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Fully quantum mechanical transport simulations for the calculation of the thermoelectric power factor in nanocomposite materials

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Abstract

Nanocomposite materials are promising candidates for the new generation of thermoelectrics due to the ability of nanoinclusions to scatter phonons and drastically reduce thermal conductivity [1]. In addition, nanoinclusions could potentially improve the power factor by introducing energy filtering. The difficulty in improving the power factor, however, is the strong reduction in electrical conductivity that these nanoinclusions introduce, which can exceed the improvements in the Seebeck coefficient. Thus, in the majority of nanocomposite materials, the power factor is reduced compared to the pristine material.

In this work we employ the fully quantum mechanical Non-Equilibrium Green's function (NEGF) transport method to calculate the electronic and thermoelectric coefficients of two dimensional materials embedded with nanoinclusions. This formalism includes electron-phonon interactions, and captures all the details of geometry, quantisation, tunnelling, and the ballistic to diffusive nature of transport in a unified way [2,3]. It is a very convenient and accurate method of providing understanding of thermoelectric transport in nanomaterials, beyond semiclassical approximations, and beyond approximations that are usually assumed in order to combine the different geometrical features of the composite structure.

A typical geometry that we simulate is shown in Fig. 1a below and can be either ordered or disordered. We show how these nanocomposites can be optimised to limit degradation in the power factor, and in some cases even provide mild improvements (Fig. 1b). We discuss how the key features in the design of nanocomposites are as follows: i) somewhat large diameter nanoinclusions (>3nm) are needed for the power factor benefit to be realised as they prevent quantum tunnelling, and the Seebeck coefficient can be increased, ii) using nanoinclusions of barrier height $V_B \sim k_B T$ above the conduction band provides a small filtering effect that can also improve the Seebeck coefficient, iii) nanocomposite structures are not severely affected by increasing porosity if the channel is degenerately doped, as long as the nanocomposite barriers are lower than the Fermi level. This means that a large number of inclusions can be used without reduction in the power factor. These guidelines would be useful in the design of nanocomposites for enhanced thermoelectric performance.

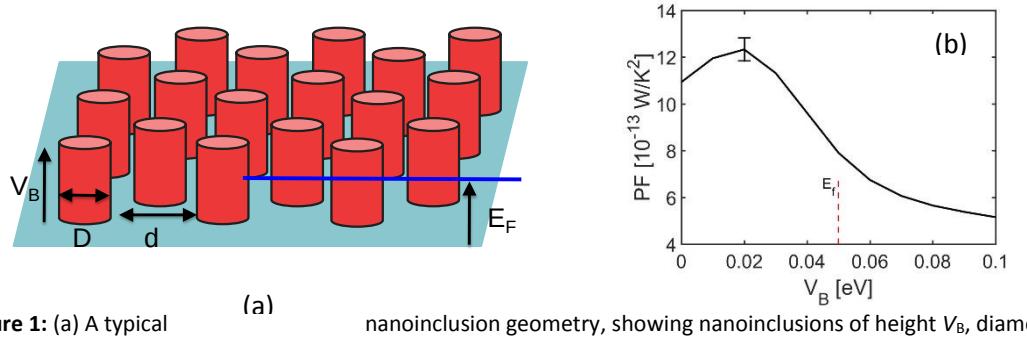

Figure 1: (a) A typical nanoinclusion geometry, showing nanoinclusions of height V_B, diameter D, average spacing d, and Fermi energy E_F (b) Power factor versus barrier height, showing a peak at $k_B T$ above the conduction band. The Fermi energy is Ef=0.05eV (red dotted line). The error bar shows the variation produced by randomising the nanoinclusions in the geometry with V_B=0.02.

References:

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