Recent progress on first-principles lattice thermal conductivity calculations

A talk by Atsushi Togo

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These years I have been working on phonon-phonon interaction and lattice thermal conductivity calculations. Recently these calculations collect more interests because the couple of first-principles calculation and linearlized phonon-Boltzmann-equation gives reasonable and systematic prediction of lattice thermal conductivities with mild computational demand. When we wanted to calculate them, already there existed a nice first-principles calculation code, therefore we only needed to develop a post-processing-type code. I will present how the code is written, how it works, and how it is used.