$N_\mathfrak{e} \geq 1$ large scale DFT/TB+NEGF calculations

Nick Rübner Papior, 3th May, Bremen

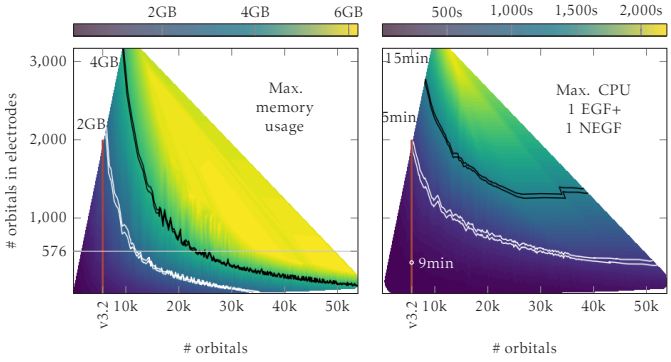

Figure 1: Left, TranSiesta memory for varying electrode (y-axis) and device size (x-axis). Right, TranSiesta time usage for equivalent systems. A linear scaling for constant electrode widths are found.

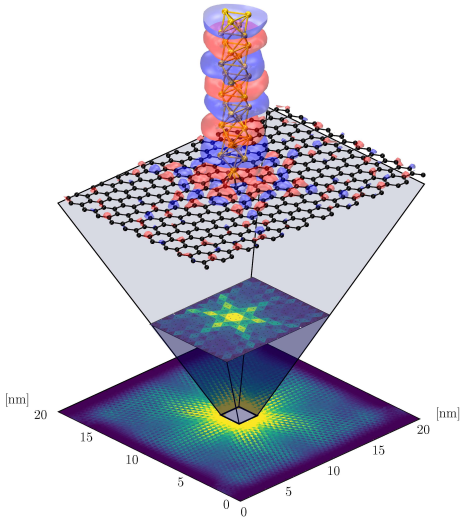

Figure 2: DFT+TB calculation with an accurate DFT STM-tip which is connected to a TB parameterized infinite graphene system to investigate the far field currents. A 6-fold symmetry is found.

I will present the recent development of $N_\mathfrak{e} \geq 1$ electrode DFT/TB+NEGF simulations which enables simulations of multiprobe physics. The specific implementation will be presented [1, 2] and the efficiency and scalability of the code (TranSiesta) will be emphasized. The code implements hybrid parallelization which easily enables efficient calculation of DFT systems with more than 10,000 orbitals under non-equilibrium, see Fig. 1 which shows the maximum memory usage with respect to system size (x-axis) and electrode size (y-axis), left. The right shows the computation time of a single SCF with NEGF.

After introduction to TranSiesta we present results based on large scale 2D-graphene systems with a Dirac Fermion microscope [3, 4]. Here we will show the extended capability of TBtrans with many custom parameters in the Hamiltonian; magnetic fields, complex absorbing potentials and $p-n$ junctions. The chosen boundary conditions have a large influence of the quantum mechanical calculations.

Lastly, a combined DFT+tight-binding calculation will be used to show the STM-tip far-field current in infinite graphene structures, see Fig. 2. We use an accurate DFT description for the STM tip-like structure and transition to a DFT parameterized tight-binding model in the far field (3rd nearest neighbour non-orthogonal model). Our findings substantiate and amend simpler tight-binding calculations.

[1] Nick R. Papior and Mads Brandbyge. "Computational Tools and Studies of Graphene Nanostructures". PhD thesis. 2016, p. 176. DOI: 10.11581/DTU:00000025.

[2] Nick Papior et al. "Improvements on non-equilibrium and transport Green function techniques: The next-generation TranSiesta". In: *Computer Physics Communications* 212 (2017). DOI: 10.1016/j.cpc.2016.09.022.

[3] Peter Bøggild et al. "A two-dimensional Dirac fermion microscope". In: *Nature Communications* 8.15783 (2017). DOI: 10.1038/ncomms15783.

[4] Gaetano Calogero et al. "Atomistic large-scale simulations of transport in ballistic graphene". In: *Carbonhagen*. Copenhagen, 2017. DOI: 10.13140/RG.2.2.27879.14242.