

# 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,  $\kappa$ , is pivotal to the search for better thermal insulators. To help find this link we present new descriptors of  $\kappa$  based on our new measure of anharmonicity,  $\sigma^A$ . Using an updated sure-independence screening and sparsifying operator (SISSO) method, we find analytical expressions with symbolic regression and generate expressions for  $\kappa_L$  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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