

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Calculations of the thermopower in materials with nano-inclusions using quantum mechanical simulations NEOPHYTOS NEOPHYTOU, School of Engineering, University of Warwick, MISCHA THESBERG, MAHDI POURFATH, HANS KOSINA, Institute for Microelectronics, Technical University of Vienna — Inclusion of nano-crystalline structures in thermoelectric materials has shown the potential to greatly enhance their thermopower. In this work we present a fully quantum mechanical simulation study of thermoelectric transport through 2D channels in the presence of 0D nano-inclusions, which effectively act as barriers for energy filtering. For this, we use the non-equilibrium Green's function (NEGF) method. We show that improved thermopower can be achieved in such structures compared to pristine geometries. We find that these materials disturb the flow of low energy electrons more compared to the flow of high energy electrons, which enhanced anisotropy and benefits the thermopower. Furthermore, we show that the largest improvements in the Seebeck coefficient can be achieved when the channels become very narrow, on the order of the nano-inclusions' feature sizes. Under such large confinement, the channel provides only a few paths for electrons to flow, and allows only high energy electrons to propagate easily, which improves filtering and, thus, increases the Seebeck coefficient.

Neophytos Neophytou
School of Engineering, University of Warwick

Date submitted: 13 Nov 2014

Electronic form version 1.4