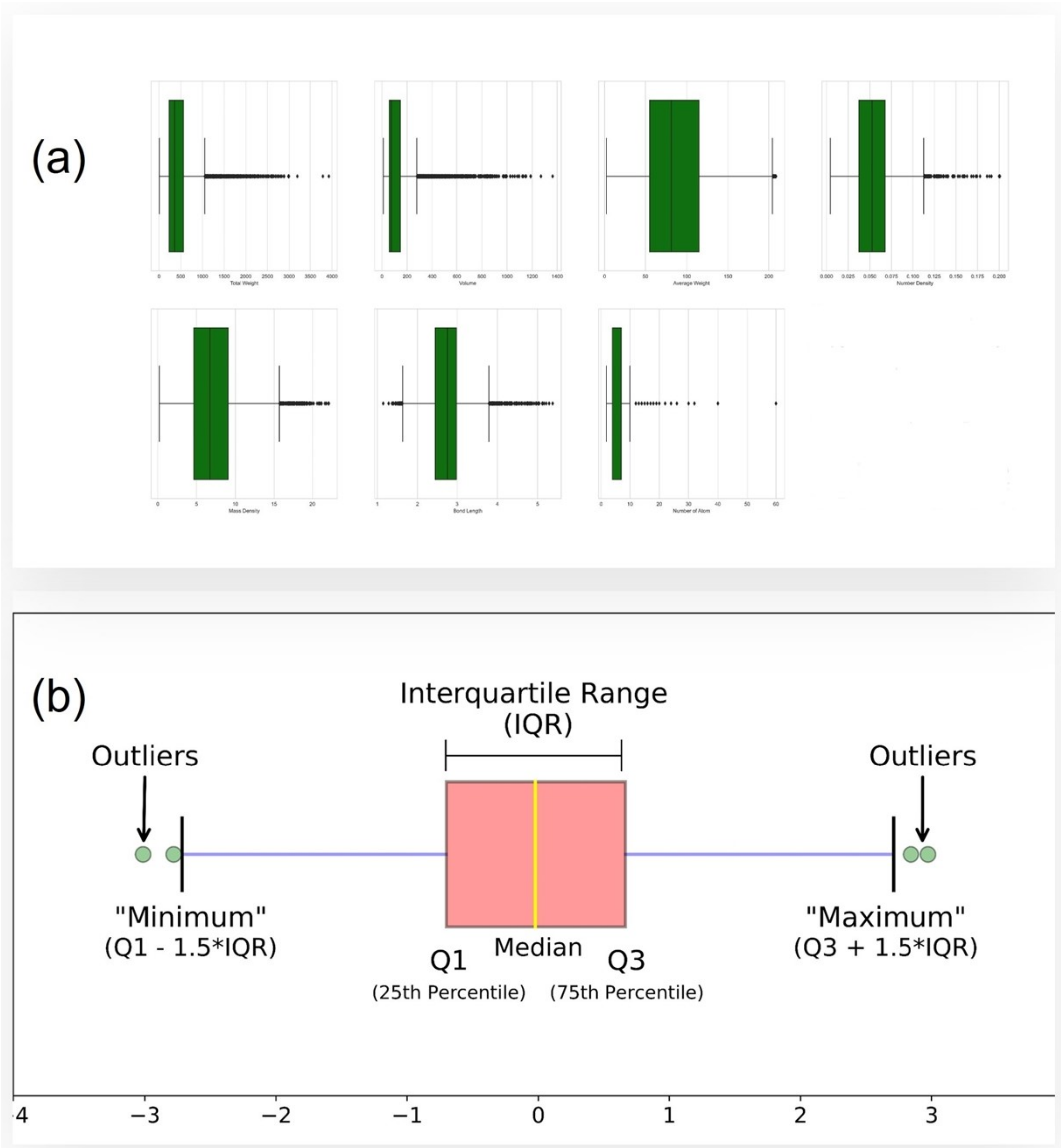

Figure S2: (a) Outliers within the independent variables for the machine learning classification models. Panel (b) explains the boxplot, showing the outliers.

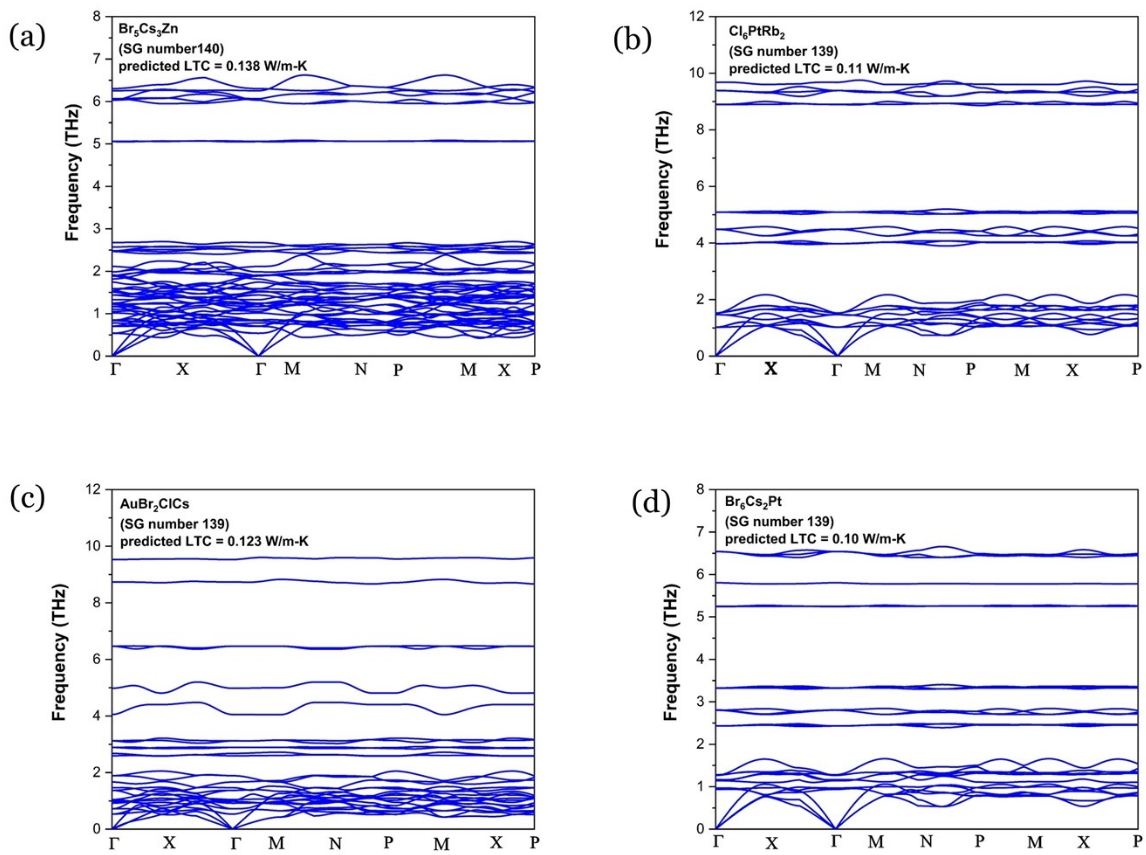

Figure S3: Phonon dispersions of selected structures (a) Br_5Cs_3Zn, (b) Cl_6PtRb_2, (c) $AuBr_2ClCs$, and (d) Br_6Cs_2Pt along high symmetry paths. The non-negative phonon dispersions prove the thermodynamic stability of the structures. The low-lying acoustic phonon frequencies are also clearly seen, which is partially responsible for their ultralow lattice thermal conductivity.

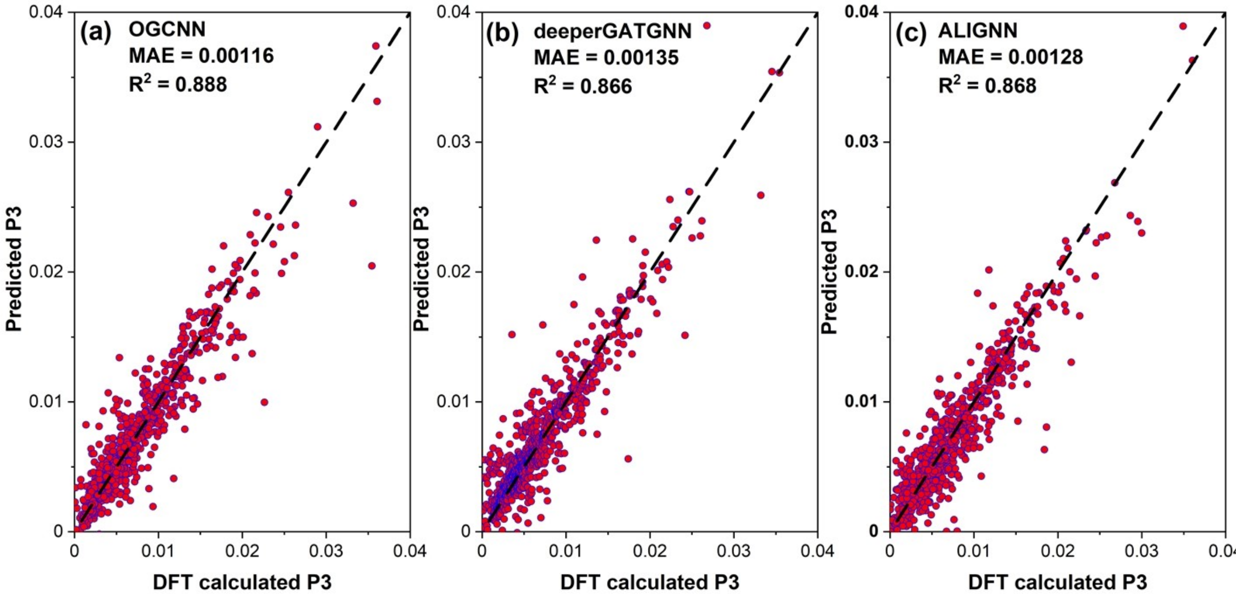

Figure S4: Testing results of P_3 parameter for the three GNN predictive models for 808 structures: (a) OGCNN, (b) deeperGATGNN, and (c) ALIGNN.

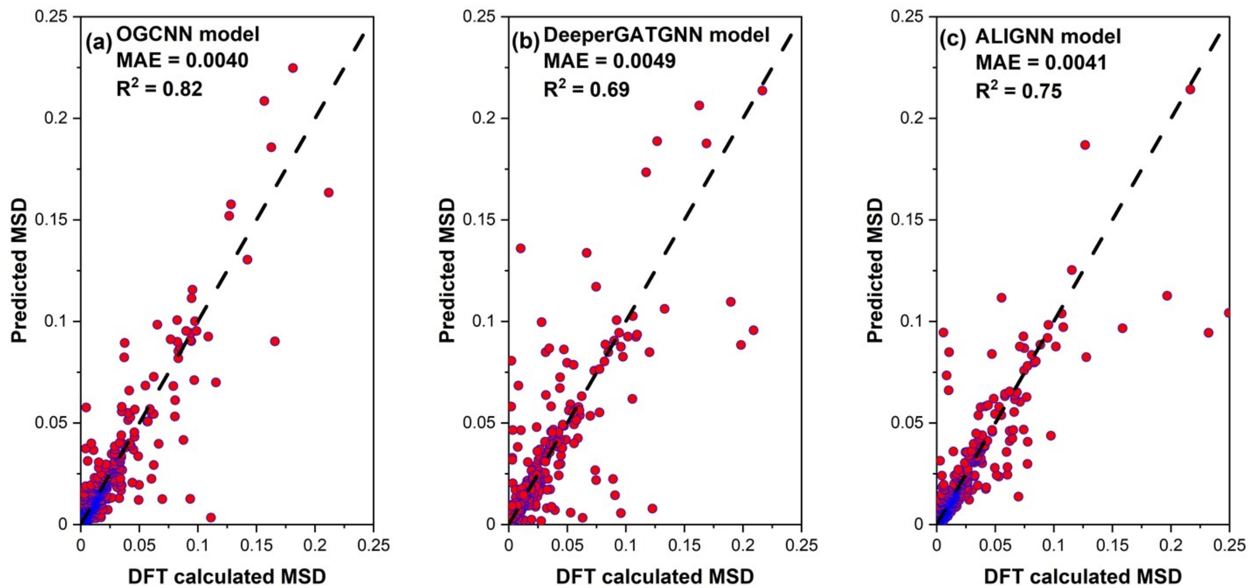

Figure S5: Testing results of mean squared displacement (MSD) of three GNN predictive models for 808 structures: (a) OGCNN, (b) deeperGATGNN, and (c) ALIGNN.

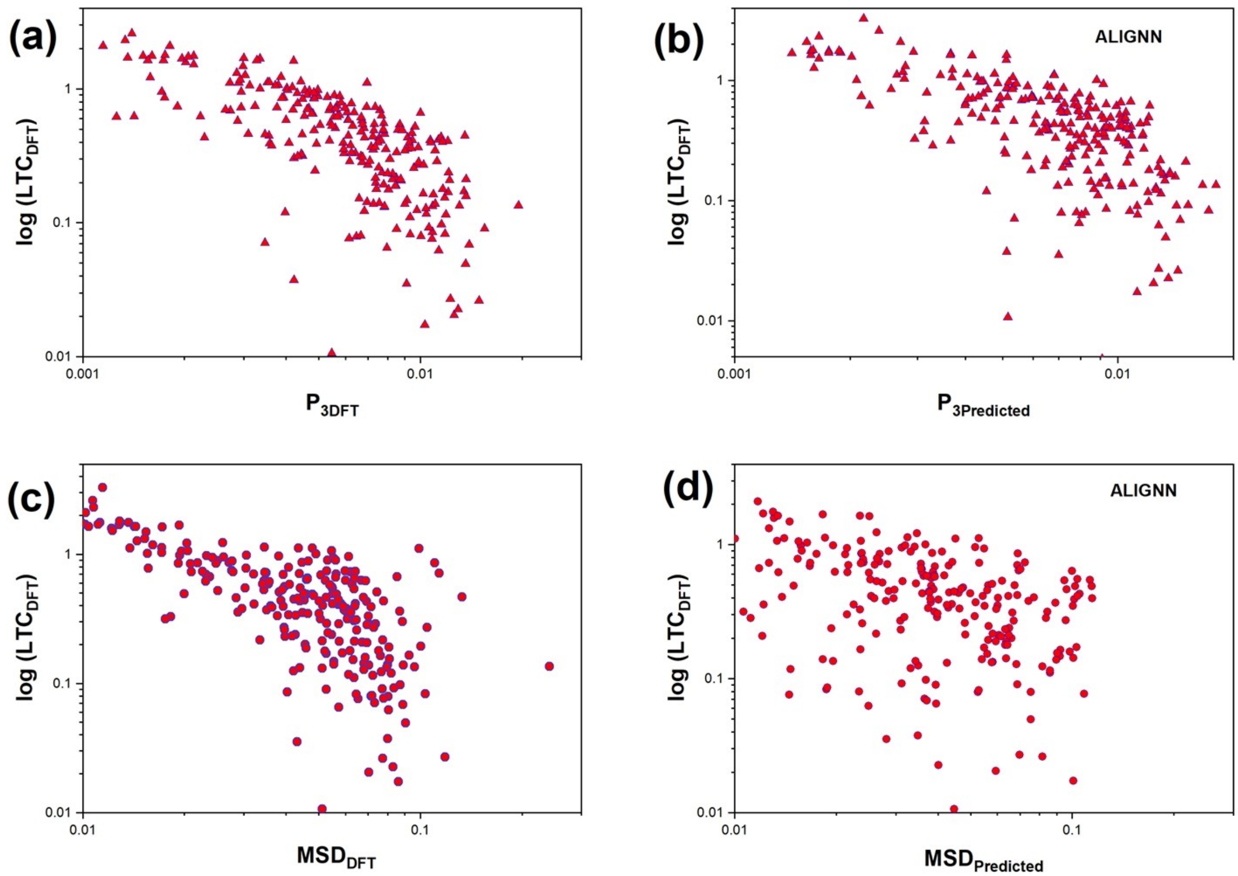

Figure S6: (a) DFT calculated P_3 parameter versus LTC, (b) ALIGNN model predicted P_3 parameter versus LTC, (c) DFT calculated MSD versus LTC, (b) ALIGNN model predicted MSD versus LTC.