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Design of thermoelectric composite materials for energy applications. MARTIN MALDOVAN, EDWIN THOMAS, Massachusetts Institute of Technology — Energy supply is becoming a major world-wide problem as fossil energy supplies decrease while energy demands increase. Thermoelectric materials, which reversibly convert thermal and electrical energy, offer the prospect of power generation and cooling by means of the rational transport of electrons and phonons. In nanocomposite materials, both quantum and classical effects provide opportunities to control the transfer of electrons and phonons. The difficulty associated with thermoelectric materials is the need to couple and optimize a variety of physical properties in order to exhibit necessary efficiencies, which are determined by the figure of merit ZT. To exhibit large efficiencies, the best thermoelectric material should possess low thermal conductivity (similar to that of a glass) and high electrical conductivity (similar to that of a perfect crystal material). In this paper we study thermoelectric materials by preparing composite materials that can provide the desired coupled physical properties. Our research concentrates on predicting and designing thermoelectric material properties using theoretical and computational methodologies. We use currently available algorithms and numerical techniques to design thermoelectric materials with increased efficiencies. The ultimate goal of our research is to develop a basic understanding of the coupled physical properties in these materials and to create a framework that allows for the systematic design, optimization, and characterization of their thermal and electric properties.

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