Imaging Electronic Currents through Graphene-Based Nanojunctions

Jean Christophe Tremblay[1*], V. Pohl[2], J. Shao[2], L.E. Marsoner Steinkasserer[2], B. Paulus[2]

[1]*Laboratoire de Physique et Chimie Théoriques, UMR7019, CNRS-Université de Lorraine, 1 Bd Arago, 57070 Metz, France*

[2]*Institut für Physikalische und Theoretische Chemie, Freie Universität Berlin, 22 Arnimallee, 14195 Berlin, Germany*

*Presenting Author E-mail: tremblay1@univ-lorraine.fr

ABSTRACT

To assist the design of efficient molecular junctions, a precise atomistic understanding of the charge transport mechanisms through nanoscaled devices is of prime importance. In this contribution, we present various simulation techniques to investigate space-resolved electron transport through graphene-based nanojunctions. On the one hand, we study coherent electronic current density in an oligo(phenylene ethynylene) derivative attached to graphene nanoribbon leads under time-dependent potential biases [1,2]. This reveals mechanistic details of the transport on time scales ranging from atto- to picoseconds, allowing to image the change from early-time scattering to quasi-static current regime. On the other hand, we investigate quasi-static charge transport in defective zigzag graphene nanoribbons using spatial maps of non-equilibrium Green's functions at finite bias voltages to understand the effect of defect dilution and of the nanojunction width on the local current densities [3].

References

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