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Field Effect Density Modulation in Nanowires for Large Thermoelectric Power Factors: A Self-Consistent Atomistic Simulation Approach

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Low-dimensional materials such as ultra-narrow nanowires have attracted significant attention as efficient thermoelectric materials because of their low thermal conductivity. Such benefits, however, although large, are reaching their limits, since thermal conductivities are already nearing the amorphous limit. Improving *ZT* through the power factor, on the other hand, is not to-date experimentally verified, despite initial suggestions. Low-dimensional materials, however, provide the possibility to achieve the required high carrier densities using field modulation techniques, such as remote doping and electrostatic gating. This removes the dopants and, thus, eliminates ionized impurity scattering, which is the strongest carrier scattering mechanism. Up to an order of magnitude higher electrical conductivity can, thus, be achieved. This is only possible in low-dimensional materials because of their large surface to volume ratio.

In this work, we employ atomistic calculations using the $sp^3d^5s^*$ tight-binding model and Boltzmann transport theory to investigate the thermoelectric properties of gated Si NWs. We couple the electronic structure calculation self-consistently to the Poisson equation for accurately capturing the effect of electrostatic gating. We simulate NWs of diameter ranging from 3nm up to 20nm, a numerically challenging task that involves several thousands of atoms in the simulation domain. We find that: i) Gated channels show a largely improved power factor, by a factor of ~5x, compared to doped channels. ii) Although the charge accumulates near the interfaces, the field is

still relatively weak, and surface roughness scattering does not degrade the performance significantly. iii) The electronic bandstructure can be modified upon gating in certain cases and the carrier mobility can be further improved. iv) Importantly, our simulations show that the benefits of gating could be observed for NW diameters even up to 40nm, which suggests that improved power factors can be achieved even for the already realized nanowire thermoelectric materials.

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