



International Workshop on Computational Nanotechnology

Session: Organic Semiconductor Devices/Soft Matter

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

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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

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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

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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