Title

Electronic transport simulations in nanostructured materials for large thermoelectric power factors

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Abstract (300 words)

Nanostructured materials have shown great potential to achieve extremely low thermal conductivities, and thus, improve thermoelectric performance. Less attention has been paid, however, in the possibility of designing nanostructured materials for improving the thermoelectric power factor. In this work, we perform large-scale, numerically intensive electronic transport simulations in nanostructured materials using the fully quantum mechanical electron transport non-equilibrium Green's function method (NEGF). We present a comprehensive simulation methodology that can address electronic transport and thermoelectric power factors in generic nanostructured geometries such as superlattices, nanocrystalline structures, structures with nano-inclusions, as well all combinations of these geometrical features. We then calculate the thermoelectric coefficients and elaborate on the main features that provide power factor enhancement, as well as the main features that degrade the performance. Specifically, we show how for optimal power factor conditions: i) the geometrical features need to be correlated with the mean-free-paths of charge carriers, ii) the thermal conductivity of the different regions needs to differ, and iii) strong variations away from idealized conditions in the height of the potential barriers built in the channel should be avoided. Furthermore, we discuss how semi-classical Monte Carlo simulations can be used to extend the simulation domain to include larger geometrical features for which NEGF might suffer from numerical difficulties, while still incorporating important quantum transport effects.