The simulation of molecular and organic devices: a critical review and a look at future development

P. Lugli, G. Csaba, C. Erlen, S. Harrer, G. Scarpa, A. Di Carlo[1], A. Pecchia[1], L. Latessa[1], A. Bolognesi[1]

Lehrstuhl für Nanoelektronik, TU München, Arcisstrasse 21 D-80333 München, Germany

[1] *Dept. Electronics Eng., University of Rome "Tor Vergata", Italy*

email: lugli@ei.tum.de website: www.nano.ei.tum.de

Molecular devices have lately attracted increasing attention due to some appealing features such as their low production cost, flexibility in the substrate choice, possibility of large area deployment, and possibly higher integration capabilities. There are actually two approaches to molecular electronics: on the one side one can mimic existing devices and substitute the active layer with an organic one. On the other, single molecules can be contacted and their transport characteristics exploited to achieve electronic functionalities. While in the former case conventional simulators can be adapted to the theoretical investigation of electronic and optoelectronic devices, in the latter case completely new approaches have to be developed.

Starting from a series of results obtained at TOV and TUM, we will critically review the state-of-the-art in the field of simulation of organic and molecular systems, by analyzing and comparing existing approaches, and looking at the open problems and possible solutions and future developments. We will describe the application of conventional device simulators to the description of organic field effect transistor (OTFT).[1-3] Here, hopping transport induce a field activated mobility which associated to the intrinsic low value of the mobility, produce unexpected phenomena. The interplay between mobility models, interface traps, grain boundaries and the nature of the contacts on the electrical characteristics of OTFT will be carried out and compared with available experimental data. Concerning the description of charge transport in molecular devices, we have developed a new code for transport computations [4,5] based on the well-known density functional tight-binding (DFTB) method, which allows an ab-initio treatment of systems comprising a large number of atoms within the self-consistent non-equilibrium Green's function approach. This technique enables the computation of the tunneling current flowing between two or more contacts in a manner consistent with the open boundaries and non-equilibrium conditions that naturally arise in coherent transport problems. Molecular dynamics simulation can be performed within the present approach, and time dependent current calculation can be calculated where the effect of molecular vibration is fully accounted [6,7]. Recently, the approach has also been extended to account for electron-phonon interaction. [8]. Our approach will be compared with other available tools, focusing on all critical aspects of electronic transport in single molecules (e.g. the role of contacts, conformational changes, and dissipation processes).

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A full journal publication of this work will be published in the Journal of Computational Electronics.

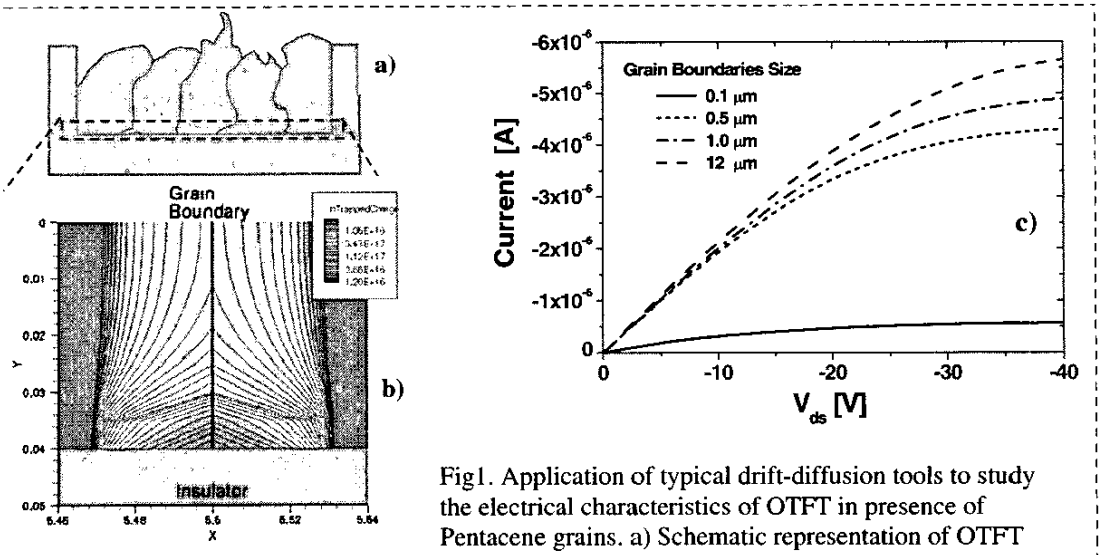

Fig1. Application of typical drift-diffusion tools to study the electrical characteristics of OTFT in presence of Pentacene grains. a) Schematic representation of OTFT with grains, b) Trapped charge density at the grain boundary, c) I-V characteristics as a function of grain size.

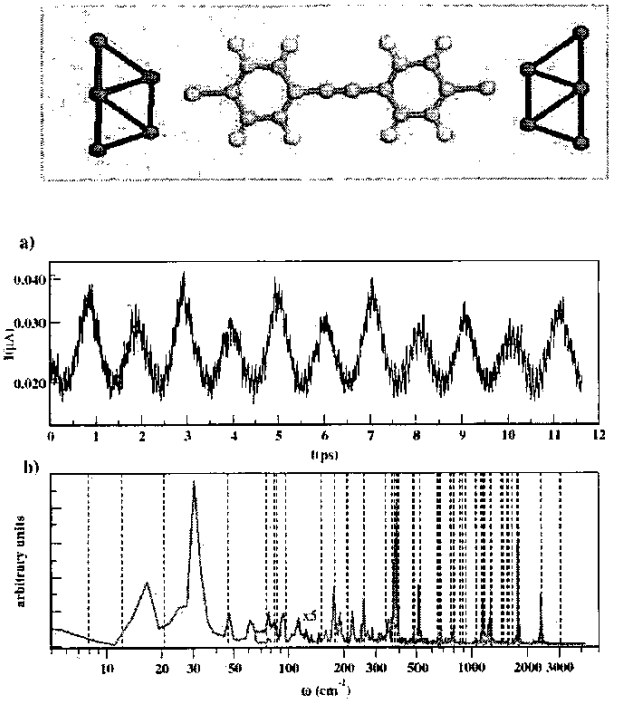

Fig. 2 . Time dependent current in molecular wires. The molecular structure is shown in the top panel together with part of the contacts. a) current obtained with the density-functional tight-binding, b) Fourier transform of the current. Vertical dashed lines represent the molecular vibrational frequencies.

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