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Thermal conductance in Si/Ge core-shell nanowires JAIME BOHORQUEZ, MASOUD BABAEIAN, MICHAEL ONTL, THUSHARI JAYASEKERA, Southern Illinois University Carbondale — We have studied the thermal conductance of Si/Ge core-shell [111]-oriented nanowires with diameters from 0.55 nm to 1.36 nm using ab initio calculations. In order to fundamentally understand the effect of atomic arrangements, we calculated the phonon conductance in a ballistic approach. Detailed analysis of phonon modes shows that thermal conductance due to selective phonon modes of Si/Ge nanowires can be suppressed by engineering the ratio of core/shell atoms. Our results suggest that, Si/Ge nanowire configurations can be engineered for optimized thermoelectric performance.

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