# Full-Band Calculations of Thermoelectric Properties of Si Nanowires and Thin Layers

Neophytos Neophytou[1,2], Hossein Karamitaheri[2,3], and Hans Kosina[2]

[1]School of Engineering, University of Warwick, Coventry, CV4 7AL, UK

[2]Institute for Microelectronics, TU Wien, Gußhausstraße 27-29/E360, A-1040 Wien, Austria

[3]Department of Electrical Engineering, University of Kashan, Kashan, 87317-51167, Iran

E-mail: N.Neophytou@warwick.ac.uk

## Abstract

Low-dimensional semiconductors are considered promising candidates for thermoelectric applications with enhanced performance because of a drastic reduction in their thermal conductivity, $\kappa_l$, and possibilities of enhanced power factors. This is also the case for traditionally poor thermoelectric materials such as silicon. This work presents atomistic simulations for the electronic, thermal, and thermoelectric properties of Si ultra-thin layers and nanowires of diameters in certain cases up to 20nm. We couple the Linearized Boltzmann theory: i) to the atomistic $sp^3d^5s^*$ tight-binding (TB) model for the electronic properties of the channels, and ii) to the modified valence-force-field method (MVFF) for the calculation of their thermal conductivity. We calculate the room temperature electrical conductivity, Seebeck coefficient, power factor, thermal conductivity, and *ZT* figure of merit of the ultra-thin Si layers and nanowires. We describe the numerical formulation of coupling TB and MVFF to the Linearized Boltzmann transport formalism, together with all relevant scattering mechanisms. The properties of low-dimensional channels are highly anisotropic, and optimized thermoelectric properties can be achieved by the choice of the appropriate transport and confinement orientations, as well as confinement length scale. We identify bandstructure engineering techniques that lead to thermoelectric power factor improvements. Finally, we show that modulation doping techniques can improve thermoelectric performance significantly.

**Keywords:** thermoelectrics, tight-binding, $sp^3d^5s^*$, modified valence-force-field, Boltzmann transport, Seebeck coefficient, silicon ultra-thin layers, silicon nanowires.