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Atomistic simulation of nanostructure effects on thermoelectric properties in Si/Ge nanowires HAIBIN SU, Caltech, PAUL VON ALLMEN, JPL, SEUNGWON LEE, JPL, TAHIR CAGIN, Texas A&M University, WILLIAM GODDARD III, Caltech — Experimental results on the thermal conductivity of superlattices demonstrate that the thermal conductivity of a superlattice can be much lower than that estimated from the bulk values of its constituent materials, and even smaller than the thermal conductivity of the equivalent composition alloys. The thermal conductivity reduction, coupled with the possible increase of the Seebeck coefficient and electrical conductivity due to quantum confinement effects in these superlattices, makes the Si/Ge superlattice system a good candidate for highly efficient thermoelectric energy conversion. Here we will combine tight-binding and atomistic molecular dynamics approaches to study the effects of nano- patterning on thermoelectric properties. The lattice contribution to the thermal conductivity, which is dominant in semiconductors, will be obtained from a Green Kubo relationship. We will calculate the electrical conductivity, the electronic contribution to the thermal conductivity, and the Seebeck coefficient using linear response theory with the empirical tight binding approach, which is suitable for the study of self-assembled nanostructures containing millions of atoms. Finally, we will discuss the systematic engineering of nanostructure to improve the figure of merit.

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