Thinking Beyond the Phonon Gas Model

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The conventional view and understanding of phonon transport, both through materials and at interfaces, is based on what is termed the phonon gas model (PGM). The PGM essentially treats the energy of phonons as analogous to gas particles that scatter from each other, boundaries or other imperfections in the system. This approach then hinges on the idea that every phonon has a well-defined velocity, which in turn is only well-defined if the atomic arrangement is periodic. There are many systems of interest, however, that do not consist of a fully periodic atomic arrangement and as a result the conventional view of phonon transport breaks down in many instances. Recently, the Atomistic Simulation & Energy (ASE) research group has developed an alternative framework for understanding phonon transport, which is based on correlation rather than scattering [1-9]. Moreover, the new framework provides individual mode contributions to thermal transport, regardless of their character, and thus treats all modes on an equal footing. The net result of this approach is then a rigorous way of assessing and understanding the role that different phonons play in heat conduction, both in the body of a material and at interfaces. This talk will present the more recently developed correlation based perspective of phonon transport and will show examples of seemingly non-intuitive behavior that is not well explained by conventional theory (i.e., the PGM), but is easily understood from a correlation based perspective.

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