Supplementary Materials

PINK: physical-informed machine learning for lattice thermal conductivity

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1. The comparison of CGCNN and other GNN models

As shown in the TABLE S 1, the d Crystal Graph Convolutional Neural Network (CGCNN) model has the lowest MAE in two out-of-distribution (OOD) cases. Additionally, it also has the second or third lowest MAE in the other three OOD cases. This indicates that CGCNN still demonstrates good generalization ability beyond the training set. We thank the reviewer for the valuable comments, and we will attempt more advanced models to further improve the predictive capability of the model.

TABLE S 1 50-fold cross-validation MAEs (log10(GPa)) of different graph neural network (GNN) models on the elasticity dataset for five different types of out-of distribution (OOD)[1].

Algorithm	LOCO	SparseXcluster	SparseXsingle	SparseYcluster	SparseYsingle
CGCNN	**0.0585**	**0.0499**	0.0895	0.0752	0.0840
MEGNet	1.4468	1.4113	1.3099	1.5659	1.4491
SchNet	1.4065	1.3455	1.2363	1.5592	1.4855
DimeNet++	1.4242	1.3562	1.3214	1.5454	1.4828
ALIGNN	0.0974	0.0834	**0.0853**	**0.0631**	**0.0450**
DeeperGATGNN	0.1173	0.1109	0.1140	0.0858	0.0807
coGN	0.1017	0.1416	0.2919	0.0823	0.1852
coNGN	0.1019	0.1417	0.2918	0.0823	0.1853

2. The relationship between κ_L and phonon group velocity.

According to the phonon gas picture, $\kappa_L = \frac{1}{3} C_V v^2 \tau$. Therefore, usually, one believes $\kappa_L \propto v^2$. However, phonon relaxation time τ in fact has a function of Debye temperature, according to the famous Klemens theory[2-3]

$$\tau^{-1} = B_1 \omega^2 T^3 \exp\left(-\frac{\theta_D}{\alpha T}\right) \#(1)$$

In above formula, θ_D is the Debye temperature, which can be expressed as[4],

$$\theta_D = \frac{\hbar v_s}{k_B}\left(\frac{3}{4\pi}\cdot\frac{N}{V}\right)^{\frac{1}{3}} \#(2)$$

Therefore, the phonon relaxation time has also a complicated relationship with group velocity.

But we fully agree with the reviewer's comments. It is worth noting that, according to main manuscript Eqs. (3, 4, 5, 6), both shear modulus G and the Grüneisen parameter γ in equation 2 are also related to phonon group velocity v, so there is a complex coupling relationship between thermal conductivity κ_L and phonon group velocity. In general, κ_L also has a corresponding direct proportional relationship with group velocity as referee mentioned.

References:

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