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Automated combinatorial method for fast and robust prediction of lattice thermal conductivity JOSE J PLATA, PINKU NATH, DEMET USANMAZ, CORMAC TOHER, Dept. of Mechanical Engineering and Materials Science, Duke University, MARCO FORNARI, Dept. of Physics, Central Michigan University, MARCO BUONGIORNO NARDELLI, Dept. of Physics, Univ. of North Texas, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics and Chemistry, Duke University — The lack of computationally inexpensive and accurate *ab-initio* based methodologies to predict lattice thermal conductivity, κ_l, without computing the anharmonic force constants or performing time-consuming *ab-initio* molecular dynamics, is one of the obstacles preventing the accelerated discovery of new high or low thermal conductivity materials. The Slack equation is the best alternative to other more expensive methodologies but is highly dependent on two variables: the acoustic Debye temperature, θ_a, and the Grüneisen parameter, γ. Furthermore, different definitions can be used for these two quantities depending on the model or approximation. Here, we present a combinatorial approach based on the quasi-harmonic approximation to elucidate which definitions of both variables produce the best predictions of κ_l. A set of 42 compounds was used to test accuracy and robustness of all possible combinations. This approach is ideal for obtaining more accurate values than fast screening models based on the Debye model, while being significantly less expensive than methodologies that solve the Boltzmann transport equation.

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