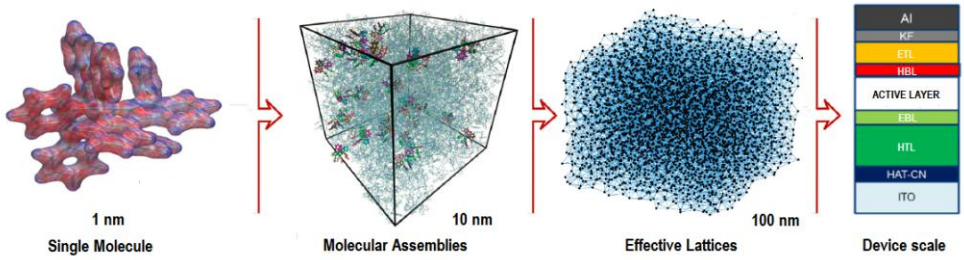
MOSTOPHOS Newsletter

Number 3, December 2016

MOdeling STability of Organic PHosphorescent OledS

Multiscale Simulation of Organic Transport



After Phillips has drop its research&development lines on displays, just before MOSTOPHOS kickoff, the project has lost its major industrial end-user. The management board has promptly addressed this problem and OSRAM, after a first expression of interest, is now officially a new project partner. OSRAM R&D expertise, especially on new lighting sources for automotive and housing, will give an important contribution to MOSTOPHOS, enhancing its exploitation potentials.

The departure of Phillips, unfortunatley, has adversely affected also the project partner company sim4tec that bankrupted in May 2016. The characterization tasks expected by sim4tec have now been taken over by FLUXIM Ltd, a Swiss company funded in 2007. Fluxim develops a powerful parameter analyzer (Paios 3.3) and simulation tools (Setfos 4.4) for transport and light coupling of OLEDs and OPVs, fitting very well into the project also opening additional potential exploitation routes of the new transport models developed within MOSTOPHOS.

About us:
MOSTOPHOS is a project addressing the problem of stability of blue emitting organic LEDs based on phosphorescent dyes in order to achieve all-organic white sources for lighting.
The challenge of the project is to provide a theoretical understanding of the dominant degradation mechanisms, that are at the basis of possible improvements.

Project kick-off: 1st June 2015.

Coordinator:

- *Max Planck Institute Polymer Res. (D)*

Project partners:

- *Consiglio Nazionale delle Ricerche (I)*
- *BASF SE (D)*
- *Universidad del Paìs Vasco (S)*
- *COSMOlogic GmbH (D)*
- *Università di Roma 'Tor Vergata' (I)*
- *Technische Universiteit Eindhoven (NL)*
- *Technische Universitaet Dresden (D)*
- *FLUXIM Ltd (Ch)* New
- *OSRAM Licht AG (D)* New

Simulations of exciton transport and exciton-polaron quenching

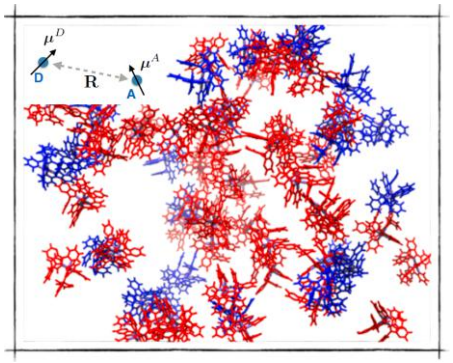


Fig. 2 MD sample of emitter (red) and DPBIC molcules (blue). Host molecules are hidden.

At University of Basque Country (UPV) exciton transport has been computed using Octopus and ORCA quantum chemistry tools. At the simplest model level Foster diffusion mechanism has been assumed. In this case a dipole-dipole approximation of the HOMO=>LUMO and HOMO=>LUMO+1 transitions have been considered. An MD sample of the emitter layer is used to extract statistics of the dipole-dipole orientations and from this a parameterization of the Foster diffusion forumala can been obtained. The spectral overlap between absorbtion and emission of each pair is considered as an experimental parameter for the moment since a reliable value of this is computationally challenging. Since the emitter layer is a mix of three compounds in which the Ir-complex DPBIC is also carrying triplets, it is important to consider all pair combinations between DPBIC (D) and emitter (E). More accurate transition densities are obtained either using a multipole expansion and local transition dipoles computed with real-time propagation TD-DFT or direct real space integration of the transition density elements, both obtained within the octopus code. These new methodologies are still under development.

The calculation of triplet-polaron quenching rates, which is clearly a key parameter for the simulation of phOLEDs, can be done on a similar level of approximation, involving transition rates between neutran and charged species. The relevant transitions are $E^*+D^+ \Rightarrow E+D^{+*}$ and $E^*+E^- \Rightarrow E+E^{-*}$. Scanning over the relative angle space it was found that E^*-D^+ has a maximal exciton coupling of 25 cm^{-1} and E^*+E^- has a maximal coupling of 40 cm^{-1}.

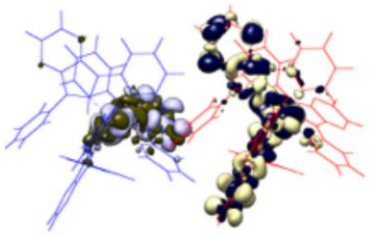


Fig. 3 Exciton-Exciton transition densities for emitter-emitter pair.

Implementation of a macroscopic drift-diffusion model

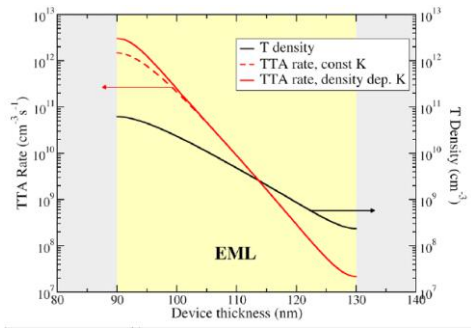


Fig. 4 Drift-Diffusion simulation of a phOLED.

At the University of "Tor Vergata", in the group of Prof. Aldo Di Carlo, a complete drift-diffusion model has been implemented in the TiberCAD simulation software. The model includes charge carrier as well as singlet and tripet exciton diffusion and their dynamics. All parameters can now be obtained and interpolated from tables provided in Monte Carlo simulations. Hence numerical models for field and concentration dependent mobilities can be used in the simulation. The hierarchical data format (HDF) has been chosen to store data and metadata necessary for the model. In the same way triplet-triplet and triplet-polaron annihilation rates as a function of host/guest fraction and exciton concentration as computed in MC runs can now be imported in the drift-diffusion simulation.

Development of a GUI for morphology simulations

In the updated version of the GUI under development in COSMOlogic, the possibility to create directories for morphologies inside the project folder is now activate. The MD simulation package GROMACS is interfaced for this purpose. The implemented calculators included simulation protocols for equilibration and production runs. For a post-processing, energy versus time step and structure per time step can be extracted from the trajectory. The format-converters have been extended to established file formats for MD simulations. Effort have been spent for a good 3D representation of the morphology.

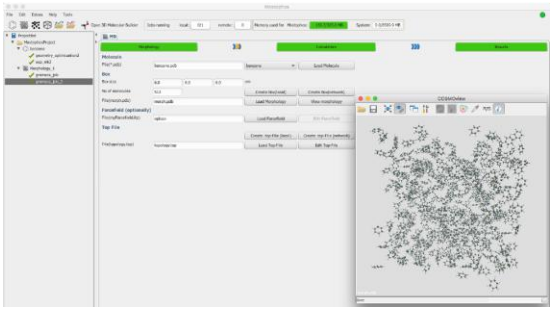


Fig. 5 Morphology simulator GUI of COSMOlogic.

Recent and upcoming events

The 18-month meeting of MOSTOPHOS took place in Mainz on November 28th and 29th.

A CECAM workshop on "Multiscale modelling of organic semiconductor: from elementary process to devices" will be held in Lyon in september 2017 co-organized by MOSTOPHOS and EXTMOS EU projects. The next MOSTOPHOS meeting (24-months) will take place on the same occasion.

Publications

[1] P. Kordt, S. Stodtmann, A. Badinski, M. Al Helwi, C. Lennartz, D. Andrienko, Parameter-free continuous drift-diffusion models of amorphous organic semiconductors, Phys. Chem. Chem. Phys., 17, 22778-22783 (2015)
[2] P. Kordt, J. M. van der Holst, M. Al Helwi, W. Kowalsky, F. May, A. Badinski, C. Lennartz, D. Andrienko, Modeling of organic light emitting diodes: from molecular to device properties, Adv. Funct. Mater., 25, 1955-1971 (2015)
[3] C. Poelking, D. Andrienko, Long-range embedding of molecular ions and excitations in a polarizable molecular environment, J. Chem. Theory Comput., 12, 4516-4523 (2016)
[4] Kordt, D. Andrienko, Modeling of spatially correlated energetic disorder in organic semiconductors, J. Chem. Theory Comput., 12, 36-40 (2016)
[5] P. Kordt, T. Speck, D. Andrienko, Finite-size scaling of charge carrier mobility in disordered organic semiconductors, Phys. Rev. B., 94, 014208 (2016)
[6] B. F. Milne, C. Kjær, J. Houmøller, M. H. Stockett, Y. Toker, A. Rubio, S. B. Nielsen, On the exciton coupling between two chlorophyll pigments in the absence of a protein environment: Intrinsic effects revealed from theory and experiment, Angew. Chemie Int. Ed. (2016)
[7] M. Mesta, H. van Eersel, R. Coehoorn, P.A. Bobbert, Kinetic Monte Carlo modeling of the efficiency roll-off in a multilayer white organic light-emitting device, Appl. Phys. Lett. 108, 133301 (2016)
[8] H. van Eersel, P.A. Bobbert, R.A. J. Janssen, R. Coehoorn, Effect of Förster-mediated triplet-polaron quenching and triplet-triplet annihilation on the efficiency roll-off of organic light-emitting diodes, J. of Appl. Physics 119, 163102 (2016)
[9] L. Zhang, H. van Eersel, P.A. Bobbert, R. Coehoorn, Clarifying the mechanism of triplet–triplet annihilation in phosphorescent organic host–guest systems: A combined experimental and simulation study, Chem. Phys. Lett. 652, 142-147 (2016)
[10] L. Zhang, H. van Eersel, P.A. Bobbert, R. Coehoorn, Analysis of the phosphorescent dye concentration dependence of triplet-triplet annihilation in organic host-guest systems, Chem. Phys. Lett. 662, 221-226 (2016)

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