ETH zürich

Charge and heat transport through graphene nanoribbon based devices

The Big Picture

Graphene nanoribbons (GNRs), narrow strips of graphene, have attracted significant interest in the last few years due to their largely modifiable band structure. As their electrical properties can be tailored by chemical design, they are predicted to find applications in a large range of electronic, optoelectronic and spintronics devices. One of such applications is as a **quantum** heat engine, in which particles, in this case electrons, are exchanged between a hot and a cold reservoir. Similar to classical heat engines, this conversion from heat to electricity is bound by the laws of thermodynamics. By exploiting the quantum nature of the GNRs, energy conversion is expected to be close to the thermodynamic limit. In recent years, significant progress has been made in the device integration of GNRs. However, their use as quantum heat engines has not been demonstrated yet. Progress on the experimental, as well as on the theoretical side is required to gain a deeper understanding of the charge and heat flow through the devices.

Short project description

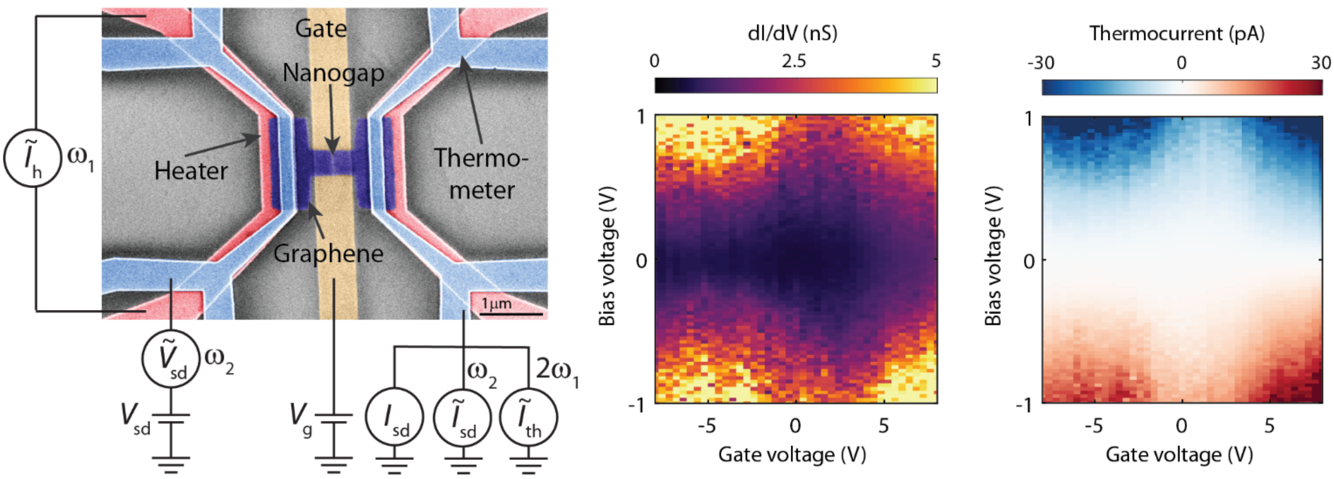
The goal of this project is to simulate charge and heat transport through graphene nanoribbon based devices. A state-of-the-art quantum transport solver called OMEN will be used for that purpose. It can treat both electrons and phonons as well as their coupling. First, device structures similar to those fabricated experimentally will be constructed atom by atom. Their properties will be first computed with density functional theory and then passed to OMEN to determine the electrical and thermal currents of the assembled graphene nanoribbons. The obtained results will finally be compared to thermoelectric measurements that are currently being performed on GNR-based devices.

Type of work

30% theory, 50% simulation, and 20% data analysis.

Prerequisites

Interest in quantum transport theory and nano-device modeling



Looking for 1 student for a semester or master project

Interested candidates please contact Prof. Mathieu Luisier (mluisier@iis.ee.ethz.ch) or Prof. Mickael Perrin (Mickael.perrin@ee.ethz.ch)