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Effect of Schottky barriers in quantum-engineered thermoelectric devices RASEONG KIM, MARK LUNDSTROM, Purdue University — Recent advancements in thermoelectric figure of merit mostly come from the substantially lowered lattice heat conduction. A question now is whether quantum engineered devices such as superlattices can provide improved electronic performance while still suppressing phonon transport. To address this question, we run quantum transport simulations using the non-equilibrium Green's function (NEGF) method. As a first step, we examine a simple one-dimensional wire and explore the effects of Schottky barrier on thermoelectric coefficients. For ballistic nanowires with no Schottky barrier, simulation results are consistent with those from the conventional analytical model. When there are Schottky barriers at the source/drain contracts, carriers must tunnel through the barrier to be injected to the channel, so the transmission decreases while the average energy of injected carriers increases. As a result, electrical and heat currents decrease while the Seebeck coefficient increases. The effects of momentum and energy relaxation scattering are also examined in the NEGF framework. Finally, the extension of this work to superlattices is discussed.

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