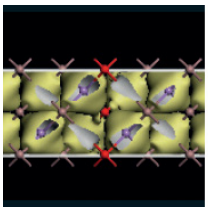

Session: Quantum Transport

(Invited) First principles calculations of electron transport in gated 2D nano-structures

M Brandbyge

Technical University of Denmark, Denmark

Devices based on stacked van der Waals heterostructures of two-dimensional (2D) materials are promising candidates for future atomically thin, flexible electronics with properties that can be tuned by the electrostatic and dielectric environment. One of the key advantages of two-dimensionality is that it allows very precise control of the carrier density and voltage drop[1] by a gate potential. However, the application of the gate potential may not only influence the transport via the carrier density in simple ways.

In this talk we present examples where we employ first principles transport calculations based on Density Functional Theory (DFT) which explicitly include the electrostatic gate potential and induced carriers. DFT is combined self-consistently with non-equilibrium Greens functions to study the effects of finite bias in devices[2], or as input to the Boltzmann equation to study bulk conductivity[3].

We consider the role of the gate geometry for the contact resistance in a stacked device where graphene is used as electrode to a MoS_2 channel[4]. We show how the contact resistance depends critically on the stacking configuration and establish a design rule for the stacking of devices based on 2D materials.

We also consider how the gate potential can induce a new flexural phonon scattering mechanism in a graphene device[5]. Gating can break the planar mirror symmetry activating one-phonon scattering from flexural phonons. Using the Boltzmann equation with parameters from DFT we calculate the mobility of graphene in a gate potential and find that this effect can have detrimental impact on the performance of a graphene device.

[1] N. Papior, T. Gunst, D. Stradi, M. Brandbyge, Phys. Chem. Chem. Phys., 18, 1025 (2016).
[2] M. Brandbyge, J-L. Mozos, P. Ordejon, J. Taylor, K. Stokbro, Phys. Rev. B 65, 165401 (2002); N. R. Papior, N. Lorente, T. Frederiksen, A. Garcia, M. Brandbyge, Comp. Phys. Comm., 212, 8, (2017).
[3] T. Gunst, T. Markussen, K. Stokbro, M. Brandbyge, Phys. Rev. B, 93, 035414 (2016).
[4] D. Stradi, N. R. Papior, O. Hansen, M. Brandbyge, Nano Lett. 17, 2660 (2017)
[5] T. Gunst, K. Kaasbjerg, M. Brandbyge, Phys. Rev. Lett. 118, 046601 (2017).