Ab initio multiscale thermal transport simulations with almaBTE

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Understanding and tailoring thermal transport is an urgent issue for many cutting edge technologies where heat poses a bottleneck to further progress, such as power electronics, nanoelectronics, interconnects, thermoelectric energy conversion, phase change memories, turbine coatings, and many other disciplines. Predictive ab initio simulation of thermal transport in these systems, from the atomic to the device level, can help understand and solve the current heat challenges.

During the past three years we have built almaBTE, an open source code capable of solving the space and time dependent Boltzmann transport equation for phonons in nano and microstructured systems, fully from first principles[1]. I will illustrate almaBTE's use in several materials and devices of technological relevance, including the role of point defects in SiC [2]and GaN [3] thermal conduction, the thermal conductivity of InAs/GaAs [4] and SiGe superlattices[5], and the design of finFETs, as well as LED and HEMT substrates [6].

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