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**Atomistic Modeling of the Thermoelectric Properties in Silicon Nanowires** ABHIJEET PAUL, GERHARD KLIMECK, Purdue University —

The thermoelectric properties of Silicon can be improved due to nano-sized structuring and modulation. The effect of crystal orientation, cross-sectional dimension and source-drain doping on Seebeck coefficient ( $S$ ) and electronic conductance ( $\sigma$ ) in silicon nanowires is studied theoretically in this work. From the electronic structure obtained using an atomistic 10 band  $sp^3d^5s^*$  Tight-Binding model with spin orbit coupling, we calculate these parameters using the Landauer formula. Conductivity increases with increasing cross-section size since the number of modes per energy increases. Different orientations show different conductivity. However, Seebeck coefficient is quite independent of the orientation and cross-section size. But, the power factor ( $S^2\sigma$ ), can be improved with size and orientation mainly due to the improvement in conductivity. In these nanowires, phonon scattering at the wire boundary further reduces the lattice thermal conductivity ( $\kappa_l$ ) which plays a positive role in improving the thermoelectric figure of merit ( $ZT$ ) bringing it close to 1 at 300K.

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