Current-induced motion of atoms on graphene

Supervisor
Mads Brandbyge, Susanne Leitherer (slei@dtu.dk)

Overview
Electronic current densities can reach high values in ballistic nanostructures where constrictions limit current. While the presence of forces induced by the current poses challenges in terms of stability and reproducibility, atomic control of the structure by external driving forces offers an enormous potential for, e.g., further downscaling, structural design and transport of material at the nanoscale. In graphene nanostructures, which are now being created using high bias voltages and currents, current-induced motion (electromigration) of adsorbates has been investigated. The ultra-high current density is shown to remove adsorbed contamination leading to cleaning of the graphene surface.

It has also been seen how the structure of edges are changed by the current/voltage. In particular, dehydrogenation of graphene edges by current has been observed, also subject to the strain applied to the constrictions.

Aim
In this project, we will calculate the current-induced inter-atomic forces in graphene nanoconstrictions using atomistic theory. Specifically, we will study driving forces on different adatoms (Au, H) placed on/in the constrictions, as well as forces on edges and impurities. Relevant for the analysis is the interplay of forces, bias voltage, the electrostatic potential profile and spatially resolved currents in the junctions.

Content
Computer simulations using tight-binding models and/or density functional theory (DFT) software.
Quantum transport using non-equilibrium Greens functions. Programming in Python.

**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