Computational atomistic studies of AC quantum transport in the THz regime

Ph.D. student position at DTU, Dept. of Physics, Denmark

The theoretical nanoelectronics group (Prof. M. Brandbyge) seeks a candidate to perform computational quantum transport studies of nano-conductors in the THz AC regime. A main target is to provide atomistic and quantum mechanical insights to link measurements to theory for various scattering mechanisms, f.ex. grain boundaries and point defects, in two-dimensional conductors. Here we will employ a newly developed multi-scale method to reach experimentally relevant length-scales[1]. Another target is to consider the THz field in scanning probe setups using our multi-electrode methods[2].

Project content:

- Electronic structure and transport calculations using Density Functional Theory (DFT) in combination with non-equilibrium Greens functions (NEGF). Development of a new AC-THz transport method.
- Development and use of tight-binding models based on DFT-NEGF parameters for large-scale calculations.
- Collaboration with experimentalists.

Essential requirements:

- M.Sc. degree in physics, materials science, chemistry, or engineering
- Solid background in theoretical solid-state physics and/or quantum chemistry.
- Good communication skills in oral and written English

Preferable experience:

- Experience with electronic structure calculation based on Density Functional Theory.
- Experience with atomistic electron transport calculations.
- Theory of electronic structure of 2D materials and interfaces.
- Good command of computational tools on linux clusters (scripting and programming)

The formal deadline is 1/10/2020, but it is likely to be extended due to the COVID. Contact mabr@dtu.dk for further information.

Apply here: https://www.dtu.dk/english/about/job-and-career/vacant-positions

[1] G. Calogero, N. Papior, M. Koleini, M. H. L. Larsen, M. Brandbyge, "Multi-scale approach to first-principles electron transport beyond 100nm", Nanoscale 11, 6153 (2019).

[2] N. R. Papior, N. Lorente, T. Frederiksen, A. Garcia, M. Brandbyge, "Improvements on non-equilibrium and transport Green function techniques: The next-generation TRANSIESTA", Comp. Phys. Comm., 212, 8, (2017).