Supplementary Materials: Lattice Thermal Conductivity Prediction using Symbolic Regression and Machine Learning

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1. Noteworthy Formulae from Symbolic Regression Models

The Symbolic Regression models generated many formulae during the training phase. Most were uninteresting. While we elected only to include the best performing formulae in the main body of this work, it would be neglectful to omit several of the more physically interesting formulae that were found by the models. Below are some of the aforementioned interesting candidates, and their average MAE and R^2 scores across both the training and validation sets.

$$\kappa_L = 3.55 \cdot \sqrt{\frac{B}{(n_p)^2 \cdot \sqrt{H}}} \tag{1}$$

$$\kappa_L = \frac{B}{H \cdot n_p^2} \tag{2}$$

$$\kappa_L = \frac{E \cdot v}{n_p} \tag{3}$$

$$\kappa_L = \frac{B}{n_p^2} \tag{4}$$

$$\kappa_L = \frac{G^{\frac{2}{3}} ln(2.60)}{ln(|n_p|) H^{\frac{1}{9}}} \tag{5}$$

$$\kappa_L = \sqrt[6]{\frac{B^3 \cdot \sqrt[H]{e} \cdot \sqrt{ln(0.45 \cdot |n|)}}{H}} \tag{6}$$

Formula	MAE	R^2
Slack-Berman	10.62	0.078
1	9.461	0.135
2	9.373	0.215
3	9.360	0.175
4	8.916	0.234
5	9.303	0.210
6	9.927	0.091

Table S1. Noteworthy formulae MAE & R^2