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Nanophononic metamaterial: Engineering local resonances in thermoelectric materials for high energy conversion performance. MAH-MOUD HUSSEIN, HOSSEIN HONARVAR, University of Colorado Boulder — Engineered manipulation of phonons can yield beneficial thermal properties in semiconducting materials. One pivotal application relates to thermoelectric materials, or the concept of converting energy in the form of heat into electricity and vice-versa. The ability to use nanostructuring to reduce the thermal conductivity without negatively impacting the power factor provides a promising avenue for achieving high values of the thermoelectric energy conversion figure-of-merit, ZT. Here, we report our latest results on a novel nanostructured material configuration that seeks to achieve this goal. Termed "nanophononic metamaterial", the configuration is based on a freestanding silicon membrane with a periodic array, or random forest, of nanopillars erected on the surface. The nanopillars qualitatively alter the base membrane phonon spectrum due to a hybridization mechanism between their local resonances and the underlying atomic lattice dispersion. Using equilibrium molecular dynamics simulations, we predict a two orders of magnitude drop in the thermal conductivity compared to the corresponding uniform membrane value despite the fact that the nanopillars add more phonon modes to the spectrum.

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