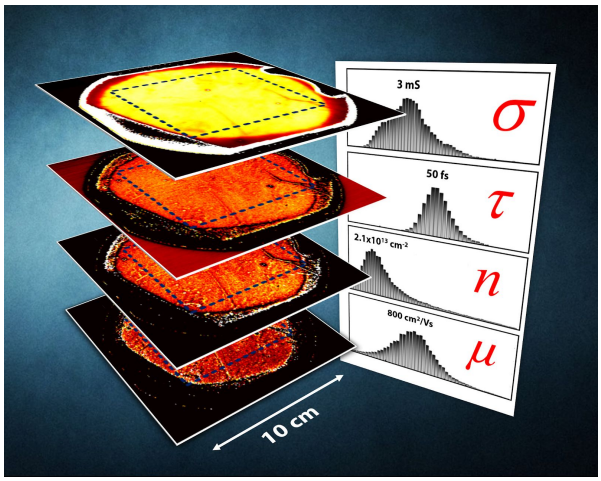
Theory for electron transport in the THz regime



Terahertz time-domain spectroscopy conductivity mapping of graphene. Credit: Bøggild, DTU

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Overview

At present there is great progress in the use of THz time-domain spectroscopy (THz-TDS) to analyse the time-resolved carrier dynamics in materials and devices. The powerful experimental techniques can e.g. provide insights into the AC conductivity of bulk materials without using electrical contacts. Combining THz-TDS with scanning probe techniques it has been possible to obtain information about electronic and atomic dynamics even at the atomic level. The THz ultrafast control of current on the atomic scale is believed to be essential for future electronic applications - so-called "light-wave" electronics.

However, the great progress in experimental techniques is not matched by theoretical understanding and modelling capabilities. The classical Drude-theory used so far to understand experiments does not give insights into the atomic scale behavior of the electrons.

Aim

The aim of this proposal is to provide atomistic quantum theory which can be compared to the experiments for nano-scale conductors. We will consider the (1) THz conductance response of different defects in two-dimensional materials, and/or (2) the resulting currents in a scanning probe experiment from THz radiation.

The project will involve interactions with experimental groups at DTU.

Content

Quantum transport using non-equilibrium Greens functions. Computer simulations using Density Functional Theory (DFT). Programming in python.

Your background (DTU courses or similar)

Mandatory:

10303 Condensed Matter Physics and Nanoscale Materials Physics

Very 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