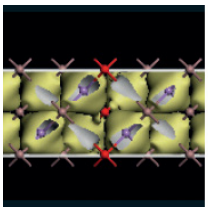

Session: Organic Semiconductor Devices/Soft Matter

(Invited) Charge and exciton dynamics in molecular aggregates: simple models from complicated ones

A Troisi

University of Liverpool, UK

We systematically approach the study of quantum dynamics problems by “model reduction”, i.e. by determining a suitable model Hamiltonian from more accurate electronic structure calculations. Several examples of this procedure will be illustrated. A global map of all molecular semiconductors will be built by reducing to the essence charge transport models based on a large set of computational exploration. A similar procedure will be used to study the exciton dynamics in biological light harvesting complexes.

(Invited) Using nanopores to sequence DNA: what can we learn from molecular dynamics

S Khalid

University of Southampton, UK

Nanopores, whether synthetic or based on proteins have been used to sequence single stranded DNA by making use of the differential partial blocking of an electric current, of the four bases. A key goal of this technology now is to optimise these pores for improved performance. Understanding the translocation of ssDNA through the confined geometry of nano-scale pores, at the atomistic and molecular level is extremely difficult using experimental methods. Computational methods such as molecular dynamics simulations offer a route to exploring the details of DNA conformational dynamics and translocation through nanopores, under an applied electric field. I will present some of our results to date.

Model parameter estimation and adaptive numerical simulation for organic thin film transistors

P Africa[1], C de Falco[1] and D Natali[2]

[1]Politecnico di Milano, Italy, [2]Istituto Italiano di Tecnologia, Italy

The accurate knowledge of relevant physical parameters is crucial to determine the predictive accuracy of numerical models for organic semiconductor devices. We present a step-by-step procedure enabling to determine critical model parameters - such as the density of states width, the carrier mobility and the injection barrier - by fitting experimental data from a sequence of relatively simple measurements to 2D numerical simulations under different regimes.

The current presentation extends the results of [1,2] where 1D models were used both for transient simulation of Metal-Insulator-Semiconductor (MIS) capacitors and for the estimating the DC transfer characteristics of Organic Thin-Film Transistors in the linear regime. The newly developed 2D simulator allows to account in a more natural way for a set of inherently two-dimensional phenomena, such as: the non-planarity of the semiconductor/insulator interface (due to the solution processing of materials); parasitic capacitances due to coupling between metal layers; the boundary condition at the semiconductor/substrate interface; contact resistance due to current-crowding effects. In order to deal with the increased complexity of numerical simulations in the new 2D setting efficient numerical methods based on a suitable a-posteriori error estimator and adaptive mesh refinement (see figure 1) have been implemented. The devices being considered in this study are shown in figure 2. Our approach is tested on a benchmark semiconducting

polymer: a very satisfactory fitting of experimental measurements is achieved and physically meaningful values for the extracted parameters are obtained, thus confirming the strategy effectiveness.

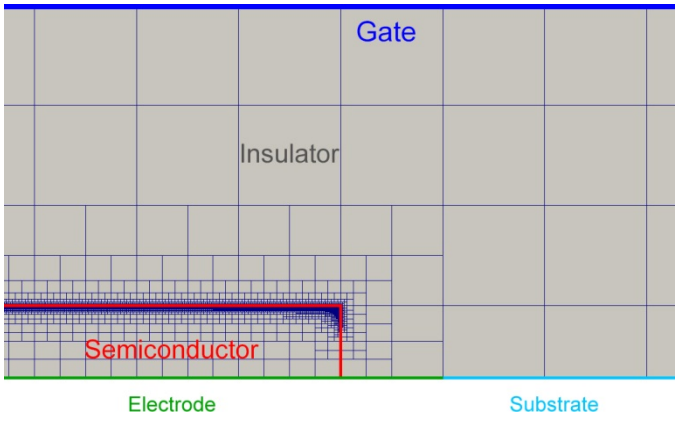

Figure 1 Example of an a-posteriori estimator driven mesh adaptation at the semiconductor/insulator interface in a benchmark MIS structure.

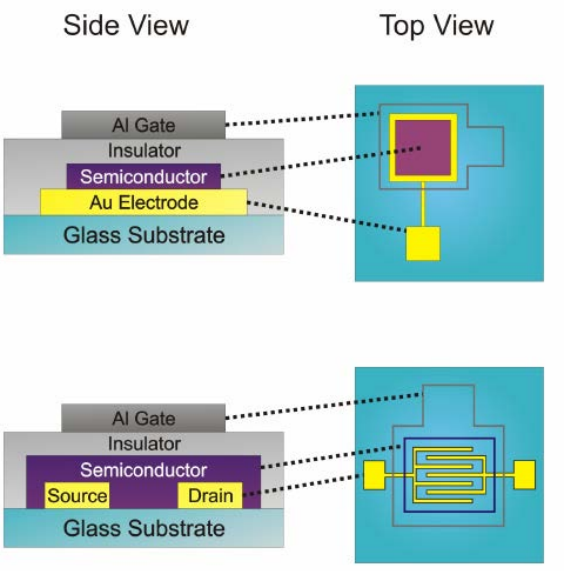

Figure 2 Top and side view of the devices used: the MIS capacitor at the top and the OTFT at the bottom. Reprinted with permission from Ref. [2]. Copyright Elsevier 2015.

[1] P. C. Africa, F. Maddalena, C. de Falco, M. Caironi, D. Natali. Simultaneous Extraction of Density of States Width, Carrier Mobility and Injection Barriers in Organic Semiconductors. Submitted, 2016.

[2] F. Maddalena, C. de Falco, M. Caironi, D. Natali. Assessing the width of Gaussian density of states in organic semiconductors. In Organic Electronics, 17, 304–318, 2015.