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Wave-particle conduction of thermal energy in thermoelectric materials MARTIN MALDOVAN, MIT — Materials that can stop heat transfer are very important for increasing the efficiency of thermoelectric materials such as skutterudites, clatharates, superlattices, nanowires, and quantum dots. The transport of thermal energy, however, is a challenging phenomenon difficult to understand and control. Currently there is no theoretical model capable of accurately describing the flow of thermal energy in nanostructures and basic physical properties such as thermal conductivity can not be predicted. This is in part due to our lack of knowledge on a fundamental physical property: whether a phonon behaves as a particle or as a wave within a nanostructured material. We present physical mechanisms governing heat transfer in semiconductor nanostructures and a quantitative wave-particle model to calculate, predict, and explain experimental observations on thermal transport properties. Comparing theoretical and experimental results, we show that phonons with frequencies above 2THz behave as particles while those with frequencies below behave as waves. We also explain the existence of a minimum thermal conductivity and the nearly temperature-independent thermal conductivity in superlattices. This opens the opportunity for the design of nanostructured materials that can control heat in optoelectronic devices or thermoelectric materials.

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