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Tenkých vrstev a nanostruktur

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TÉMA

Multiprobe NEGF calculations & molecular projected transport

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I will present the recent development of N≥1 electrode 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 calculations of 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 (yaxis), left. The right shows the computation time of a single SCF with NEGF. Using the N electrode capability I will present initial 3 terminal results based on 2Dgraphene interconnects [3].

After having introduced the NEGF method I expand on usage of some of the implemented methods. In particular the addition of gates and extraction of projected molecular transport, see Fig. 2. Projections enable spectroscopy of molecular eigenstates and the identification of the electron carrying pathways. They will provide an intuitive understanding of the physics governing the transport properties of the junction. I will analyze the transport projection of the C60 molecule in a close packed Cu surface [4]. Importantly the projection is not limited to molecules and it will be shown that a generic projection onto k-resolved eigenstates is also possible.
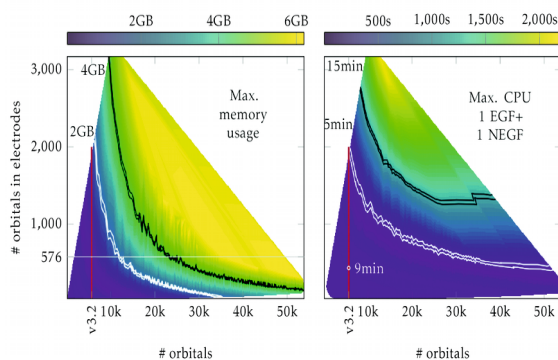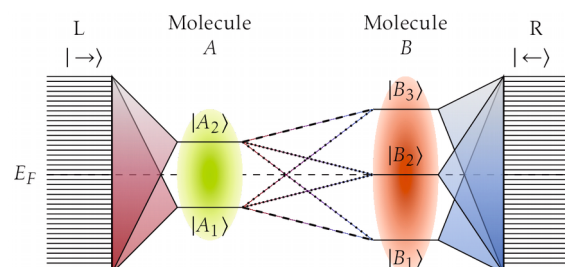

Fig. 1: Memory/Time use of 2-terminal

Fig. 2: Transmission projection of molecule eigenstates.

[1] Papior, PhD thesis (2016)
[2] Papior, et al. Computer Physics Communications, 212, 8–24 (2017).
[3] Jacobsen, et al., Carbon. 101, 101-106 (2016)
[4] Schneider, et al., Journal of Physics Condensed Matter 27, 015001 (2014).

odborný garant: *Hector Vazquez, PhD.*