MOSTOPHOS Newsletter

Number 6, June 2018

MOdeling STability of Organic PHosphorescent OledS

The last stages of the project

MOSTOPHOS project has reached its endings. A number of managment issues afflicted its progress, essentially due industrial partners defections and on-the-fly substitutions. Indeed, the initial consortium had onboard industries such as BASF, an external member as relevant as Phillips as well as several SMEs such as sim4tec. However, since the very beginning it was evident that a big hurricane was investing the European OLED and display manufacturing sector. Phillips decision to quit the field determined BASF decisions to sell its IP portfolio and adversly impacted SMEs such as sim4tec. Ultimately, this jeopardized the prosecution of the whole project, as substitutions were initially not obvious, expecially after month 18th. Certainly, thanks to a good management and decisions process it was possible to find new partners: FLUXIM Ltd has taken over sim4tec in the characterization of stacks and CYNORA has substituted BASF in materials manufacturing.

From a scientific point of view we can say that MOSTOPHOS has been a successful project. In this final newsletter we review the major achievments. The final goal was to develop a multiscale environement available to industrial developments hence maintained by a software company, in our case COSMOlogic. Scientific progresses concerned the refinement of all steps in the simulation process, including accurate energy levels, disorder, charge and exciton transfer rates, injection rates, development of an efficient off-lattice Monte Carlo, up in the scale to device-oriented drift-diffusion models and optical models.

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)*
- *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)*
- *CYNORA GmbH (D)*

CYNORA stack simulations

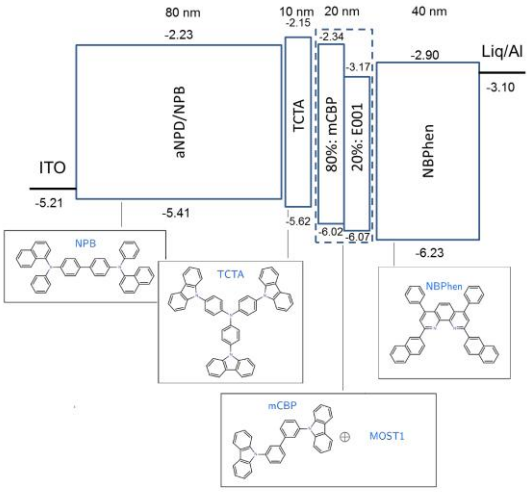

Fig. 1 Blue OLED stack of CYNORA based on TADF.

FLUXIM tools such as Setfos and Phelos allows for a thourough characterization of OLED devices.
In Fig. 2 are reported the measured angular dependent emission of the OLED for bot s and p polarized light. The tools allows to simulate the real device operating condition with a drift-diffusion model coupled to an electro-magnetic simulation. A comparison between simulated and measured optical response is shown on the top of Fig. 1.

The blue OLED stack produced at CYNORA is represented in Fig. 1. This stack is based on the Thermally Activated Delayed Fluorescence (TADF) mechanism that up-convert triplet excitons back to singlets via a reverse intersystem crossing. As such this device is not properly a phosphorescent OLED, as was the original Ir-complex DPBIC in the BASF stack, however all the multiscale workflow developed in the MOSTOPHOS project can be applied to this new type of materials. Indeed, TADF have been considered as a third generation OLED after Adachi et al. breakthrough in 2012. These materials hold the promise of low driving voltage, low power and long lifetime.

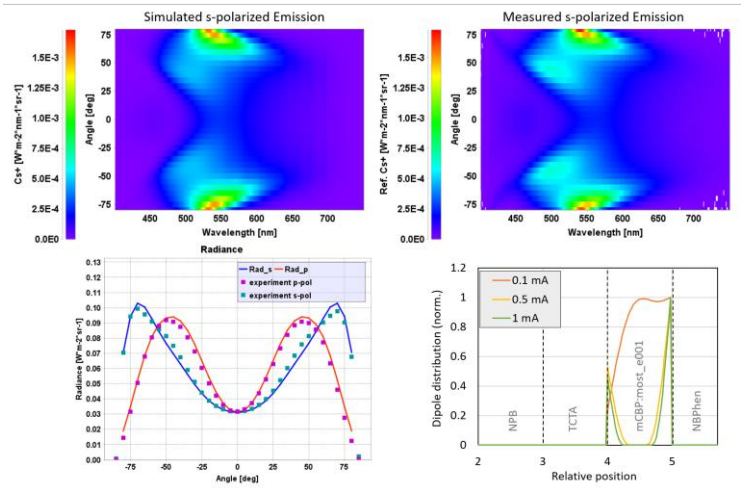

Fig. 2 Optical characterization and simulations by FLUXIM.

Transfer rates

Energy levels are computed using the VOTCA package developed at Max Planck. The energy levels of gas-phase molecules are computed with Espresso, typically using the B3-LYP hybrid functional. Condensed phase renormalizations are obtained with the help of an MD simulation comprising ~4000 molecules. The polarizable force-field developed in the MOSTOPHOS project accurately accounts for the polaron self-energy and disorder. An example of the level position and Gaussian disorder broadening for the emitter host/guest mixture are shown in Fig. 3. Since the emitter molecule (MOST1 in Fig.1) is polar, disorder in the emitter can be as large as 200 meV. The shift of almost 0.8 eV of the predicted electron affinities might be correct since Cyclic Voltammetry EAs tend to be overestimated.

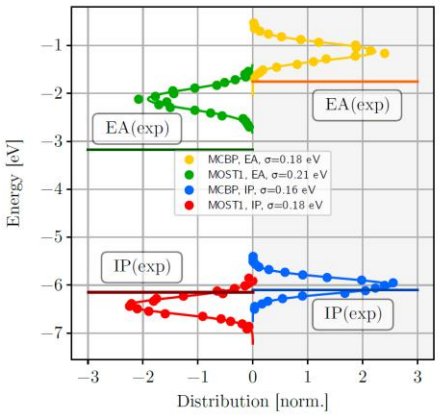

Fig. 3 Predicted levels and gaussian disorder.

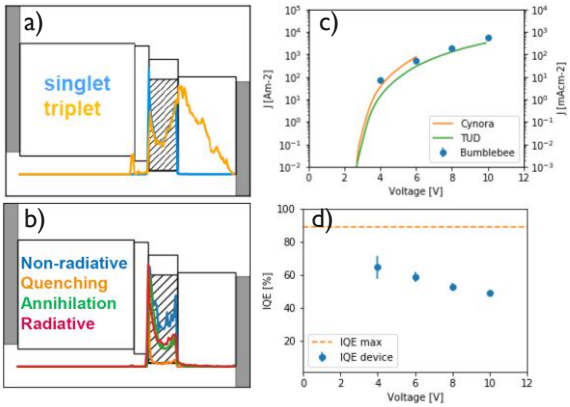

Fig. 4 Monte Carlo Simulations. a) Distribution of excitons; b) distribution of loss processes; c) I-V characteristics; d) Internal quantum efficiency.

Charge transfer as well as exciton transfer rates are computed using the Marcus approach and inserted in a Monte Carlo solver. The most important development of the MOSTOPHOS project was the extension of the Bumblebee tool of TU Eindhoven is to treat realistic molecular geometries rather than a regular square lattice of sites (off-lattice simulations). This is a non-trivial step since Coulomb interactions are computed much more efficiently on a regular lattice. Results of the MC simulations are shown in Fig. 4.

Another important work performed in the MOSTOPHOS project has been to asses the validity of the Marcus type approach for transfer rates. As possibly expected, since most of the reorganization energies are linked to internal vibrational degrees of freedom Marcus is not quite accurate. Surprisingly tunneling effect produce a rate that looks like a Miller-Abrahms in functional form.

Software Environment

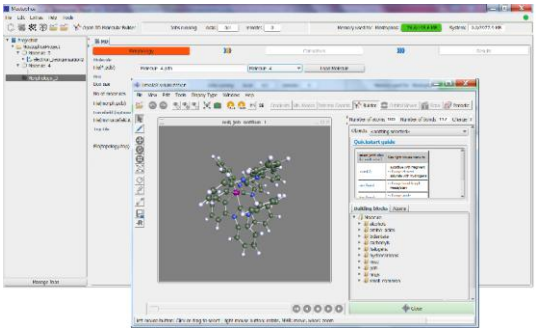

Fig. 5. A snapshot of the simulation environement

COSMOlogic has developed a fully functional simulation environement able to compute electronic properties using TURBOMOLE, build amorphous structures with the help of VOTCA tools to build supercells that can be equilibrated with GROMACS MD simulation tools. Reorganization energies charge-transfer integrals and transfer rates can then be computed. The tool can also run VOTCA integrated kinetic MC in order to extract mobility parameters and can setup input structures for exciton transfer calculations using OCTOPUS.

All resulted parameters can be used in MC simulations performed at device level or into effective drift-diffusion models.

Upcoming events

The 36-months closing and review meeting will taken place in Eindhoven on the 14-15th may 2018.

Publications

[1] A. Lorenzoni, A. Mosca-Conte, A. Pecchia, F. Mercuri, "Nanoscale morphology and electronic coupling at the interface between indium tin oxide and organic molecular materials", Accepted by Nanoscale

[2] N. B. Kotadiya, H. Lu, A. Mondal, Y. Ie, D. Andrienko, P.W. M. Blom, G.-J. A. H. Wetzelaer, "Universal strategy for Ohmic hole injection into organic semiconductors with high ionization energies, Nature Materials", 17, 329-334, 2018

[3] P.-A. Will, E. Birgit, S. C. Fuchs, R. Scholz, S. Lenk, S. Reineke, "Scattering quantified: Evaluation of corrugation induced outcoupling concepts in organic light-emitting diodes, Organic Electronics 58, 250 (2018)

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