Title

Electronic transport simulations in nanocomposites – exploring the features that optimize the thermoelectric power factor.

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Abstract (1500)

Nanocomposite materials have shown the potential to provide much larger Seebeck coefficients, and in certain cases higher power factors, compared to pristine materials. In order for power factor improvements to be realized, however, key elements regarding the geometrical features of the nanocomposite geometry, the underlying electrostatic potential, and the local properties of the different materials phases need to be properly designed and controlled to some degree. In this work, we discuss our current efforts in developing large scale, comprehensive simulation tools based on transport methods from fully quantum mechanical (Non-Equilibrium Green's Functions) to semiclassical (Monte Carlo) to describe electronic transport in nanocomposites. Multi-physics approaches to combine elements of the two methods are also discussed. As an example we perform an optimization study of the thermoelectric power factor in superlattices and elaborate on the main features that provide power factor enhancement, as well as the main features that degrade the performance. Specifically, we show that for optimal 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 build in the channel should be avoided.