PROJECT FINAL REPORT

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1 Final publishable summary report

1.1 Executive summary

White Organic Light-Emitting Diodes (OLEDs) are potentially highly efficient large-area light sources, which can be used for lighting applications in hitherto unprecedented ways, such as light-emitting flexible foils. In principle, there seems to be no fundamental obstacle towards 100 lm/W efficiency, beyond that of fluorescent lamps. However, in practice the ever-increasing complexity of OLEDs hampers further progress towards that goal, in part because reaching this efficiency goal is only of practical interest in combination with durability, colour stability and tunability, and ease of fabrication. For the further development of efficient white OLEDs, the availability of an experimentally validated predictive opto-electronic device model is crucial. At the start of the project, such a model was not available. State-of-the-art “first generation” models, based on conventional understanding of transport and photo-physical processes, are insufficient for realistic OLEDs based on structurally disordered organic semiconductors.

Within the AEVIOM project (2008-2011, www.aeviom.eu) a paradigm shift in OLED modelling was realized by introducing a “second generation” OLED model which takes the consequences of the disordered nature of realistic organic semiconductor OLED materials into account. A fundamental basis was created by carrying out advanced three-dimensional (3D) supercomputer Monte Carlo charge transport and recombination modelling studies. Intensive experimental studies have been used to demonstrate the high importance of taking the disordered nature of the organic semiconductor materials into account, and to validate the models developed. Furthermore, various novel experimental simulation-software-assisted techniques were developed to study OLED materials and devices, providing e.g. accurate measurements of the mobility functions, the light emission profile, the singlet-exciton fraction, the built-in voltage and the injection barriers. The 3D-results were “translated” to accurate one-dimensional expressions, and using these expressions fast PC-software tools were developed. Applications of this second-generation OLED modelling tool have been demonstrated for a complete “hybrid-white” OLED, based on experimentally determined hole and electron mobility functions, using the world’s first full 3D Monte Carlo OLED modelling as a benchmark. The model has also been used to support OLED lifetime and color stability studies. Predictive modelling has been demonstrated for single-layer OLEDs, and the realization of such a demonstration is in good progress for multilayer OLEDs.

The project results have been presented in 31 published and accepted papers in peer-reviewed high-quality international journals, and have been disseminated via more than 90 other channels (oral and poster presentations at conferences, in workshops, at exhibitions, websites, digests). A large number of additional publications is expected. Commercial OLED simulation PC-software containing much of the AEVIOM second-generation modelling has recently become available from Fluxim (SETFOS3.2-software, March 2011), and will become available from sim4tec in the first half of 2011 (SimOLED-software). This is expected to contribute to the rational, timely and efficient development of advanced OLED device structures with breakthrough performance.

1.2 Description of project context and objectives

In this section, the project context and objectives as formulated at the start of the project are presented.

White Organic Light-Emitting Diodes (OLEDs) are potentially highly efficient large-area light sources, which can be used for general and intelligent lighting applications in hitherto unprecedented ways, such as light-emitting flexible foils. Fig. 1(a) shows the difference in form factor between OLEDs and conventional light sources. In the past three years, the luminous efficacy of laboratory prototype white OLEDs has shown a very fast, fivefold increase. At present, world-record values are 60 – 65 lm W^{-1} (including a scattering layer for improved light-outcoupling), a factor of four larger than that of incandescent lamps. This is shown in fig. 1(b), in which a comparison is made with the luminous efficacy of conventional light sources (incandescent lamps and fluorescent tubular lamps) and with inorganic LEDs. There is a **great societal need** in achieving durable and affordable light sources with a high luminous efficacy. At present, 10-15 % of the global energy production is used for lighting, corresponding to 2100 TWh per year, and corresponding to 250 billion Euro (of which 25 % for Europe). The need for lighting is expected to increase strongly in the near future, realistically by a factor of 2 within the next two decades [1]. In view of the huge cost of lighting, the waste of precious energy involved in many of today's electrical lamps, and the resulting environmental impact due to the annual amount of greenhouse gas (CO_2) produced, there is a strong need for more efficient and thereby more environmentally friendly light sources. The prospect of realizing a breakthrough in this direction is achievable by OLED technology. The successful development of OLED white light sources can greatly extend the societal impact of solid-state lighting technology. *In principle*, there seems to be no fundamental obstacle towards a 100 lm W^{-1} efficiency, beyond that of fluorescent lamps. However, *in practice* the ever-increasing complexity of OLEDs now hampers further progress towards that goal. "Conventional" OLEDs, such as shown in fig. 2(a), already contain ~10 organic layers, whereas advanced so-called stacked devices (fig. 2(b)) can contain more than 20 layers.

(a) 

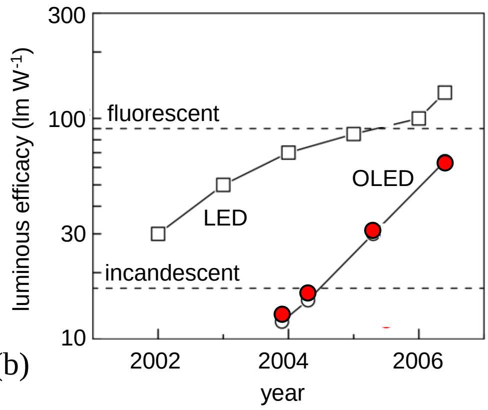
(b) 

Figure 1.1

(a) White and yellow (middle) OLEDs as compared to conventional light sources (compact fluorescent lamp, incandescent lamp and fluorescent TL).

(b) Development of the luminous efficacy of white OLEDs (closed circles), as compared to that of white inorganic LEDs (open squares) and commercial tubular fluorescent lamps and incandescent lamps. All LED and OLED data points refer to laboratory prototypes. The data given are only meant to indicate the development. From [2].

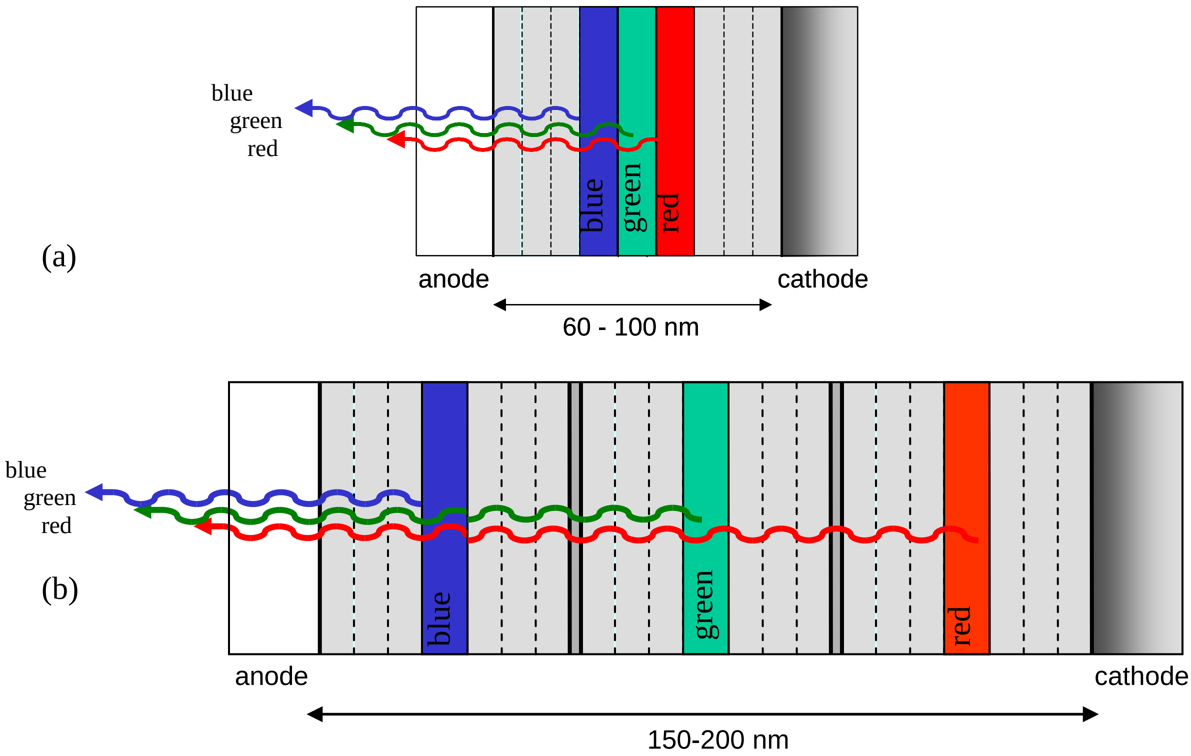


Figure 1.2

(a) *Layer structure of a white OLED, containing nine different organic semiconducting layers, with a central light-emitting layer that contains blue, green and red sublayers. In actual devices, the order of the emissive layers may be different.*

(b) *Layer structure of a so-called "stacked" OLED, containing separate blue, green and red emitting subunits, each separated by a very thin transparent interlayer. The total layer structure comprises more than 20 organic semiconducting sublayers. Some sublayers have a thickness of approximately 10 nm (approximately 10 molecules), or less.*

So far, the development of OLEDs was to a large extent a semi-empirical trial-and-error process, in which organic semiconducting materials were selected on the basis of their known or partially known separate properties. It has recently become clear that this a roadblock for further development. Due to the complex layer compositions and structures, an efficient and rational OLED design is no longer possible without the availability of an *experimentally validated* comprehensive OLED device model. Such a model is not available at this time. Therefore, we specify our main objective as follows:
The main objective of this project is to develop a powerful numerical simulation tool for achieving breakthroughs in white OLED technology. The underlying comprehensive model will be validated experimentally, and applied to advanced OLED device structures in order to enable breakthroughs in white OLED efficiency, lifetime, and manufacturing cost.

The model is the result of what may be called a **'paradigm shift'** in the way we understand the functioning of high-performance OLEDs, and in the way of translating that understanding into a model with high impact on OLED performance. Therefore, we call our model a **"second generation" OLED model**, whereas existing OLED models, which are presently being commercialized, may be called "first generation" OLED models. The paradigm shift in our understanding of how OLEDs function is the result of a recent breakthrough in our insights in the effect of **disorder** of the organic semiconductors on the functioning of OLEDs. It is obvious that in the absence of disorder, a device model can be one-dimensional (1D): the current density in the OLED is then the same at any point on the OLED area. This is a basic assumption in the present, first generation models. These models take the effect of disorder only partly into account, by including certain effects on the electron and hole mobility. However, it has recently become clear that the use of first generation models can lead to important misconceptions and numerically large errors. The reason is that the disorder leads, in fact, to a highly **filamentary current density** in OLEDs. This is illustrated by fig. 1.3, which shows the current density in a realistic (electrode / organic layer / electrode) structure, as obtained from an advanced three-dimensional calculation, carried out using a supercomputer. For simplicity, the current density shown here is due to only one type of charge carrier (holes). The calculation has been done for an area of 40×40 molecules (i.e. 40 nm × 40 nm, typically), and the thickness of the organic layer is 20 molecules (20 nm, typically). The figure shows that the current is confined to rather narrow filamentary pathways, instead of being uniform. In this realistic example, 50 percent of the current is confined to only a few percent of the device area.

The **urgency** of developing a second generation model as a crucial breakthrough-step towards high-performance OLED technology becomes already apparent by analyzing in more detail the results of calculations such as those shown in fig. 1.3. Furthermore, we have found from pilot calculations that that discrepancies in quantitative predictions between first and second generation models can be one order of magnitude or more for realistic devices, due to modifications of the mechanisms of charge carrier transport within the organic layers, and near interfaces. Moreover, it should be emphasized that we are just beginning to understand the full impact of disorder on OLED performance. It is highly plausible, although presently not yet proven, that due to the filamentary nature of the current density of electrons and holes, recombination does not take place uniformly over the surface area of the device, but instead in small areas, almost of the scale of one molecule. At these points, the energy density in the device is locally very large. As a result, the probability of the occurrence of structural changes that lead to a defect (e.g. breaking of double bonds, so that the molecule does not conduct a current anymore) is locally more strongly enhanced than would be expected from a first generation model. The microscopic-scale processes that ultimately limit the OLED device lifetime can therefore only be understood using a second generation OLED model.

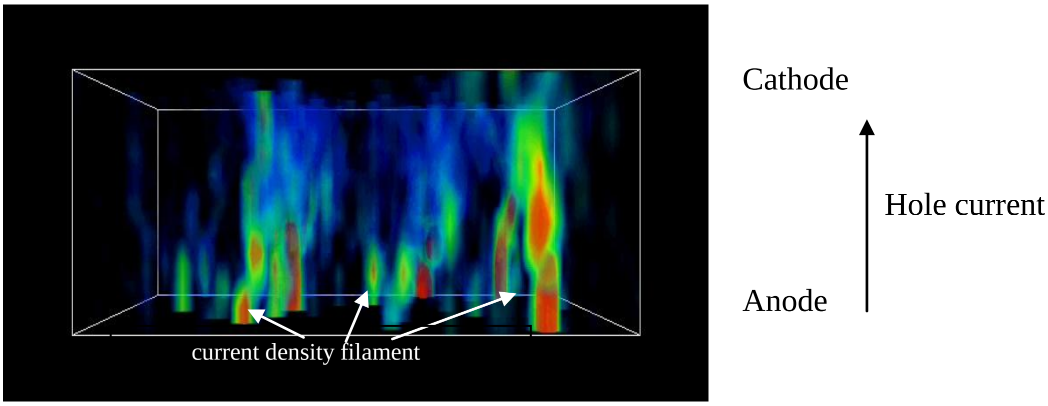


Figure 1.3
*Current density filaments in a 20 nm thick and 40×40 nm large segment (indicated by the white box contour lines) of an OLED-type device. In this advanced fully 3-dimensional calculation, there is only a hole current, from the anode to the cathode. The applied voltage is 2 V. In the figure, regions with decreasing current density become more transparent. In the current density filaments shown, the current density is at least 6 times larger than the average value. In the center of some of the filaments, it is more than 30 times larger than the average current density (J.J.M. van der Holst, Phys. Rev. B **79**, 085203 (2009)).*

Full support for our statement that there is an urgent need for developing a second generation OLED model is given in a workshop report **"Basic Research Needs for Solid-State Lighting",** by the U.S. Department of Energy [5]. A panel, formed by twelve leading U.S. OLED researchers concluded:

"*Since disorder is pervasive in organic films, immediate improvements in OLED performance are likely to be achieved upon understanding the relative impact of the various kinds of disorder. Quantifying disorder will lead to a better understanding of its origin and will enable the community to design materials that help inject and transport charge more efficiently. Improved modeling will help guide materials synthesis and device development efforts. Controlling energetic disorder will improve charge injection and transport in the bulk of the films and also help confine excitons away from quenchers, both of which lead to higher OLED efficiency. Achieving injection from air-stable metals will enable devices with reduced encapsulation requirements and reduced manufacturing cost. Finally, control of disorder will benefit not only OLEDs, but also other organic electronic technologies, such as solar cells."*

The **focus in the project** will be on small-molecule OLEDs for white-light applications, and the project will cover all relevant electronic transport and exciton physics aspects of these devices. However, we will also investigate polymer OLEDs, which we consider as excellently suited for exploring many of the consequences of disorder. The results of the project will be equally relevant to small-molecule and polymer OLED devices, and they will be even relevant beyond the field of OLEDs, e.g. for organic field-effect transistors based on disordered materials and for organic photovoltaic cells.

The main objective of the project, that has already been stated above, is specified further by the following **more specific objectives**:

1. To develop an advanced 3D-numerical OLED device model that has a transparent and sound physical basis, so that accurate predictions can be derived from it concerning OLED efficiency and concerning lifetime-limiting processes, based on a critical analysis of experiments that probe the electrical transport and photophysics.
2. To derive from this model a practical easy-to-use 1D-numerical method for steady-state and transient (a.c.) current-voltage-luminance calculations, that still has essentially the full functionality of the 3D model, and that will be the basis of a versatile and indispensable tool for rational OLED development.
3. To apply the model in order to make experimentally validated recommendations towards the realization of a breakthrough in white OLED efficiency and lifetime, and towards drastic simplifications of the manufacturing process.

[1]. *Towards a Bright Future for Europe*, Strategic Research Agenda in Photonics (2006). Available from the EU Photonics21 technology Plaform, www.photonics21.org.

[2]. R. Coehoorn and H. Boerner, *Encyclopedia of Materials: Science and Technology*, ed. K.H.J. Buschow et al., Elsevier (2008). ISBN: 0-08-043152-6.

[3]. Philips: P.W.M. Blom and M.C.J.M. Vissenberg, Mat. Sc. Eng. **27**, 53-94 (2000). IBM: J. Campbell Scott et al., Synth. Met. 111-112, 289 (2000), and B. Ruhstaller et al., J. Appl. Phys. **89**, 4575 (2001). Siemens: J. Staudigel *et al*., J. Appl. Phys. **86**, 3895 (1999).

[4]. Los Alamos: P.S. Davids, A.S. Saxena and D.L. Smith, J. Appl. Phys. 78, 4244 (1996); Lausanne: H. Houili et al., Comp. Phys. Comm. 156, 108-122 (2003); D. Berner et al., Phys. Stat. Sol. (a) **202**, 9 (2005). Bath: A.B. Walker et al., J. Phys. Cond. Matt. **14**, 9825 (2002).

[5]. "Basic Research Needs for Solid-State Lighting", p. 106, U.S. Department of Energy (2006). The report can be obtained from http://www.sc.doe.gov/bes/reports/files/SSL_rpt.pdf. The names of the panel members are given on p. 193.

1.3 Main S&T results and foregrounds

The development of a powerful numerical simulation tool for achieving breakthroughs in white OLED technology, which has been the overall objective of AEVIOM, requires that the simulation methods developed are not only *descriptive* but also *predictive*. Predictive simulation makes computer-aided-design possible of optimized OLED stacks on the basis of a model which contains a parameterized description of the performance of all elements, obtained from dedicated studies on simplified structures. An overview of the steps taken in the AEVIOM project to realize this goal is shown in Figure 1.4. In the remainder of this section, we discuss each of these steps in more detail, and we give a complete although brief explanation on all published contributions to these steps made by AEVIOM. References are given to the list of publications contained in table 2.1. It should be emphasized that much work is still in (good) progress, and that many more publications are expected. This includes the public reporting on the demonstration of predictive white OLED modelling.

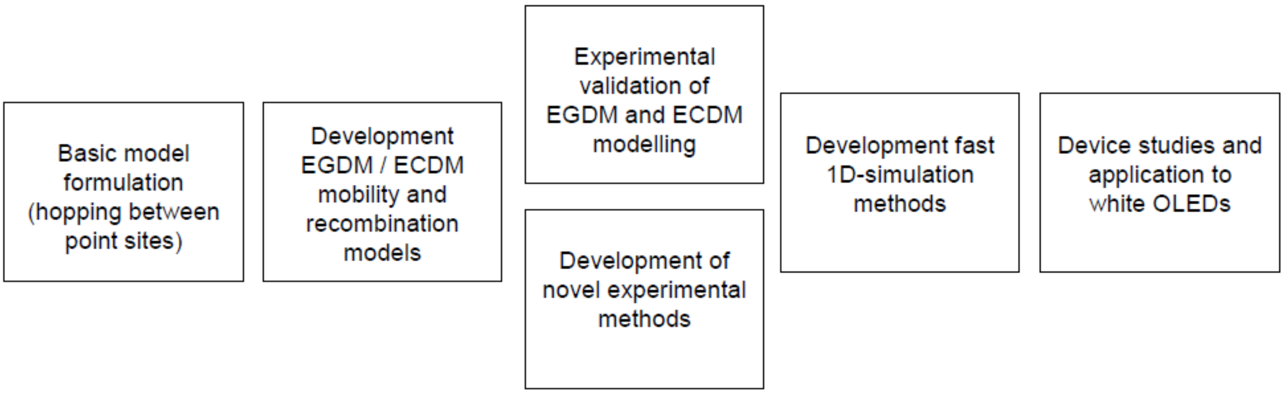


Figure. 1.4.
Schematic overview of the steps taken in the AEVIOM project to develop a predictive white OLED simulation tool.

1.3.1. Decision about the level of detail within which the molecular structure of real OLEDs is taken into account

Already at the beginning of the project, we have decided to model the transport and recombination processes in OLEDs as if the charge-carrier and exciton transport takes place due to hopping in between **“point-sites”.** The molecular-scale details (orientation distributions, shape of the HOMO and LUMO wavefunctions, etc.) are thus neglected.

1.3.2. Development of models for the charge-carrier mobility and recombination process taking the disordered energy level structure in relevant OLED materials into account

We have developed mobility and recombination models for two basic types of energetic disorder, viz. the “Extended Gaussian Disorder Model” (**EGDM**) and the “Extended Correlated Disorder Model” (**ECDM**). In both cases, the density of states (DOS) formed by the energy levels which contribute to the transport has a Gaussian shape. Within the EGDM, there is no spatial correlation between the energy levels on nearest neighbour molecular sites, whereas in the ECDM such a correlation is present. Whereas the EGDM had been developed before the start of the project [F.A. Pasveer *et al.*, Phys. Rev. Lett. **94**, 206601 (2005)), the development of the ECDM is one of the highlights of AEVIOM [17]. In both cases, the word "Extended" refers to the inclusion of the dependence of the mobility on the charge-carrier density. This important effect was neglected in the already existing "Gaussian Disorder Model" and "Correlated Disorder Model".

From Monte Carlo calculations, a model for the EGDM and ECDM **recombination** rates was developed [11]. It was found that the standard Langevin expression can be used, but only if the electron and hole mobilities used are not taken equal to the values obtained from single-carrier device studies, but corrected for the presence of the other carrier (i.e. using "bipolar mobilities").

It was also found that for including the effect of **deep trap states** on the mobility it is not necessary to develop yet another transport model, but that this can be included using a "multiple-trap-and-release" approach in the EGDM and the ECDM. The charge carriers reside part of the time in the deep trap states, and part of the time in the states forming the Gaussian DOS. The mobility is proportional to the latter time-fraction [23,24]. It was discovered that then a correction must be made to include the effect of an applied field. This leads to "**field-induced-detrapping**", and therefore to an enhanced mobility. A general and easy-to-use method for describing that effect in the case of the EGDM was developed [13].

1.3.3. Development of fast one-dimensional OLED device simulation methods

In order to be able to use these results of three-dimensional supercomputer modelling in fast PC-simulations, we have made developed several types of one-dimensional OLED device methods containing the EGDM and ECDM and including additional elements such as the presence of traps and interfaces.

As a first step, we have developed a **1D-method for modelling the current density (*J*) *versus* voltage (*V*) curves of single-carrier single-layer devices**, using a continuum solution of the 1D-drift-diffusion equation [6]. This method is found to be computationally very efficient and accurate, and has been used as a numerical benchmark for novel methods developed later. Using this method it was shown how Gaussian disorder affects the $J(V)$ curves, and that a realistic degree of disorder can give rise to apparent mobilities that vary over more than 2 orders of magnitude with the layer thickness if the current-voltage curves are incorrectly analyzed in terms of the often-used drift-only Mott-Gurney formula. Many of the results of this work were used in the user notes of the first release of SETFOS (version 3.0) containing elements of the EGDM (2009).

The results of this 1D-method were critically compared with the results of full 3D device-modelling, and were found to be in excellent agreement for a large range of values of the disorder parameter and the injection barrier [8]. In this 3D-device modelling study for the first time the **filamentary nature of current density** was quantified. It was shown how the current density of an ensemble of nominally identical (small) OLEDs can show a wide distribution, dependent on the disorder, due to the spatial randomness of the current pathways. For small injection barriers a slight difference was found between the 3D and 1D results. This was shown to be due to the **Coulomb repulsion** between the carriers close to the electrodes [15]. In future 1D-models, this effect should be included.

Subsequently, an **EGDM double-carrier OLED model** was developed, making use of a 1D-Master Equation approach within which a solution is obtained of the drift-diffusion-recombination problem on a discrete series of molecular sites [10]. The model is also applicable to multilayer structures, and to cases with trap states. It was found that due to disorder the width of the "recombination zone" (the region in a single-layer OLED within which a large recombination rate is found) can be much smaller than in the absence of disorder. Furthermore, the model provides physically transparent descriptions of the dependence of the mobility and the recombination rate on the electric field as obtained from three-dimensional modeling.

Speed is critical to the success of any commercial OLED simulation tool. For all realistic modelling cases (apart from the single-layer single carrier case studied in ref. 6), OLED simulations involve a many-step iterative solution method until steady state is reached. Technically different solutions methods have been investigated, showing that a **drastic reduction of the total calculation time** is possible following a strategy combining the Gummel-method (for the first few iterations) with the Newton method (for completing the convergence) [21]. This advantage is particularly relevant for numerically challenging devices. The fast method developed for solving the steady-state drift-diffusion equation (EGDM) was shown to yield excellent agreement with the results obtained earlier in refs. 6 and 8, and is the basis of future commercial OLED simulation tools. It was successfully extended to **fast transient EGDM modelling**, yielding dark-injection transients and capacitance-voltage curves [25], methods which are both frequently used to study the mobility.

1.3.4. Experimental determination of the applicability of the EGDM and ECDM for OLED-relevant organic semiconductor materials

Our studies on a large number of OLED-relevant small-molecule materials have led to the following picture:

(1) Hole and electron transport in **small-molecule** organic semiconductors is best described using the **ECDM** without and with and exponential trap DOS, respectively.

(2) Hole and electron transport in **polymer** semiconductors is best described using the **EGDM** without and with and exponential trap DOS, respectively.

We do not yet know how generally applicable this picture is, and there is at present no well-founded model from which the occurrence of an exponential electron trap DOS can be explained. The evidence was obtained from systematic studies of the $J(V)$ characteristics of single-carrier and single-layer test devices, in which the electrodes are chosen such that injection of the second carrier is negligible. Variation of the temperature and layer thickness was found to be necessary to obtain an accurate description of the mobility function within the EGDM or the ECDM model. Hole and electron transport in a blue-emitting polymer (PF-TAA, polyfluorene with 7.5 mol-% copolymerized triaryamine hole transporting units) was found to be well described using the EGDM [7,9,4]. For the application-relevant small-molecule materials α-NPD [20] and BAlq [18] the ECDM was found to be most appropriate. For some cases explicit proof was given that "first-generation" modelling, within which the carrier density dependence of the mobility is neglected, is not appropriate [7,20]. The use of molecularly doped injection layers, thereby creating symmetric devices, was found to be particularly useful in such studies [5]. It was also found from these studies that, for the cases studied, hole transport could be described well without assuming a trap DOS, whereas for electron transport the assumption of an exponential trap DOS was necessary. The picture given above is supported by our unpublished work on a large number of other small-molecule organic semiconductors.

1.3.5. Novel experimental methods

The "basic" experimental method for obtaining descriptions of the mobility and recombination functions in OLED materials is the measurement of the voltage dependence of the current density and current efficiency, carried out for sufficiently simple devices as a function of the temperature and of the thickness of all layers involved. The work carried out in AEVIOM has shown that this can only be done in a simulation-assisted manner, using EGDM and ECDM software for solving the "inverse" problem. In some cases, this task is still very difficult, in view of the large number of degrees of freedom involved. Moreover, in the case of multilayer devices, crucial additional required information is the energy level landscape, i.e. the position of the HOMO and LUMO (top of the Gaussian DOS) in all materials. These energies determine the injection barriers at the electrodes and the internal (organic-organic) barriers (if present). Whereas the HOMO can be determined using UPS, an appropriate method for determining the LUMO is not routinely available. The only direct method, inverse UPS, is only available in a few laboratories, and is far from routine due to the potential damage of the materials by the high-intensity electron beams used.

For these reasons, the availability of additional experimental techniques is crucial. Within AEVIOM, **we have developed or refined various experimental techniques which can be routinely applied and which help realize the goal of predictive OLED modelling.**

Measurement of capacitance-voltage ($C(V)$) curves in single-layer devices studied at low frequencies was found to reveal a distinct peak at the effective onset voltage. From the peak voltage and the peak intensity **the injection barriers at both interfaces can be deduced**, as well as the built-in voltage [2]. This also provides a relatively simple method for studying the effect of a change of injection conditions during ageing.

A well-known alternative method for determining the built-in voltage, and therefore for obtaining information about the injection barriers, is electroabsorption. It was found that the conventional analysis of electroabsorpion experiments, within which the voltage at which the effective internal electric field as probed optically is zero is assumed to be equal to the built-in voltage, is incorrect by in some cases more than 0.5 eV, viz. if the injection barrier at the injection electrode is only small. **A refined method was developed for analyzing electroabsorption experiments**. It was applied to PF-TAA, for which it was shown to be in excellent agreement with independent results from $J(V)$ and $C(V)$ curves [12].

Perhaps the most sensitive independent method for determining the validity of an OLED device model is the measurement of the light emission profile across the active layer. Furthermore, the light-outcoupling efficiency is a strong function of the position of the emission zone. For both reasons, the availability of a method for accurately determining the emission profile is very important. Actually, such a “measurement” is quite indirect, as this is again an “inverse” problem. The profile has to be deduced from the angular and polarization dependent emission spectra of OLEDs. In the literature, many elements of such an analysis had already been proposed and demonstrated seperately. In AEVIOM, a combination of all such elements was developed and the **measurement of the OLED emission profile with nanometer-scale resolution** was demonstrated for blue and red-emitting polymer OLEDs based on PF-TAA and NRS-PPV, respectively [1]. Elements included are the use of a combined semi-classical - quantum-mechanical microcavity model for properly treating the radiative decay probability, a normalization of the experimental data so that the method also provides the internal (source) emission spectrum, self-absorption, birefringence, use of the full angular dependence of the emission, use of a glass hemisphere to couple out light from more internal modes, and enhancement of the resolution by making use of a fit-profile method to reduce the effective number of degrees of freedom of the solution by employing the monotonicity of the solution. An extensive study was carried out of the applicability of various alternative algorithms and for various types of source spectra [16], and the effect of properly including in the forward modelling the **dependence of the exciton radiative lifetime on the position in the microcavity** was investigated [26,29,30].

The ultimate internal quantum efficiency of OLEDs is reached using phosphorescent emitters. However, blue phosphorescent emitters have limited operational lifetime. Therefore, ofter “hybrid-white” solutions are investigated, using fluorescent blue emitters. It is usually assumed that the fraction of (radiative) singlet excitons formed is then only 25%, the quantum-statistical limit. However, this is actually an issue of intense debate, in particular for polymers. In AEVIOM, **a method from which the singlet fraction can be deduced has been refined.** A combination of forward electroluminescence (EL) and reverse photoluminescence measurements is used, as proposed earlier, and the approach is improved by including the (important) effect of the different light-outcoupling efficiencies in both experiments. For PF-TAA, this has resulted in a measured singlet fraction in the range 10-25% [14]. An independent study for the same material, based on a combination of electrical modelling and EL measurements, also carried out in AEVIOM, led to 22% [22].

1.3.6. OLED device studies and applications to white OLEDs

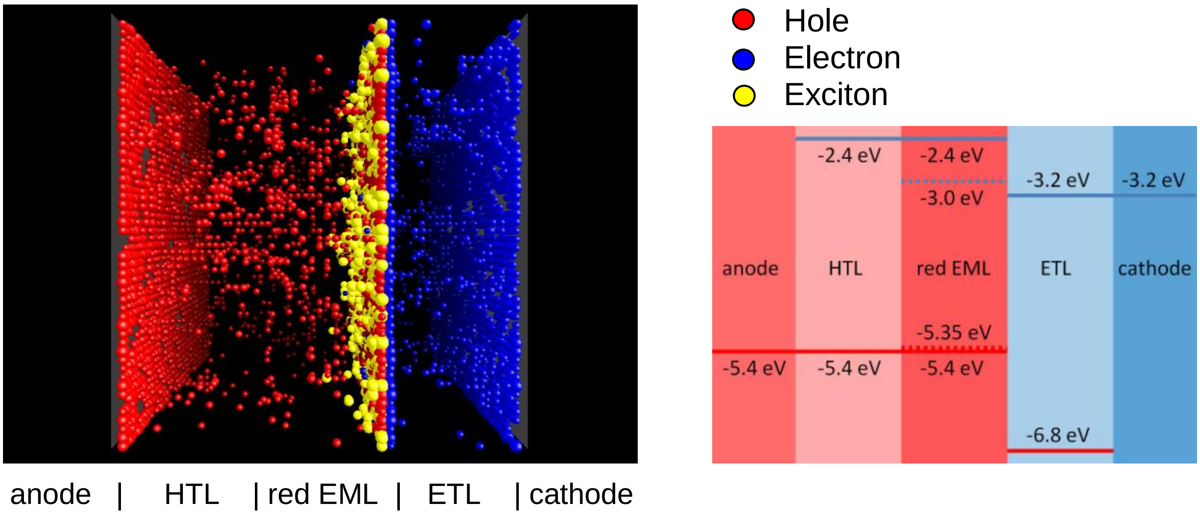
For the first time **predictive EGDM single-layer OLED modelling was demonstrated,** by carrying out a study of blue-emitting PF-TAA based OLEDs [22]. For a wide range of temperatures, the current density was found to be in excellent agreement with the current density expected from the seperately determined electron and hole mobility functions, and a distinct maximum in the current efficiency as a function of the voltage was predicted quite accurately and explained as an effect of a voltage dependent emission zone. This study also led to a quantitative determination of the singlet fraction, as mentioned already above.

The polymer PF-TAA is an example of a wide class of polyfluorene and polybispirofluorene based green and blue emitting polymers within which the hole transport is optimized by the copolymerization of amine-based hole-transporting units (HTUs). A study within which two different types of such blue-emitting HTUs was used, with different contributions to the hole mobility, randomly dispersed, and for a wide range of concentrations of both units, showed that it is possible optimize the voltage dependence of the current efficiency such that it is optimal at a certain chosen value as required for a certain application [19]. **Tuning the material composition in order to optimize the efficiency was thus demonstrated.** Modelling using the EGDM, making use of the same methodology as used in ref. 21, was found to provide excellent understanding of the observed trends in the voltage and composition dependence of the efficiency.

Applications of EGDM and ECDM modelling to multilayer OLED modelling, the development of a predictive white-OLED simulation tool and its application to the efficiency, lifetime and color stability have been the subject of AEVIOM-studies which have not yet been made public. Good progress has been shown in internal reports. This collaborative work continues even after the end of AEVIOM. Two elements of this work have already been presented. Firstly, the functioning of **ambipolar (electron *and* hole conducting) interlayers**, used to separate in hybrid white OLEDs the fluorescent blue and (e.g.) green or yellow phosphorescent layers, was intensively studied experimentally for the case of 1:1 α-NPD/BAlq systems [3]. Secondly, a demonstration of the progress made on 3D trilayer OLED device modelling, which shows already much of the advances made, has been given in the form of a **video publicly available on YouTube**:
http://www.youtube.com/watch?v=HVmQtyTOjWQ . An explanation of what is shown in this video is included in the box below.

Progress on OLED simulation has been presented in ref. 27, a view on the **applicability of various options for OLED stacks** (hybrid white versus all-phosphorescent, e.g.) and results of experimental studies of such OLEDs have been given in ref. 28. And a view on the **development of OLED technology for lighting applications** has been given in ref. 31.

In 3D modelling of charge transport in OLED materials either a Master Equation (ME) is solved for the average occupational probabilities of the sites in the presence of an electric field or a direct Monte-Carlo (MC) simulation is performed for the motion of the charge carriers. **It has been established within AEVIOM that Monte Carlo simulations are possible for complete multilayer OLEDs**, including injection by electrodes, all effects of Coulomb interactions (image-charge effects, space-charge effects, short-range attractions or repulsions), organic-organic interfaces, and traps.



The figure gives an example of the results of an AEVIOM Monte Carlo study for a three-layer OLED with a red dye in the middle, emissive, layer. The OLED consists of three 10 nm thick organic layers with the indicated energy-level diagram. The left (right) layer is the hole- (electron-) transporting layer. The middle emissive layer contains 10% of red emitting dye molecules (energy levels indicated by the dots). The size of the spheres indicates the time-averaged occupation of a site by a hole (red), an electron (blue), or the number of recombination events that has occurred at that site (yellow). Because of the specific choice of HOMO and LUMO energies, hole and electrons predominantly meet at the interface between the emissive and electron-conducting layer. A cubic site lattice was used, with a 1 nm lattice constant and spatially correlated energetic disorder. For a movie of this simulation, see http://www.youtube.com/watch?v=HVmQtyTOjWQ (F.W.A. van Oost and P.A. Bobbert, Eindhoven University of Technology).

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1.4 Potential impact and main dissemination activities and exploitation results

In section 1.3, the scientific and technical advances made by AEVIOM have been highlighted. Much scientific impact was created, by 31 papers (published or accepted) in peer-reviewed high-quality international journals. Furthermore, the work has been disseminated via more than 90 other channels (oral and poster presentations at conferences, in workshops, at exhibitions, websites, digests). A large number of additional publications is expected.

Commercial OLED simulation PC-software containing much of the AEVIOM second-generation modelling has recently become available from Fluxim (SETFOS3.2-software, March 2011), and will become available from sim4tec in the first half of 2011 (SimOLED-software). Figure 1.5 shows as an example a screen picture of the Fluxim software. Philips expects that this will contribute to the rational, timely and efficient development of advanced OLED device structures with breakthrough performance.

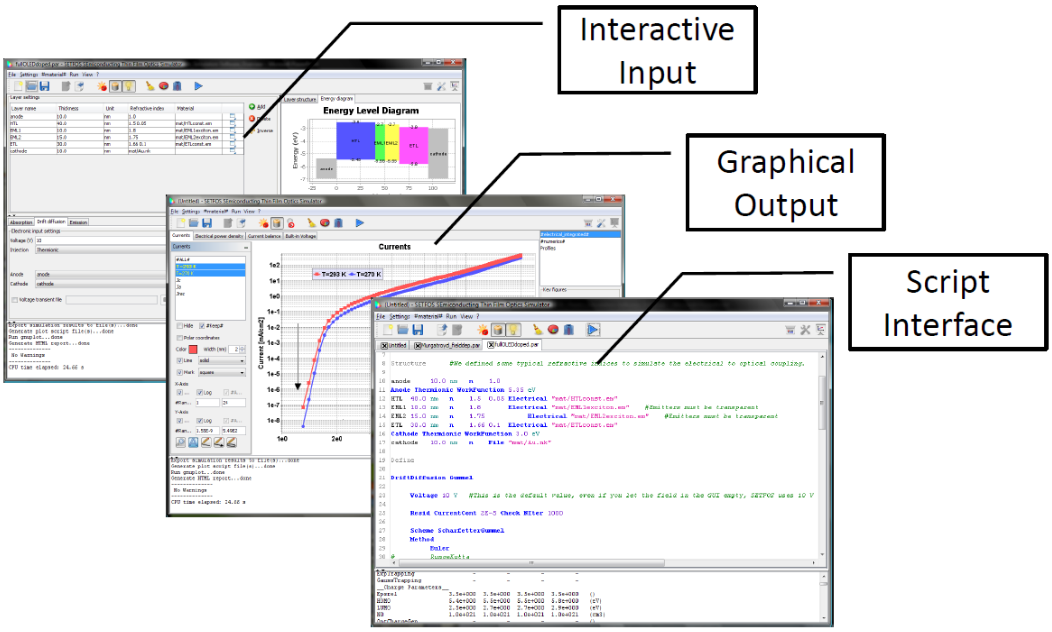

Figure 1.5
Screenshots of the versatile simulation software SETFOS, commercialized by Fluxim, showing three different views for input, output and advanced scripting.

Awards
In November 2009, recognition for the relevance and impact of AEVIOM was obtained by the granting of the yearly **NanoNed Innovation Award (2009)** to dr. Siebe van Mensfoort (PRE and EUT) for his contributions to the development of OLED device modelling and his collaboration within AEVIOM with Fluxim, leading to SETFOS3.0 containing for the first time EGDM modelling: http://w3.tue.nl/nl/nieuws/artikel/?tx_ttnews[tt_news]=8755&tx_ttnews[backPid]=55392&cHash=bfef73d252
This generated much publicity (e.g. coverage on approximately 30 websites, etc.), in which the collaboration with Fluxim was in most cases explictly mentioned. NanoNed is a Dutch public-private partnership program (2005-2011) on nanotechnologies.

In June 2010, dr. Siebe van Mensfoort obtained for his PhD thesis research on OLED device modelling the **third DSM Science and Technology Award**, an international (North-Germany, Belgium, The Netherlands) award in recognition of “outstanding young researchers (PhD students

and those who have recently obtained their PhD) who are conducting innovative research with clear potential for practical applications”:
http://www.dsm.com/en_US/html/da/Winners_North_2010.htm
See figure 1.6.

Figure 1.6.
Dr Siebe van Mensfoort (right) among the winners of the DSM Science and Technology Award 2010, handed over by the DSM Chief Innovation Officer dr. Rob van Leen (one-but-right).

Press-release
In March 2010, Philips issued a press release under the title **“Philips novel method accelerates progress in OLED lighting efficiency”**, after the publication of the article “*Measuring the shape of the emission profile in organic light-emitting diodes with nanometre resolution”* in Nature Photonics” (first authors S.L.M van Mensfoort and M. Carvelli, ref. 1 in section 1.3):
http://www.newscenter.philips.com/main/research/news/press/2010/100315-oled.wpd ,
In this press release the support of the AEVIOM project was explicitly mentioned.

1.5 Project public website and contact details beneficiaries

The project public website is www.aeviom.eu .

The project logo is shown in the figure below.

The project beneficiaries and their contact details are included in the table. The AEVIOM website includes links to the institute or company websites.

Partner	**Contact names**
Philips Research Laboratories Eindhoven	prof. dr. R. Coehoorn (project leader) reinder.coehoorn@philips.com
Technische Universität Dresden	prof. dr. K. Leo leo@iapp.de
Sim4tec	dr. R. Nitsche robert.nitsche@sim4tec.com
University of Cambridge	prof. dr. N. Greenham ncg11@cam.ac.uk
Zurich University of Applied Sciences	prof. dr. B. Ruhstaller ruhb@zhaw.ch
FLUXiM	prof. dr. B. Ruhstaller ruhb@zhaw.ch
University of Groningen	prof. dr. P.W.M. Blom p.w.m.blom@rug.nl
Eindhoven University of Technology	dr. P.A. Bobbert p.a.bobbert@tue.nl
Philips Research Laboratories Aachen	dr. H.P. Loebl hans-peter.loebl@philips.com

Figure 1.6
AEVIOM project logo.

2 Use and dissemination of foreground

The project has so far resulted in **31 published or accepted papers** (including one book chapter), and one submitted paper (approved by the other project members). An overview is given in table 2.1, sorted according to the journal impact factor. The highest impact factor publications have appeared in Nature Photonics (1), Physical Review Letters (1), Applied Physics Letters (3) and Physical Review B (10).

In addition, dissemination has taken place in the form of **89 oral or poster presentations** at conferences, workshops etc. An overview is given in table 2.2, sorted chronologically. The audience addressed was in most cases scientific or industrial. In a few talks also the wider public was addressed. The AEVIOM results have furthermore been disseminated via the public website www.aeviom.eu and via a publication in the EU Photonics Newsletter.

Important channels for disseminating our results are not only the scientific papers or scientific talks at conferences, but also the **workshops and conference exhibition booths** at which the SMEs Fluxim and Sim4tec have been in contact with their customers. Figures 2.1 and 2.2 give an impression.

Figure 2.1
(Left) sim4tec booth at Plastic Electronics Conference and Exhibition 2010 (Dresden Germany); (right): entrance to SID exhibition hall with SimOLED advertising panel.

Figure 2.2
(Left) Participants of the ISW'10 workshop organized by Fluxim and ZUAS in Winterthur in July 2010. (Right) Hands-on simulation exercises at the ISW'10.

Table 2.1. *List of scientific (peer reviewed) publications, sorted in journal impact factor (hightest impact factor first).*

No.	Title	Main author	Title of the periodical or the series	Number, date or frequency	Publisher	Place of publication	Year of publication	Relevant pages	Permanent identifiers (if available)	Is/Will open access provided to this publication?
1	*Measuring the shape of the emission profile in organic light-emitting diodes with nanometre resolution*	S. L. M. van Mensfoort	Nature Photonics	4	Nature Publ. Group		2010	329	10.1038/nphoton. 2010.32	NO
2	*Determination of injection barriers in organic semiconductor devices from capacitance measurements,*	S.L.M. van Mensfoort	Phys. Rev. Lett.	100	APS		*2008*	086802	10.1103/PhysRevLett. 100.086802	YES
3	*Balanced ambipolar charge carrier mobility in mixed layers for application in hybrid white organic light-emitting diodes*	Gregor Schwartz	Appl. Phys. Lett.	93	AIP		2008	073304	10.1063/1.2973151	YES
4	*Analysis of hole transport in a poly-fluorene based co-polymer - evidence for the absence of correlated disorder*	R.J. de Vries	Appl. Phys. Lett	94	AIP		2009	163307	10.1063/1.3119317	YES
5	*Single carrier devices with electrical doped layers for the characterization of charge-carrier transport in organic thin-films*	Matthias Schober	Appl. Phys. Lett.	97	AIP		2010	013303	10.1063/1.3460528	YES
6	*Effect of Gaussian disorder on the voltage dependence of the current density in sandwich-type devices based on organic semiconductors,*	S.L.M. van Mensfoort	Phys. Rev. B	78	APS		2008	085207	10.1103/PhysRevB. 78.085207	NO
7	*Hole transport in polyfluorene-based sandwich-type devices: quantitative analysis of the role of energetic disorder*	S.L.M. van Mensfoort	Phys. Rev. B	78	APS		2008	085208	10.1103/PhysRevB. 78.085208	NO
8	*Modeling and analysis of the three-dimensional current density in sandwich-type single-carrier devices of disordered organic semiconductors*	J.J.M. van der Holst	Phys. Rev. B	79	APS		2009	085203	10.1103/PhysRevB. 79.085203	NO

9	*Electron transport in polyfluorene-based sandwich-type devices: quantitative analysis if the effects of disorder and electron traps*	S.L.M. van Mensfoort	Phys. Rev. B.	80	APS		2009	033202	10.1103/PhysRevB. 78.085208	NO
10	*Effects of disorder on the current density and recombination profile in single layer and multilayer organic light-emitting diodes*	R. Coehoorn	Phys. Rev. B.	80	APS		2009	085302	10.1103/PhysRevB. 80.085302	NO
11	*Electron-hole recombination in disordered organic semiconductors: Validity of the Langevin formula*	J. J. M. van der Holst	Phys. Rev. B	80	APS		2009	235202	10.1103/PhysRevB. 80.235202	NO
12	*Relation between the built-in voltage in organic light-emitting diodes and the zero-field voltage as measured by electro-absorption*	R. J. de Vries	Phys. Rev. B	81	APS		2010	125203	10.1103/PhysRevB. 81.125203	NO
13	*Field-induced detrapping in disordered organic semiconducting host-guest systems*	J. Cottaar,	Phys. Rev. B	82	APS		2010	205202	10.1103/PhysRevB. 82.205203	NO
14	*Determination of the exciton singlet-triplet ratio in single layer organic light-emitting diodes*	M. Carvelli	Phys. Rev. B	83	APS		2011	075203	10.1103/PhysRevB. 83.075203	NO
15	*Monte-Carlo study of charge transport in organic sandwich-type single-carrier devices: effects of Coulomb interactions*	J.J.M. van der Holst	Phys. Rev. B	83	APS		2011	085206	10.1103/PhysRevB. 83.085206	NO
16	*Analysis of the emission profile in organic light-emitting devices*	B. Perucco	Optics Express	18			2010	pp. A246-A260	10.1364/OE. 18.00A246	YES
17	*Carrier density and field dependent charge-carrier mobility in organic semiconductors with correlated Gaussian disorder*	M. Bouhassoune	Organic Electronics		Elsevier		2009	437-445	10.1016/j.orgel. 2009.01.005	NO
18	*Electron transport in the organic small molecule material BAlq - the role of correlated disorder and traps*	S. L. M. van Mensfoort	Organic Electronics	11	Elsevier		2010	1408	10.1016/j.orgel. 2010.05.014	NO
19	*Tuning the voltage dependence of the efficiency of blue organic light-emitting diodes based on fluorene–amine copolymers*	S. Harkema	Organic Electronics	11	Elsevier		2010	755	10.1016/j.orgel. 2010.01.015	NO
20	*Hole transport in the organic small molecule material α-NPD - evidence for the presence of correlated disorder*	S. L. M. van Mensfoort	J. Appl. Phys.	107	AIP		2010	113710	10.1063/1.3407561	NO

21	*Numerical simulation of charge transport in disordered organic semiconductor devices*	E. Knapp	J. Appl. Phys	108	AIP		2010	054504	10.1063/1.3475505	NO
22	*Predictive modeling of the current density and radiative recombination in blue polymer-based light-emitting diodes*	S. L. M. van Mensfoort,	J. Appl. Phys. (accepted)		AIP		2011			NO
23	*Charge transport in disordered organic host-guest systems: effects of carrier density and electric field,.*	Y.Y. Yimer	J. Phys. Cond. Matt.	20			2008	335204	10.1088/0953-8984/20/33/335204	NO
24	*Charge transport in disordered organic host–guest systems: Effects of carrier density and electric field*	Y.Y. Yimer	Synth. Met.	159	Elsevier		2009	2399	10.1088/0953-8984/20/33/335204	NO
25	*Numerical Analysis of Steady-State and Transient Charge Transport in Organic Semiconductor Devices*	E. Knapp	Optical and Quantum Electronics (accepted)				2011		10.1007/s11082-011-9443-1	YES
26	*Numerical analysis of exciton dynamics in organic light-emitting devices and solar cells*	D. Rezzonico	J. Photon. Energy	1			2011	011005	10.1117/1.3523314	YES
27	*Comprehensive simulation of light-emitting and light-harvesting organic devices*	B. Ruhstaller	Proc. of the SPIE Conference	Vol. 7051	SPIE		2008		10.1117/12.802447	NO
28	*White OLEDs for lighting applications*	Peter Loebl	Proceedings of SPIE, Photonic Devices and Applications,	Vol. 7415,	SPIE		2009	74151A-1	10.1117/12.828574	NO
29	*The influence of the optical environment on the emission profile and methods of its determination*	B. Perucco	Proc. SPIE	7722	SPIE		2010	14	10.1117/12.853989	NO
30	*Analysis of Exciton Distributions in OLEDs: The Influence of Optical Modes and Energetic Disorder*	B. Ruhstaller	SID Proceedings	P-198	SID		2010	P-198		NO
31	*High efficiency OLEDs for Lighting applications - completing the Solid State Lighting portfolio*	C. Verschuren	Book chapter (accepted)		Springer		2011			NO
32	*Differentiation of interface and bulk contributions to the limitation of charge-carrier transport in organic thin-film devices*	M. Schober	(submitted)							NO

Table 2.2. *List of other dissemination activities.*

No.	Type of activities	Main leader	Title	Date	Place	Type of audience
1	FOM-Physics Veldhoven-2008 Conference	S.L.M. van Mensfoort	New light on recombination in OLEDs - the role of disorder	23/01/2008	Veldhoven, NL	Scientific
2	DPG conference, Berlin, Germany	R. Nitsche	Advanced modeling of optoelectronic characteristics of OLEDs	26/02/2008	Berlin	Scientific
3	SPIE-Europe Conference, Strasbourg	R. Coehoorn	Towards an experimentally validated second generation OLED model **(invited)**	09/04/2008	Strasbourg	Scientific
4	Printed Electronics Conference,	R. Nitsche	Electrical and Optical Simulation of OLED Devices	09/04/2008	Dresden, Germany	Scientific, Industry
5	Studium Generale, Eindhoven University of Technology	R. Coehoorn	Light from organic semiconductors	07/05/2008	Eindhoven	Scientific, Civil Society
6	SID2008	R. Nitsche	Combined electrical and optical simulation of OLED devices	21/05/2008	Los Angeles, USA	Scientific, Industry
7	Royal Netherlands Academy of Sciences (KNAW), Amsterdam	R. Coehoorn	Light from organic semiconductors - nanoscience for the development of a novel light source	26/05/2008	Amsterdam	Scientific, Civil Society
8	International Krutyn Summer School (OLLA)	R. Nitsche	Workshop on OLED simulation	28/05/2008	Krutyn, Poland	Scientific
9	International Krutyn Summer School (OLLA),	E. Huber	Mobility models for OLED device simulation	28/05/2008	Krutyn, Poland	Scientific
10	International Krutyn Summer School	M. Schober	Simulation of electrical OLED behavior	30/05/2008	Krutyn, Poland	Scientific
11	University of Cambridge	R. Coehoorn	Towards a second generation OLED model **(invited)**	10/06/2008	Cambridge, UK	Scientific
12	1st International User Workshop 2008	D. Rezzonico	Simulation of light-emitting and light-harvesting organic devices	7-8/8/2008	Winterthur, Switzerland	Scientific, Industry
13	SPIE Optics & Photonics Conference,	B. Ruhstaller	Comprehensive simulation of light-emitting and light-harvesting organic devices (Invited)	10/8/2008	San Diego, USA	Scientific, Industry
14	7th Int. Conf. on electroluminescence of molecular materials and related phenomena (ICEL-7)	P.A. Bobbert	Advanced modeling of charge transport in OLEDs	05/09/2008	Dresden	Scientific

15	International Conference on Electroluminescence ICEL-7, Dresden, Germany	R. Nitsche	Combined electrical and optical simulation of OLED devices	05/09/2008	Dresden	Scientific
16	International Conference on Electroluminescence ICEL-7, Dresden, Germany	R. Nitsche	Workshop on OLED simulation	06/09/2008	Dresden	Scientific
17	BASF Ludwigshafen	P.A. Bobbert	Advanced modeling of charge transport in OLEDs **(invited)**	11/09/2008	Ludwigshafen	Scientific, Industry
18	Organic Semiconductor Conference 2008, Frankfurt, Germany	D. Rezzonico	Comprehensive simulation of light-emitting and light-harvesting organic devices **(invited)**	29/9/2008	Frankfurt	Scientific, Industry
19	Workshop on OLED and OPV simulation	D. Rezzonico		14/10/2008	Taipeh, Taiwan	Scientific, Industry
20	Workshop on OLED and OPV simulation	D. Rezzonico		16/10/2008	Seoul, Korea	Scientific, Industry
21	International Conference on Vacuum Technology (Gent)	K. Leo	Highly Efficient Organic Devices	18/11/2008	Gent (B)	Scientific
22	Fall Meeting Materials Research Society (Boston)	R. Coehoorn	Towards a second generation OLED model **(invited)**	03/12/2008	Boston (US)	Scientific
23	Organic and Large Area Electronics Cluster Meeting	R. Coehoorn	The AEVIOM project	13/01/2009	Brussels (B)	Scientific, Industry
23	Physics@FOM Veldhoven, The Netherlands	J.J.M. v.d. Holst	Advanced modeling of electronic processes in OLEDs	21-22/01/2009	Veldhoven (NL)	Scientific
24	DPG Tagung, Dresden, Germany	D. Rezzonico	(Exhibition booth)	25/03/2009	Dresden	Scientific
25	DPG Frühjahrstagung, Dresden, Germany	R. Nitsche	Optical Modelling of Organic Light Emitting Diodes	25/03/2009	Dresden	Scientific
26	DPG Tagung, Dresden, Germany	Evelyne Knapp	Advanced Simulation Methods for Charge Transport in OLEDs	25/03/2009	Dresden	Scientific
27	NanoDay 2009, Lyngby, Denmark	P.A. Bobbert	Advanced Modeling of Electronic Processes in OLEDs	06/05/2009	Lyngby	Scientific
28	Eindhoven University of Technology (Symposium Future Challenges of Organic Electronics)	R.J. de Vries	Towards a predictive model for small-molecule multilayer OLEDs	12/05/2009	Eindhoven	Scientific
29	Eindhoven Univ. of Techn. (Symposium Future Challenges of Organic Electronics)	M. Carvelli	Measuring the light emission profile in OLEDs	12/05/2009	Eindhoven	Scientific
30	University Duisburg / Essen Germany	Peter Loebl	White OLEDs	28/05/2009	Duisburg	Scientific
31	SID 2009,	R. Nitsche	Presentation booth at exhibition area	31/05 – 05/06/2009	San Antonio, USA	Scientific, Industry
32	OLED100 Summer School	R. Coehoorn	The development of an experimentally validated OLED device model	04/06/2009	Krutyn (Poland)	Scientific
33	International Krutyn Summer School	A. Elsner	Modeling of optoelectronic characteristics of OLEDs	06/06/2009	Krutyn, Poland	Scientific
34	ICOE2010, Liverpool	J.J.M. v.d. Holst	Modelling of transport and injection in single-carrier devices of disordered organic semiconductors	15/06/2009	Liverpool (UK)	Scientific

35	Leiden University (Symposium 100th anniversary birthday prof. H.B.G. Casimir)	R. Coehoorn	Light from organic semiconductors	26/06/2009	Leiden (NL)	Scientific, Civil Society
36	Fluxim International User Workshop	D. Rezzonico	Several sessions on optical and electronic device simulation	30/6 & 1/7/2009	Winterthur (CH)	Scientific, Industry
37	SPIE Annual Meeting	Peter Loebl	White OLEDs for lighting applications.	04/08/2009	San Diego (US)	Scientific, Industry
38	BASF	R. Coehoorn	Effects of disorder on the current density and recombination in OLEDs based on polymer and small-molecule organic semiconductors	7/08/2009	Ludwigshafen	Scientific, Industry
39	BASF	R.J. de Vries	Towards a full understanding of the charge transport in white OLEDs - The role of correlations	17/08/2009	Ludwigshafen (D)	Scientific, Industry
40	Pro*Doc Workshop	Evelyne Knapp	Charge Transport in OLEDs	18/08/2009	Disentis (CH)	Scientific
41	ECME Conference Copenhagen	M. Carvelli	The role of outcoupling efficiency on the experimental determination of the exciton singlet : triplet ratio in OLEDs	09/09/2009	Copenhagen (DK)	Scientific
42	ECME Conference Copenhagen	R.J. de Vries	Determination of the presence of correlatated disorder in organic semiconductors	09/09/2009	Copenhagen (DK)	Scientific
43	ECME Conference Copenhagen	J.J.M. van der Holst	Modeling of transport and injection in single-carrier devices of disordered organic semiconductors	09/09/2009	Copenhagen (DK)	Scientific
44	Printed Electronics Asia, Tokyo, Japan	D. Rezzonico	Design of Multilayer Solar Cells and Light-Emitting Devices	30/9 & 1/10/2009	Tokyo (Japan)	Scientific, Industry
45	OSC 2009, London, UK	R. Nitsche	Optimization of OLED performance by optical modelling	30/09/2009	London (UK)	Scientific, Industry
46	IMID 2009, Seoul, Korea	R. Nitsche	Optimization of OLED performance by optical modelling; Workshops on OLED simulation (Japan, Korea)	14/10/2009	Seoul (S. Korea)	Scientific, Industry
47	Setfos New Version Release Seminar	D. Rezzonico	Setfos	29/10/2009	Tokyo, Japan	Scientific, Industry
	Plastic Electronics Europe, Dresden, Germany	R. Nitsche	Optimization of OLED performance by optical modelling; presentation, booth at exhibition area	29-30/10/2009	Dresden (D)	Scientific, Industry
48	OTEC, Inha University, Incheaon, South Korea	Daniele Rezzonico	OLED Simulation with Setfos 3	3/11/2009	Incheaon (S. Korea)	Scientific
49	MicroNano Conference Delft	J.J.M. van der Holst	Advanced modeling of organic light-emitting diodes	05/11/2009	Delft (NL)	Scientific
50	Seoul National University	Daniele Rezzonico	Design of Multilayer Solar Cells and Light-Emitting Devices	1/12/2009	Seoul (S. Korea)	Scientific
51	Physics@FOM2010 conference	J.J.M. van der Holst	Electron-hole recombination in disordered organic semiconductors: Validity of the Langevin formula	22-23/01/2010	Veldhoven, The Netherlands	Scientific
52	Physics@FOM2010 conference	F.W.A. van Oost	Advanced modeling of organic light-emitting diodes	22-23/01/2010	Veldhoven, The Netherlands	Scientific
53	CECAM Workshop	E. Knapp	Simulation of Charge Transport in Organic Semiconductor Devices	01/02/2011	Lausanne	Scientific

54	Dutch Scientific meeting on Chemistry related to Physics & Material Sciences	P.A. Bobbert	Field-induced detrapping: electric-field dependence of the charge-carrier mobility in host-guest systems	16/02/2010	Veldhoven, The Netherlands	Scientific
55	SPIE-Europe Conference	R.J. de Vries	Investigation of the presence of correlated disorder in organic semiconductors	09/04/2010	Brussels	Scientific, Industry
56	SPIE-Europe Conference	M. Schober	Single carrier devices with electrical doped layers	09/04/2010	Brussels	Scientific, Industry
57	SPIE-Europe Conference	M. Carvelli	Determination of the light emission profile in small molecule based double layer OLEDs	09/04/2010	Brussels	Scientific, Industry
58	SPIE-Europe Conference	P.A. Bobbert	Advanced modeling of charge transport and recombination in organic light-emitting diodes	09/04/2010	Brussels	Scientific, Industry
59	SPIE-Europe Conference	B. Perucco	The influence of the optical environment and energetic disorder on the shape of emission zones in OLEDs and methods of their determination	12/4/2010	Brussels	Scientific, Industry
60	Printed Electronics Europe	R. Nitsche	Numerical simulation software for organic electronics	12/4/2010	Dresden, Germany	Scientific, Industry
61	Int. Symp. Functional π-electron systems, Atlanta	J.J.M. van der Holst	Advanced modeling of charge injection, transport, and recombination in organic light-emitting diodes	23-28/05/2010	Atlanta (US)	Scientific
62	Int. Symp. Functional π-electron systems, Atlanta	F.W.A. van Oost	Monte-Carlo modeling of organic light-emitting diodes	23-28/05/2010	Atlanta (US)	Scientific
63	Int. Symp. Functional π-electron systems,	J. Cottaar	Field-induced detrapping: electric field dependence of charge-carrier mobility in host-guest systems	23-28/05/2010	Atlanta	Scientific
64	SID Symposium,	M. Lu	Exciton Distributions in OLEDs: Influence of Optical Modes and Energetic Disorder	25/5/2010	Seattle, USA	Scientific, Industry
65	Society for Information Displays	P.Loebl	OLEDs for lighting applications	27/05/2010	Seattle	Scientific, Ind.
66	LOPE-C	D. Rezzonico	Design of Multilayer Organic Solar Cells and Light emitting Devices	31/5/2010	Frankfurt	Scientific, Industry
67	OLED100 Summerschool	P.Loebl	White OLEDs for lighting	06/06/2010	Krutyn, Poland	Scientific
68	SOLED Optics and Photonics Congress	E. Knapp	Impedance Analysis of Organic Light-Emitting Devices with Disorder	22/06/2010	Karlsruhe	Scientific, Industry
69	SOLED Optics and Photonics Congress	B. Perucco	The influence of the optical environment and energetic disorder on the shape of emission zones in OLEDs and methods of their determination	22/6/2010	Karlsruhe	Scientific, Industry
70	SLN/Opera Optoelectronics Meeting	B. Ruhstaller	Simulation Software for Organic Electronics	25/6/2010	Basel	Scientific, Industry
71	SETFOS Workshop	R. Coehoorn	Second generation OLED device modelling: from supercomputer studies to industrial applications	30/06/2010	Winterthur	Scientific, Industry
72	SETFOS Workshop	M. Carvelli	Determination of the light emission profile in small-molecule-based double-layer OLEDs	30/06/2010	Winterthur	Scientific, Industry
73	Center for NanoMaterials Research Day	J. Cottaar	Field-induced detrapping: electric-field dependence of charge-carrier mobility in host-guest systems	30/06/2010	Eindhoven	Scientific
74	Center for NanoMaterials Research Day	J.J.M. van der Holst	Electron-hole recombination in disordered organic semiconductors: validity of the Langevin formula	30/06/2010	Eindhoven	Scientific

75	12th Int. Symposium on Light Sources and White LED – 3 Conference	M. Carvelli	Spatial resolution of the light-emission profile in single-layer organic light-emitting diodes	12/07/2010	Eindhoven	Scientific, Industry
76	12th Int. Symposium on Light Sources and White LED – 3 Conference	R. Coehoorn	Towards a predictive model for organic light-emitting diodes: current density, recombination and light emission	12/07/2010	Eindhoven	Scientific, Industry
77	12th Int. Symposium on Light Sources and White LED – 3 Conference	R.J. de Vries	Novel insights in the electron and hole mobility in organic semiconductors used in OLEDs for lighting applications	12/07/2010	Eindhoven	Scientific, Industry
78	SPIE Optics + Photonics	D. Rezzonico	Numerical analysis of exciton dynamics in organic light-emitting devices and solar cells	2/8/2010	San Diego, USA	Scientific, Industry
79	NUSOD	E. Knapp	Numerical Analysis of Steady-State and Transient Charge Transport in Organic Semiconductor Devices	07/09/2010	Atlanta, USA	Scientific
80	HOPV Workshop,	B. Ruhstaller	Advanced simulation of OLEDs and organic solar cells	5/10/2010	Castello, Spain	Scientific, Industry
81	IMID	R. Nitsche	Tuning OLED performance by numerical simulations	13/10/2010	Kintex, Korea	Scientific, Industry
82	Plastic Electronics Conference	R. Nitsche	Predictive OLED simulation – just a dream?	19/10/2010	Dresden, Germany	Scientific, Industry
83	Int. Conf. on Electroluminescence	R. Coehoorn	Effects of charge-carrier relaxation on the transient mobility in organic semiconducting devices – modelling and experiment	19/10/2010	Ann Arbor, US	Scientific
84	Int. Conf. on Electroluminescence	M. Carvelli	Determining the light emission profile near the organic-organic interface in small-molecule-based double-layer OLEDs	20/10/2010	Ann Arbor, US	Scientific
85	Int. Conf. on Electroluminescence	R.J. de Vries	Relation between the built-in voltage in organic light-emitting diodes and the zero-field voltage as measured by electroabsorption	20/10/2010	Ann Arbor, US	Scientific
86	Int. Conf. on Electroluminescence	P.A. Bobbert	Advanced modeling of charge injection, transport, and recombination in organic light-emitting diodes	20/10/2010	Ann Arbor, US	Scientific
87	Physics@FOM2011 conference	M. Carvelli	Determining the light emission profile near the organic-organic interface in small-molecule-based double-layer OLEDs	18/01/2011	Veldhoven, The Netherlands	Scientific
88	Physics@FOM2011 conference	R.J. de Vries	Method for an accurate extraction of materials parameters that determine the mobility in OLEDs	18/01/2011	Veldhoven, The Netherlands	Scientific
89	Physics@FOM2011 conference	J. Cottaar	Field-induced detrapping: Electric-Field dependence of the charge-carrier mobility in host-guest systems	18/01/2011	Veldhoven, The Netherlands	Scientific
90	website	R. Coehoorn	AEVIOM public website www.aeviom.eu	2008-2011		
91	digest	R. Nitsche	Tuning OLED performance by numerical simulations, IMID/IDMC/ASIA DISPLAY-2010 DIGEST, 42, 295 (2010)	13/10/2010	Kintex, Korea	Scientific, Industrial
91	article	R. Coehoorn	EU Photonics Newsletter	Feb. 2010		
92	youtube movie	P.A. Bobbert	http://www.youtube.com/ watch?v=HVmQtyTOjWQ	Dec. 2010		

The overview in tables 2.1 and 2.2 gives only the present status (15/3/2011). **Many publications based on the AEVIOM results are still in the pipeline.** In Deliverable report D5.2 an overview has been given. This is copied below, in table 2.3.

Table 2.3. Confidential. *Planned publications or other dissemination activities based on AEVIOM (2011).*

PRE

We plan to write journal publications on at least the following subjects:

- "Determining the light-emission profile near the organic-organic interface in small-molecule-based double-layer OLEDs".
- "Method for a fast extraction of parameters which describe the mobility in OLEDs"
- "Spatial resolution of the light-emission profile in single-layer OLEDs"
- "Electron mobility in NET-5 and spiro-DPVBi"
- "Efects of energetic disorder on the low-frequency differential capacitance of organic light-emitting diodes"
- "Modeling of the transient mobility in disordered organic semiconductors".

The progress realized in the AEVIOM project will furthermore be disseminated in an invited book chapter on "second-generation OLED modelling" (ed. W. Bruetting *et al.*), at an OLED100.eu Summerschool (Dresden, May 2011), and at various national and international conferences.

TUD

We plan to write two papers and to give a talk at the MRS-conference in San Francisco (2011). The journals, topics and author listst (expected) are:

- (For Appl. Phys. Lett.) "Differentiation of interface and bulk contributions to the limitation of charge-carrier transport in organic multilayer devices", Matthias Schober, Merve Anderson, Michael Thomschke, Johannes Widmer, Mauro Furno, Reinhard Scholz, Björn Lüssem and Karl Leo.
- (For J. Appl. Phys.) "A quantitative description of hole-transport in a white organic light-emitting diode", Matthias Schober, Merve Anderson, Michael Thomschke, Johannes Widmer, Mauro Furno, Reinhard Scholz, Björn Lüssem and Karl Leo.
- (For MRS, talk) "Characterization of charge transport in organic light-emitting diodes", Matthias Schober, Merve Anderson, Michael Thomschke, Johannes Widmer, Mauro Furno, Reinhard Scholz, Björn Lüssem and Karl Leo.

UCAM

We envisage three eventual papers on the optical probing work:

- Electromodulation spectroscopy of the α-NPD devices and of α-NPD doped with phosphorescent emitters.
- Electromodulation studies of n- and p-type doped organic small molecule materials.
- Analysis of the electromodulation spectra of multilayer OLED structures.

Sim4tec

The planned dissemination activities in 2011 include:

- Conference participation SID 2011, USA.
- Conference participation IMID 2011, Korea.
- Conference participation Plastic Electronics 2011, Dresden.
- Regular customer visits and workshops / trainings at the customer site.

EUT

The planned dissemination activities at EUT in 1011 involve

- Submission of a paper on the effects of Coulomb interaction on charge transport in single-carrier organic devices (submitted on 13/1/2011)

- Writing of a paper on charge transport across organic-organic interfaces and translation to a one-dimensional model
- Writing of a paper on a novel percolation theory for charge transport in organic semiconductors, including the consideration of Marcus-type hopping
- Writing of a paper on recombination in a single-layer OLED; comparison Monte-Carlo results with results of drift-diffusion calculations
- Presentation of AEVIOM results at ECME2011 (European Conference on Molecular Electronics

ZUAS/Fluxim

Results from AEVIOM will be disseminated by ZUAS on different conferences and workshops:

- E. Knapp, B. Ruhstaller, "Simulation of Charge Transport in Organic Semiconductor Devices", CECAM Workshop on First Principles Theory and Modeling in Organic Electronics at EPFL, Lausanne (2011).

Upcoming Publications:

- E. Knapp, B. Ruhstaller, "Impedance Modeling of Organic Semiconductor Devices", manuscript in preparation.
- E. Knapp, B. Ruhstaller, „Numerical Analysis of Steady-State and Transient Charge Transport in Organic Semiconductor Devices“, Optical and Quantum Electronics, accepted for publication.
- B. Ruhstaller, et al, “Advanced Numerical Simulation of Organic Light-emitting Devices”, chapter in INTECH book on Optoelectronic Devices and Properties, in press.
- D. Rezzonico, et al. “Numerical analysis of exciton dynamics in organic light-emitting devices and solar cells”, J. of Photonics for Energy, in press.

Fluxim

Similar to the year 2010, Fluxim again plans to attend several European and international conferences and exhibitions (e.g. E-MRS, LOPE-C, PV Expo etc.). Moreover, an International Simulation Workshop will again be co-organized with the ZUAS in Winterthur for scientific exchange and for training end-users and getting feedback from the community.

University Groningen

Publication planned on transport in blue polymers forming a host-guest system, with hole-transporting units, and on red and green dye-doped systems contained in the AEVIOM stack.

No **patents or trademarks** have resulted from the project (table 2.4). However, much **exploitable foreground knowledge** has been created (table 2.5). In that table, this has been split in two categories: (i) the general models developed and (ii) the simulation-assisted experimental methods and ways of working developed. Subdividing this further here does not seem useful, as the information would quickly become quite technical. The impact is as follows:

- The models developed have had strong scientific impact, as is visible from the large number of publications, but have also created the basis for commercial 2nd generation OLED software tools made available by Fluxim and soon also by sim4tec. The **impact which this will have on industry (including Philips) has been described in deliverable report D5.2**. Briefly: this software will be a necessary tool for rationally and time-effectively developing high-efficiency, long-lifetime and low-cost OLEDs.
- The simulation-assisted experimental methods will be adopted as standard ways of working by the partners, including Philips. Moreover, novel software tools supporting their use are expected to be developed by the SMEs in the coming years, so that **AEVIOM has created novel opportunities for their differentiation and growth.**

Table 2.4. *List of applications for patents, trademarks, registered designs etc.*

Type of IP Rights:	Confidential Click on YES/NO	Foreseen embargo date dd/mm/yyyy	Application reference(s) (e.g. EP123456)	Subject or title of application	Applicant (s) (as on the application)
-	-	-	-	-	-

Table 2.5. *Overview of exploitable foreground knowledge created in AEVIOM.*

Type of Exploitable Foreground	Description of exploitable foreground	Confidential Click on YES/NO	Foreseen embargo date dd/mm/yyyy	Exploitable product(s) or measure(s)	Sector(s) of application	Timetable, commercial or any other use	Patents or other IPR exploitation (licences)	Owner & Other Beneficiary(s) involved
General advancement of knowledge and of software methods	3D-Modelling based understanding of transport and recombination in materials with Gaussian disorder (EGDM, ECDM, trap distributions), translated to fast 1D-models.	NO	-	This is the basis for commercial PC software based on 1D-modelling (Fluxim, sim4tec).	1. Lighting, displays	2009 (first release in 2nd generation OLED modelling: SETFOS software). 2011 (more complete 2nd generation SETFOS3.2 release; 2nd generation sim4tec release).		Knowledge generated from 3D-modeling by partners working in WP1 (EUT, PRE) has been translated to 1D-models used by all partners to experimentally validate OLED models and by the partners in WP3 (ZUAS, Fluxim, sim4tec) to develop fast PC software which forms the basis of commercial OLED software, licensed to industry.
General advancement of knowledge	Various simulation-assisted experimental methods for characterizing OLEDs, including measurement of the emission profile, injection barriers, built-in voltage, internal field, single-fraction, relaxation effects, parameter extraction).	NO	-	Potential new elements of commercial software (Fluxim, sim4tec)	1. Lighting, displays	…..		Knowledge generated in all work packages by all AEVIOM partners.

3 Report on societal implications

Replies to the following questions will assist the Commission to obtain statistics and indicators on societal and socio-economic issues addressed by projects. The questions are arranged in a number of key themes. As well as producing certain statistics, the replies will also help identify those projects that have shown a real engagement with wider societal issues, and thereby identify interesting approaches to these issues and best practices. The replies for individual projects will not be made public.

A General Information *(completed automatically when **Grant Agreement number** is entered.*

Grant Agreement Number:	213708
Title of Project:	AEVIOM
Name and Title of Coordinator:	Prof. dr. R. Coehoorn

B Ethics

1. Did your project undergo an Ethics Review (and/or Screening)? • If Yes: have you described the progress of compliance with the relevant Ethics Review/Screening Requirements in the frame of the periodic/final project reports? Special Reminder: the progress of compliance with the Ethics Review/Screening Requirements should be described in the Period/Final Project Reports under the Section 3.2.2 *'Work Progress and Achievements'*	***No***
2. Please indicate whether your project involved any of the following issues (tick box) :	
RESEARCH ON HUMANS	
• Did the project involve children?	
• Did the project involve patients?	
• Did the project involve persons not able to give consent?	
• Did the project involve adult healthy volunteers?	
• Did the project involve Human genetic material?	
• Did the project involve Human biological samples?	
• Did the project involve Human data collection?	
RESEARCH ON HUMAN EMBRYO/FOETUS	
• Did the project involve Human Embryos?	
• Did the project involve Human Foetal Tissue / Cells?	
• Did the project involve Human Embryonic Stem Cells (hESCs)?	
• Did the project on human Embryonic Stem Cells involve cells in culture?	
• Did the project on human Embryonic Stem Cells involve the derivation of cells from Embryos?	
PRIVACY	
• Did the project involve processing of genetic information or personal data (eg. health, sexual lifestyle, ethnicity, political opinion, religious or philosophical conviction)?	
• Did the project involve tracking the location or observation of people?	
RESEARCH ON ANIMALS	
• Did the project involve research on animals?	
• Were those animals transgenic small laboratory animals?	
• Were those animals transgenic farm animals?	

• Were those animals cloned farm animals?	
• Were those animals non-human primates?	
RESEARCH INVOLVING DEVELOPING COUNTRIES	
• Did the project involve the use of local resources (genetic, animal, plant etc)?	
• Was the project of benefit to local community (capacity building, access to healthcare, education etc)?	
DUAL USE	
• Research having direct military use	
• Research having the potential for terrorist abuse	

C Workforce Statistics

3. Workforce statistics for the project: Please indicate in the table below the number of people who worked on the project (on a headcount basis).

Type of Position	Number of Women	Number of Men
Scientific Coordinator	0	1
Work package leaders	0	5
Experienced researchers (i.e. PhD holders)	0	10
PhD Students	1	9
Other	0	0

4. How many additional researchers (in companies and universities) were recruited specifically for this project?	5
Of which, indicate the number of men:	4

D Gender Aspects

5. Did you carry out specific Gender Equality Actions under the project? ○ No

6. Which of the following actions did you carry out and how effective were they?

	Not at all effective				Very effective
❑ Design and implement an equal opportunity policy	x	○	○	○	○
❑ Set targets to achieve a gender balance in the workforce	x	○	○	○	○
❑ Organise conferences and workshops on gender	x	○	○	○	○
❑ Actions to improve work-life balance	x	○	○	○	○
○ Other:					

7. Was there a gender dimension associated with the research content – i.e. wherever people were the focus of the research as, for example, consumers, users, patients or in trials, was the issue of gender considered and addressed?

- ○ Yes- please specify
- x No

E Synergies with Science Education

8. Did your project involve working with students and/or school pupils (e.g. open days, participation in science festivals and events, prizes/competitions or joint projects)?

- ○ Yes- please specify
- x No

9. Did the project generate any science education material (e.g. kits, websites, explanatory booklets, DVDs)?

- x Yes- please specify – public website www.aeviom.eu containing links to published work.
- ○ No

F Interdisciplinarity

10. Which disciplines (see list below) are involved in your project?

- ○ Main discipline[1]: 1.2
- ○ Associated discipline[1]: 1.1
- ○ Associated discipline[1]: 1.3

G Engaging with Civil society and policy makers

11a Did your project engage with societal actors beyond the research community? *(if 'No', go to Question 14)*

- ○ Yes
- x No

11b If yes, did you engage with citizens (citizens' panels / juries) or organised civil society (NGOs, patients' groups etc.)?

- x No
- ○ Yes- in determining what research should be performed
- ○ Yes - in implementing the research
- ○ Yes, in communicating /disseminating / using the results of the project

[1] Insert number from list below (Frascati Manual).

11c	**In doing so, did your project involve actors whose role is mainly to organise the dialogue with citizens and organised civil society (e.g. professional mediator; communication company, science museums)?**	○ ○	n.a.

12. Did you engage with government / public bodies or policy makers (including international organisations)

- x No
- ○ Yes- in framing the research agenda
- ○ Yes - in implementing the research agenda
- ○ Yes, in communicating /disseminating / using the results of the project

13a Will the project generate outputs (expertise or scientific advice) which could be used by policy makers?

- ○ Yes – as a **primary** objective (please indicate areas below- multiple answers possible)
- ○ Yes – as a **secondary** objective (please indicate areas below - multiple answer possible)
- x No

13b If Yes, in which fields?

13c If Yes, at which level? (n.a.)

- ○ Local / regional levels
- ○ National level
- ○ European level
- ○ International level

H Use and dissemination

14. How many Articles were published/accepted for publication in peer-reviewed journals?	**30**
To how many of these is open access[2] provided?	**-**
How many of these are published in open access journals?	**-**
How many of these are published in open repositories?	**-**
To how many of these is open access not provided?	**30**
Please check all applicable reasons for not providing open access:	
x publisher's licensing agreement would not permit publishing in a repository ❑ no suitable repository available ❑ no suitable open access journal available ❑ no funds available to publish in an open access journal ❑ lack of time and resources ❑ lack of information on open access ❑ other[3]: ……………	

15.	**How many new patent applications ('priority filings') have been made?** *("Technologically unique": multiple applications for the same invention in different jurisdictions should be counted as just one application of grant).*	**-**

16. Indicate how many of the following Intellectual	Trademark	**-**

[2] Open Access is defined as free of charge access for anyone via Internet.
[3] For instance: classification for security project.

Property Rights were applied for (give number in each box).	Registered design	-
	Other	-

17. How many spin-off companies were created / are planned as a direct result of the project?	-
Indicate the approximate number of additional jobs in these companies:	-

18. Please indicate whether your project has a potential impact on employment, in comparison with the situation before your project:

x	Increase in employment, or	x	In small & medium-sized enterprises
x	Safeguard employment, or	x	In large companies
❑	Decrease in employment,	❑	None of the above / not relevant to the project
❑	Difficult to estimate / not possible to quantify		

19. For your project partnership please estimate the employment effect resulting directly from your participation in Full Time Equivalent (*FTE = one person working fulltime for a year*) jobs:	*Indicate figure:*
Difficult to estimate / not possible to quantify	x

I Media and Communication to the general public

20. As part of the project, were any of the beneficiaries professionals in communication or media relations?

○ Yes x No

21. As part of the project, have any beneficiaries received professional media / communication training / advice to improve communication with the general public?

○ Yes x No

22 Which of the following have been used to communicate information about your project to the general public, or have resulted from your project?

x	Press Release	x	Coverage in specialist press
❑	Media briefing	❑	Coverage in general (non-specialist) press
❑	TV coverage / report	❑	Coverage in national press
❑	Radio coverage / report	❑	Coverage in international press
❑	Brochures /posters / flyers	❑	Website for the general public / internet
❑	DVD /Film /Multimedia	❑	Event targeting general public (festival, conference, exhibition, science café)

23 In which languages are the information products for the general public produced?

❑	Language of the coordinator	x	English
❑	Other language(s)		