The thermoelectric effect in novel nanostructured materials from ballistic quantum transport calculations

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**Overview**

The thermoelectric effect refers to the conversion between an electrical potential and a temperature difference. That is, one can either use the effect for ‘solid state’ cooling/heating, or for harvesting electrical energy from an external temperature gradient. The thermoelectric ‘figure of merit’ for a material is called $ZT$ and for the best known thermoelectric alloys it is usually around 1. Graphene is by itself not a great thermoelectric material, but it has previously been shown that when nanostructured, the heat conductivity of graphene is suppressed and the Seebeck coefficient enhanced, such that it may be relevant for nano-sized thermoelectric devices. Recently, a new type of nano-structured graphene was synthesized - the nanoporous graphene. We have previously investigated this material’s electronic properties, but not the phononic properties nor the Seebeck coefficient. We suspect that due to its unique structure - resembling a series of nanoribbons connected by thin ‘molecular bridges’ - that it could either directly or by modification become a high $ZT$ material.

**Aim**

The aim of this project is to calculate the thermoelectric figure of merit ($ZT$) for nanoporous graphene. This will require calculation of both electronic and phononic transport properties. We will then investigate possible modifications to the material to further enhance the figure.

**Content**


**Your background (DTU courses or similar)**

*Mandatory:*
10303 Condensed Matter Physics and Nanoscale Materials Physics

*Relevant:*
10325 Quantum mechanical modelling of nanoelectronics
10323 Quantum transport theory
10321 Nano-2: Nanosystems engineering
10302 Electronic Structure Methods in Material Physics, Chemistry and Biology