

Supplementary Information for

Machine-Learning-Assisted Discovery of 212-Zintl-phase Compounds with Ultra-low Lattice Thermal Conductivity

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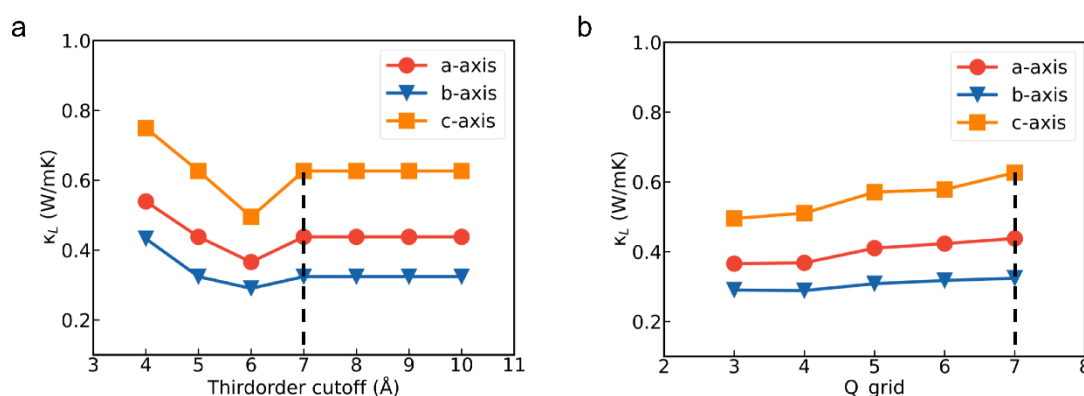


Figure S1. Convergence test of the third-order cutoff (a), and the q grids (b) of the TDEP calculation.

Table S1. The details of the database as well as the references. (See [TableS1.pdf](#))

Table S2. The optimized hyperparameters for the ML models.

Symbol	Definition	Value
n_estimators	The number of boosting stages to perform	453

learning_rate	Adjustment the contribution of each tree	0.07
max_depth	The maximum depth of the individual regression estimators	3

Table S3. The details of the predicted results.

Formula	Temperature (K)	κ_L (W/(mK))
Ca ₂ CdP ₂	300	3.418999291
	400	2.622836393
	500	2.13224968
	600	1.864276224
	700	1.59660608
	800	1.343485272
	900	1.316505932
	1000	1.305298445
Sr ₂ ZnP ₂	300	2.103014068
	400	1.613324079
	500	1.322628937
	600	1.141592994
	700	0.813907198
	800	0.525875164
	900	0.501868052
	1000	0.495753319
Sr ₂ ZnAs ₂	300	1.276798589
	400	1.043000778
	500	0.948903528
	600	0.872226682
	700	0.661412228
	800	0.463096048
	900	0.451040705
	1000	0.445703501
Sr ₂ ZnBi ₂	300	1.560371412
	400	1.24105267
	500	1.006770516
	600	0.843030479
	700	0.742227151
	800	0.474955594
	900	0.441875716
	1000	0.436557762
Sr ₂ CdAs ₂	300	2.277186172
	400	1.786981374
	500	1.359191182
	600	1.225550508
	700	1.163023743
	800	1.035981407

	900	1.020572827
	1000	1.01014287
Ba ₂ ZnBi ₂	300	1.034144346
	400	0.897010956
	500	0.866224312
	600	0.690121451
	700	0.699817386
	800	0.526505901
	900	0.505775346
	1000	0.500457392
Ba ₂ CdAs ₂	300	1.124192111
	400	0.8439103
	500	0.749626657
	600	0.660855075
	700	0.607433838
	800	0.454958862
	900	0.449877248
	1000	0.437217754
Eu ₂ ZnP ₂	300	2.879037083
	400	2.216380811
	500	1.970393072
	600	1.670651611
	700	1.515454436
	800	1.359146627
	900	1.34458557
	1000	1.333378083
Eu ₂ ZnBi ₂	300	1.426441981
	400	1.1879422
	500	1.020322726
	600	0.819434962
	700	0.697180325
	800	0.404016503
	900	0.38991408
	1000	0.389136551
