Atomic-Scale Modeling of Carbon Transistors

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We present atomic-scale simulations which compare the characteristics of transistors made of carbon nanotubes (CNT) [1] and graphene nanoribbons (GNR) [2]. We studied the properties of a semi-conducting CNT attached to metallic electrodes and controlled by a triple back gate. We find that the performance of the device is weakened by quantum tunneling and show that it is related to inefficient control by the back gate. For the GNR transistor we use a structure comprising of two metallic GNRs separated by a semiconducting GNR. We find only weak quantum tunneling and show that the GNR has much better transistor characteristics compared to the CNT.

In addition, we will show that while short graphene nanoribbons operate based on pure ballistic tunneling, the transport properties in longer ribbons exhibit characteristics of thermionic emission.

The calculations were performed with Atomistix ToolKit (ATK) from QuantumWise. ATK is a software package comprising a number of simulation methods for atomic-scale modeling of nanostructures. It collects first-principles, semi-empirical and classical methods in a homogeneous interface, and uses non-equilibrium Greens functions (NEGF) to model the transport properties of nanostructures under an applied bias. Certain features of the software and their relevance for the studied systems will also be discussed in the presentation.

[1] H. H. B. Sørensen, P.C. Hansen, D.E. Petersen, S. Skelboe and K. Stokbro, *Efficient wave function matching approach for quantum transport calculations*, Phys. Rev. B **79**, 205322 (2009).
[2] K. Stokbro, D. E. Petersen, S. Smidstrup, M. Ipsen, A. Blom and K. Kaasbjerg, *Semiempirical model for nanoscale device simulations*, Phys. Rev. B **82**, 075420 (2010).
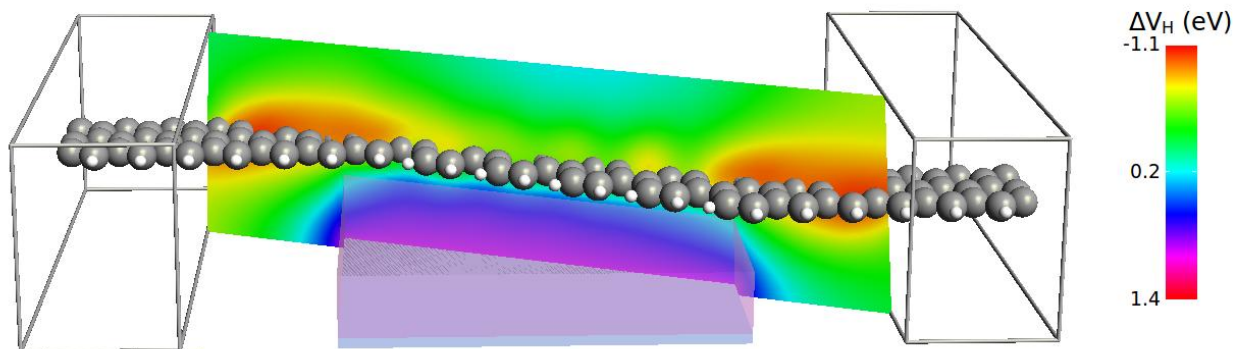
Graphene nanotransistor consisting of two metallic zigzag nanoribbons connected by a semiconducting armchair ribbon. The nanoribbons are passivated with hydrogen, and the width of the ribbons are is 7 Å. The device is sitting on top of a dielectric and the transport is controlled by an electrostatic backgate. The contour plot illustrates the Hartree potential for a gate potential of −1 V.