Contribution ID: **48** Type: **Talk**

Uncovering the Relationship Between Thermal Conductivity and Anharmonicity with Symbolic Regression (12 min talk + 3 min discussion)

Wednesday, 14 April 2021 17:30 (15 minutes)

Quantitatively understanding the link between anharmonicity and thermal conductivity, κ, is pivotal to the search for better thermal insulators. To help find this link we present new descriptors of κ based on our new measure of anharmonicity, σ^{A}. Using an updated sure-independence screening and sparsifying operator (SISSO) method, we find analytical expressions with symbolic regression and generate expressions for κ_L that are competitive with those previously reported in the literature using only a third of the primary features. Finally, we discuss the implications of the new models on future materials design.

Poster title

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