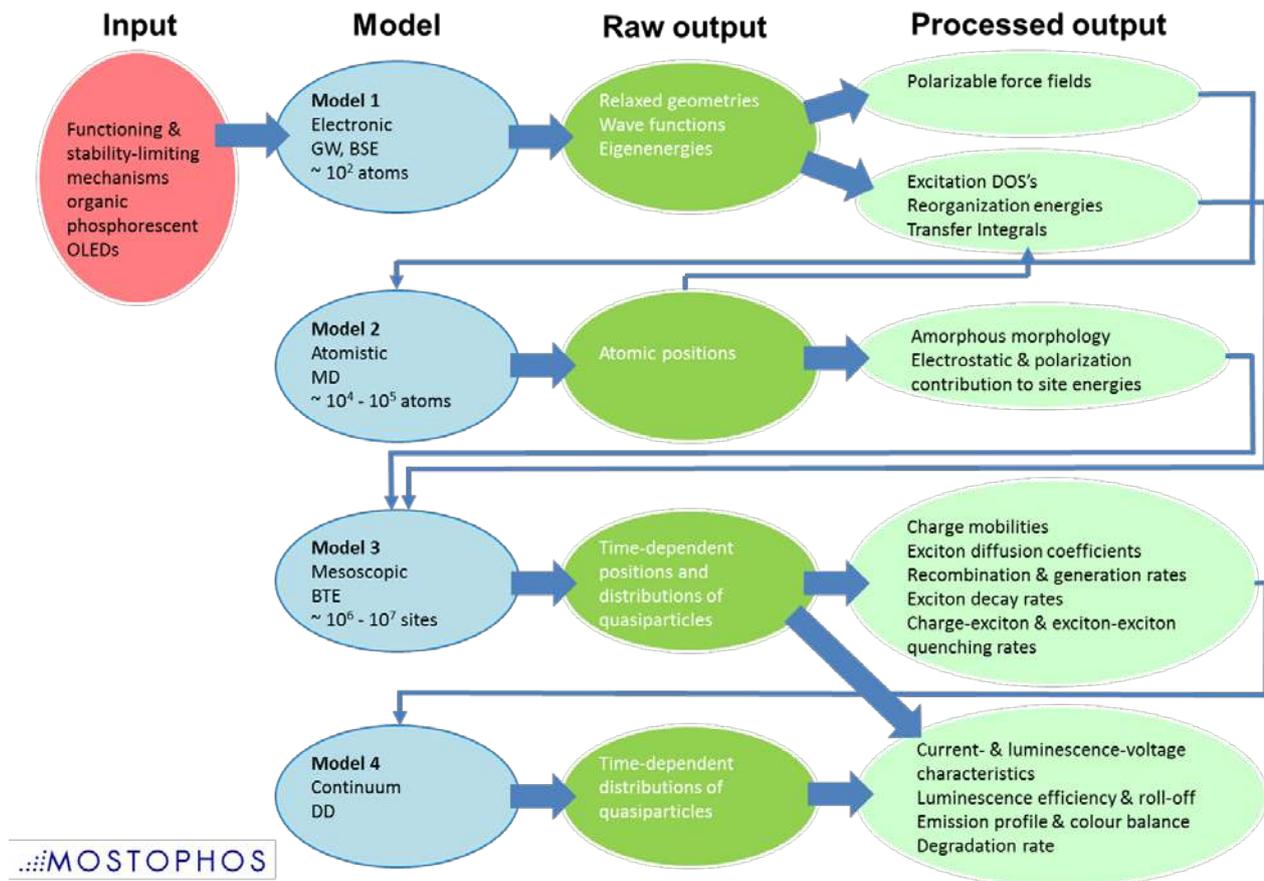


MOSTOPHOS: Modelling stability of organic phosphorescent light-emitting diodes

Version Date: 2015.11.13. *Last updated 2016.08.16.*

THE SIMULATION GENERAL DESCRIPTION									
1	<p>USER CASE</p> <p>The user wants to model the functioning and the stability-limiting mechanisms under operational conditions of organic phosphorescent light-emitting diodes fabricated by vacuum deposition.</p>								
2	<p>CHAIN OF MODELS</p> <table border="1"> <tbody> <tr> <td>MODEL 1</td> <td> <p><u>Electronic model</u>: Ab initio quantum-mechanical model for electron, hole, and exciton energies and wavefunctions; for transfer rates of electrons, holes and excitons, formation of excitons, exciton quenching by charge-exciton and exciton-exciton interactions, radiative and non-radiative decay of excitons, and material degradation. Parameterization of polarizable force-fields for intra- and inter-molecular forces. 1.1.2, 1.1.3, 1.2.2, and 1.3.1. in ROMM.</p> </td> </tr> <tr> <td>MODEL 2</td> <td> <p><u>Atomistic model</u>: Molecular dynamics simulations of atomistic morphologies of vacuum deposited organic semiconductor layers, using the force-fields from Model 1. Evaluation of the solid-state contribution to site energies (electrostatic and induction). 2.3.1 in ROMM.</p> </td> </tr> <tr> <td>MODEL 3</td> <td> <p><u>Statistical Electronic transport model (applied to mesoscale)</u>: <i>Discrete</i> description of dynamics of quasiparticle densities: electrons, holes and excitons, formation of excitons, exciton quenching by charge-exciton and exciton-exciton interactions, radiative and non-radiative decay of excitons, and material degradation, given the rates from Model 1 and morphologies from Model 2. 1.4.1 in ROMM.</p> </td> </tr> <tr> <td>MODEL 4</td> <td> <p><u>Continuum model</u>: <i>Continuum</i> description of dynamics of density of electrons, holes and excitons, formation of excitons, exciton quenching by charge-exciton and exciton-exciton interactions, radiative and non-radiative decay of excitons, and material degradation, based on the output of Model 3. 1.4.1 in ROMM.</p> </td> </tr> </tbody> </table>	MODEL 1	<p><u>Electronic model</u>: Ab initio quantum-mechanical model for electron, hole, and exciton energies and wavefunctions; for transfer rates of electrons, holes and excitons, formation of excitons, exciton quenching by charge-exciton and exciton-exciton interactions, radiative and non-radiative decay of excitons, and material degradation. Parameterization of polarizable force-fields for intra- and inter-molecular forces. 1.1.2, 1.1.3, 1.2.2, and 1.3.1. in ROMM.</p>	MODEL 2	<p><u>Atomistic model</u>: Molecular dynamics simulations of atomistic morphologies of vacuum deposited organic semiconductor layers, using the force-fields from Model 1. Evaluation of the solid-state contribution to site energies (electrostatic and induction). 2.3.1 in ROMM.</p>	MODEL 3	<p><u>Statistical Electronic transport model (applied to mesoscale)</u>: <i>Discrete</i> description of dynamics of quasiparticle densities: electrons, holes and excitons, formation of excitons, exciton quenching by charge-exciton and exciton-exciton interactions, radiative and non-radiative decay of excitons, and material degradation, given the rates from Model 1 and morphologies from Model 2. 1.4.1 in ROMM.</p>	MODEL 4	<p><u>Continuum model</u>: <i>Continuum</i> description of dynamics of density of electrons, holes and excitons, formation of excitons, exciton quenching by charge-exciton and exciton-exciton interactions, radiative and non-radiative decay of excitons, and material degradation, based on the output of Model 3. 1.4.1 in ROMM.</p>
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3	<p>PUBLICATION ON THIS SIMULATION</p>								
4	<p>ACCESS CONDITIONS</p> <p>The programs VOTCA, GROMACS, Octopus, Abinit, Quantum Espresso, and Yambo used in MOSTOPHOS are open source codes. The programs Turbomole, Bumblebee and TiberCAD are commercially distributed by the companies Cosmologic (www.cosmologic.com) Simbeyond (www.simbeyond.com) and tiberlab s.r.l. (www.tiberlab.com).</p>								

Workflow of the MOSTOPHOS project, illustrating the models, their interdependencies via input/output, and experimental validation.



Rationale for the choice of models in this workflow: we are aiming at materials pre-screening, hence the link of device properties to chemical structures must be retained. Complete ab initio description of the system is, however, computationally prohibitive, therefore we adopt a multiscale ansatz: classical atomistic models for morphologies (M2) and statistical quasiparticle description for drift-diffusion (M3), both parametrized using first-principles (M1). Phenomena which are difficult to describe with a mesoscopic model (M3) (heat balance, light in- and out-coupling) are then incorporated at a continuum model (M4).

Model 1

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED		
1.1	ASPECT OF THE USER CASE TO BE SIMULATED AND HOW IT FORMS A PART OF THE TOTAL USER CASE	The user wants to calculate from first principles energies of neutral and charged excitations of organic semiconducting molecules, the rates of transfer processes of these excitations between molecules, and the stability of the products of these processes. This information is then used in Model 3. The user wants to develop parameterized force-fields for intra- and inter-molecular forces, which are used as input in Model 2.
1.2	MATERIAL	Organic semiconducting molecules, including phosphorescent dyes in the emission layers of organic light-emitting diodes. The organic layers grown by vacuum deposition, leading to a disordered conformation and packing of the molecules. The <i>ab initio</i> model requires types of atoms as input.
1.3	GEOMETRY	Single molecules and pairs of molecules.
1.4	TIME LAPSE	Up to picoseconds.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	
1.6	PUBLICATION ON THIS SIMULATION	

2 GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Electronic model: Higher-level ab initio models (ROMM 1.1.2)
2.1	MODEL ENTITY	Quasiparticles (electrons, holes, excitons).
2.2	MODEL PHYSICS/CHEMISTRY EQUATION PE'S	Equations <ol style="list-style-type: none"> Dyson equation (in the GW approximation). Bethe-Salpeter equation (BSE).
		Physical quantities for each equation <ol style="list-style-type: none"> Quasiparticle wave functions. Green function (G), self-energy (Σ), dynamically screened interaction (W).
MATERIALS RELATIONS	Equations	<ol style="list-style-type: none"> Equation for dielectric function completes the Dyson equation and Bethe-Salpeter equations. Electrons/holes are described via single-particle green functions, excitons by two-particle green functions.
	Physical quantities/descriptors for each MR	<ol style="list-style-type: none"> Quasiparticle wave functions. Coulomb interaction.
2.4	Simulated input	None

3 SPECIFIC COMPUTATIONAL MODELLING METADATA			
3.1	NUMERICAL SOLVER	Eigensolver, propagator, GW and BSE solvers.	
3.2	SOFTWARE TOOL	Octopus (www.tddft.org/programs/octopus), Abinit (www.abinit.org), Quantum Espresso (www.quantum-espresso.org), Yambo (www.yambo-code.org), VOTCA (www.votca.org)	
3.4	TIME STEP		
3.5	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION	Abinit, Quantum Espresso, Turbomole (DFT), Yambo (GW): wavefunctions and density are represented in plane-wave basis.
		MATERIAL	Pseudopotentials: representation on regular real-space grid (Octopus) and

		RELATIONS	in plane-wave basis (Quantum Espresso). Dielectric functions: representation in plane-wave basis (Yambo).
		MATERIAL	The material is represented by the locations of its atoms.
		BOUNDARY CONDITIONS	Absorbing boundary conditions or use of Coulomb cut-off under periodic boundary conditions to prevent interaction of periodic images.
		ADDITIONAL SOLVER PARAMETERS	Eigensolver: <ol style="list-style-type: none"> 1. Convergence of density. 2. Convergence of eigenstates. 3. Convergence of forces. 4. Maximum number of iterations. Propagator: <ol style="list-style-type: none"> 1. Maximum number of iterations. 2. Method for approximation of the evolution operator.
3.6	PUBLICATION		

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	Atoms in Model 2 and quasiparticles in Model 3
4.2	METHODOLOGIES	<ul style="list-style-type: none"> • The ab initio forces following from the calculations are parameterized (calculation of values in a FF formula from the literature), leading to polarizable force-fields. This information is the input to Model 2. • The distribution of the energies of excitations leads to densities of states of quasiparticles (DOS) that are input to Model 3. • The conformational dependent excitation energies lead to reorganization energies that are input to Model 3. • The charge and exciton transfer rates between two neighbouring organic molecules are calculated on the basis of the Fermi-golden rule for wave functions of the initial and final states. This information is input to Model 3.
4.3	MARGIN OF ERROR	30%.

Model 2

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED		
1.1	ASPECT OF THE USER CASE TO BE SIMULATED and how it forms a part of the total user case	The user wants to calculate the amorphous morphology of a layer of organic semiconducting molecules, possibly with phosphorescent dye molecules added.
1.2	MATERIAL AND ITS PROCESSING	Organic molecular semiconductors, including phosphorescent dyes in the emission layers of organic light-emitting diodes. The organic layers are grown by vacuum deposition, leading to a disordered conformation and packing of the molecules. The microscopic amorphous morphologies obtained from Model 2 are used as input for (i) pairs of molecules in Model 1 and (ii) the mesoscale morphologies, represented by the molecular centres of mass, in Model 3. If required, a stochastic expansion method is applied to expand the microscopic morphologies to mesoscale morphologies.
1.3	GEOMETRY	Multilayered structure.
1.4	TIME LAPSE	Picoseconds.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	
1.6	PUBLICATION	

2 GENERIC PHYSICS OF THE MODEL EQUATION			
2.0	MODEL TYPE AND NAME	Atomistic model: Classical molecular dynamics (MD) (ROMM 2.3.1).	
2.1	MODEL ENTITY	Atoms.	
2.2	MODEL PHYSICS/CHEMISTRY EQUATION PE'S	Equations	1. Newton's equation of motion.
		Physical quantities for each equation	1. Spatial coordinates and velocities of all atoms. 2. Forces, partial multipoles, polarizabilities.
MATERIALS RELATIONS		Equations	1. Equation for intra- and intermolecular force-field for atoms. 2. Equation for the interaction cut-offs of the force field.
		Physical quantities/descriptors for each MR	1. Forces, positions of atoms, dihedral angles. 2. Positions of atoms, dihedral angles.
2.4	Simulated input	Ab-initio calculated values for forces fields from Model 1.	

This part is similar to the description on input files to simulation software and requires understanding of the underlying architecture of the data in certain class of solvers for the models.

3 SPECIFIC COMPUTATIONAL MODELLING METADATA			
3.1	NUMERICAL SOLVER	Velocity-Verlet algorithm	
3.2	SOFTWARE TOOL	GROMACS (www.gromacs.org).	
3.4	TIME STEP	0.01fs	
3.5	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION	Newton's equations of motion are applied to the set of atomic coordinates and solved numerically by time discretization using a Verlet algorithm. An analogue of the Poisson equation is solved for polarizable force-fields by optimizing induced multipoles.

		MATERIAL RELATIONS	The material-specific electrostatic potential and interaction potential are represented as a sum over atomic-coordinate based force-field functions, making use of distributed multipoles, polarizabilities, and bonded constants.
		MATERIAL	The material is represented by the locations of its atoms.
		BOUNDARY CONDITIONS	The calculations are done on a representative unit cell with periodic boundary conditions.
		ADDITIONAL SOLVER PARAMETERS	<ol style="list-style-type: none"> 1. Verlet list cutoff. 2. Number of self-consistent iterations, tolerance. 3. Ewald sum grid.
3.6	PUBLICATION		[1] B. Hess, C. Kutzner, D. van der Spoel, and E. Lindahl, J. Chem. Theory Comput. 4, 435 (2008).

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	The amorphous morphology obtained in the present model is used as input to Model 3.
4.2	METHODOLOGIES	The polarizable force-field is employed to calculate electrostatic and polarization contributions to the site energies used in Model 3.
4.3	MARGIN OF ERROR	Margin of error: typically within 10%, mostly due to the error in the material relations (force-field parameters, basis set size).

Model 3

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED		
1.1	ASPECT OF THE USER CASE TO BE SIMULATED and its role in the and how it forms a part of the total user case	The user wants to analyse at the mesoscale all the electronic processes under DC bias relevant for the functioning and material degradation of phosphorescent organic light-emitting diodes. Photons are generated in the device.
1.2	MATERIAL	Organic molecular semiconductors, including phosphorescent dyes in the emission layers of organic light-emitting diodes. The microscopic morphologies of the used materials are obtained from Model 2 (Manufacturing has been done by vacuum deposition)
1.3	GEOMETRY	Layers of several nanometres thick of (mixtures of) organic molecular semiconductors, each with a specific function: injection layers for electrons and holes, transport and blocking layers for electron and holes, emissive layers with dyes, exciton-blocking layers, etc.
1.4	TIME LAPSE	Up to tens of microseconds.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	A DC voltage is applied to the device.
1.6	PUBLICATION	

2 GENERIC PHYSICS OF THE MODEL EQUATION			
2.0	MODEL TYPE AND NAME	Quasiparticle model: statistical semi-classical transport model (ROMM 1.4.1).	
2.1	MODEL ENTITY	Quasiparticles.	
2.2	MODEL PHYSICS/CHEMISTRY EQUATION PE'S	Equations	1. Boltzmann transport equation (BTE) describing how quasiparticles (charged and neutral excitations) hop between sites representing molecules.
		Physical quantities for each equation	1. Transfer rates of all hopping transfer processes; spatial profile of quasiparticles (charges, excitons), electric field and temperature.
MATERIALS RELATIONS		Equations	Equations for the material-specific rates k of all hopping transfer process to complete BTE.
		Physical quantities/descriptors for each MR	Material-specific energies and molecular reorganization energies of charged and neutral excitations, exciton binding energies, intermolecular electronic couplings, dielectric constant.
2.4	SIMULATED INPUT	<ul style="list-style-type: none"> Amorphous morphology calculated with Model 2. Energies and molecular reorganization energies of charged and neutral excitations, exciton binding energies, intermolecular electronic couplings, calculated with Model 1. The microscopic information about DOS of charged and neutral excitations, the reorganization energies, and the rates of transfer processes of these excitations are obtained from Model 3. 	

3		SPECIFIC COMPUTATIONAL MODELLING METADATA	
3.1	NUMERICAL SOLVER	Kinetic Monte Carlo (kMC).	
3.2	SOFTWARE TOOL	Bumblebee (www.simbeyond.com).	
3.4	TIME STEP	Typically a nanosecond.	
3.5	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION	The BTE is solved by executing at each time step a hopping transfer process from one site to another, chosen randomly with a probability proportional to its rate. Time is proceeded in each step by a time interval chosen from an exponential distribution with a decay time equal to the inverse of the sum of the rates of all possible hopping transfer processes.
		MATERIAL RELATIONS	Material- and excitation-specific transfer rates are used (Marcus transfer for electrons and holes, Förster transfer for singlet excitons, and Dexter transfer for triplet excitons). The material-specificity in these transfers comes in via the material-specific electronic energies and reorganisation energies for electrons, holes, and singlet and triplet excitons, exciton binding energies, and intermolecular couplings.
		MATERIAL	The material is represented as a collection of molecular point sites at which charged (electrons and holes) and uncharged (singlet and triplet excitons) can reside. Each site has specific electronic energies and reorganisation energies for electrons, holes, and singlet and triplet excitons, and a specific exciton binding energy. Every pair of sites has specific intermolecular couplings for charge or exciton transfer. The dielectric properties of each material is represented by its dielectric constant. A specific material degradation scenario is chosen (example: an exciton-charge quenching event leads with a certain probability to disfunctioning of a molecule).
		BOUNDARY CONDITIONS	In the direction of current flow the boundary conditions are determined by the work functions of the electrode materials and the applied bias voltage. Periodic boundary conditions are used in the lateral directions perpendicular to the current flow.
		ADDITIONAL SOLVER PARAMETERS	<ol style="list-style-type: none"> 1. Maximum length of run. 2. Criterion for reaching steady state. 3. Criterion for reaching sufficient accuracy of physical quantity to be calculated.
3.6	PUBLICATION		

4		POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	The output of the model is used to determine the form and values of parameters in the Material Relations in the continuum Model 4 (finite differences)	
4.2	METHODOLOGIES	<p>- The raw output of the program is a time record of all charge hopping, exciton recombination, transfer, quenching, and radiative and non-radiative decay events. By spatial and temporal averaging, relations are determined for the following physical quantities:</p> <ol style="list-style-type: none"> 1. Electron mobility. 2. Hole mobility. 3. Singlet exciton diffusion coefficient. 4. Triplet exciton diffusion coefficient. 5. Electron-hole recombination and generation rates. 6. Singlet exciton decay rate. 7. Triplet exciton decay rate. 8. Charge-exciton quenching rates. 9. Exciton-exciton quenching rates. <p>The following relations and values found will be used as Material Relations of Model 4:</p> <ol style="list-style-type: none"> 1. Current-voltage characteristics. 2. Luminescence-voltage characteristics. 3. Luminescence efficiency as a function of voltage. 	



		<ol style="list-style-type: none">4. Colour balance.5. Efficiency roll-off (decrease of efficiency with increasing current).6. Emission profile.7. Degradation rate. <p>These properties are used to benchmark the results of Model 4.</p>
4.3	MARGIN OF ERROR	20-30%.

Model 4

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED		
1.1	ASPECT OF THE USER CASE TO BE SIMULATED and how it forms a part of the total user case	The user wants to analyse at the μ -macro scale all the processes relevant for the functioning and material degradation of phosphorescent organic light-emitting diodes. Heat is generated in the device.
1.2	MATERIAL	Organic molecular semiconductors, including phosphorescent dyes in the emission layers of organic light-emitting diodes.
1.3	GEOMETRY	Stacked OLED structure including electrons and holes transport layers, blocking layers and emission layers. Layers thickness ranges from a few nanometres up to tens of nanometres.
1.4	TIME LAPSE	N/A: Reaching the steady state is simulated.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	The device in its in-service conditions is simulated: a voltage is applied and the transport of electrons, holes and excitons, as well as exciton formation, exciton-charge quenching and exciton-exciton quenching in the whole device are simulated.
1.6	PUBLICATION	

2 GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum model: semiclassical steady-state drift-diffusion (DD) model (ROMM 4.2)
2.1	MODEL ENTITY	Density of quasiparticles in finite volumes
2.2	MODEL PHYSICS/CHEMISTRY EQUATION PE'S	Equations Tightly-Coupled PEs: <ol style="list-style-type: none"> Poisson equation for the electrostatic potential. Drift-diffusion equation for electrons. Drift-diffusion equation for holes. Diffusion equation for singlet excitons. Diffusion equation for triplet excitons.
		Physical quantities for each equation <ol style="list-style-type: none"> Electrostatic potential, charge density. Current and charge density of electrons. Current and charge density of holes. Current and density of singlet excitons. Current and density of triplet excitons. Current and charge density of quasiparticles.
MATERIALS RELATIONS		Equations <ol style="list-style-type: none"> Relation for dielectric constant, completes Poisson equation. Relation for electron mobility, completes drift-diffusion equation electrons. Relation for hole mobility, completes drift-diffusion equation holes. Relation for diffusion coefficient singlet excitons, completes diffusion equation for singlet excitons. Relation for diffusion coefficient triplet excitons, completes diffusion equation for singlet excitons. Relation for electron-hole recombination and generation rate, completes drift-diffusion equations electrons and holes and diffusion equations excitons. Relation for singlet exciton decay rate, completes diffusion equation for singlet excitons. Relation for triplet exciton decay rate, completes diffusion equation for singlet excitons.

		<ul style="list-style-type: none"> 9. Relations for charge-exciton quenching, complete diffusion equations for singlet and triplet excitons. 10. Relations for exciton-exciton quenching rates, complete diffusion equation for singlet and triplet excitons.
	Physical quantities/ descriptors for each MR	<ul style="list-style-type: none"> 1. Dielectric constant. 2. Electron mobility. 3. Hole mobility. 4. Singlet exciton diffusion coefficient. 5. Triplet exciton diffusion coefficient. 6. Electron-hole recombination and generation rates. 7. Singlet exciton decay rate. 8. Triplet exciton decay rate. 9. Charge-exciton quenching rates. 10. Exciton-exciton quenching rates.
2.4	SIMULATED INPUT	<p>Relations for the following quantities calculated with the mesoscopic Model 3 are the material input relations of the continuum Model 4:</p> <ul style="list-style-type: none"> 1. Electron mobility. 2. Hole mobility. 3. Singlet exciton diffusion coefficient. 4. Triplet exciton diffusion coefficient. 5. Electron-hole recombination and generation rates. 6. Singlet exciton decay rate. 7. Triplet exciton decay rate. 8. Charge-exciton quenching rates. 9. Exciton-exciton quenching rates.

3 SPECIFIC COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	Finite element discretization of the continuum problem (FEM) and Newton's method
3.2	SOFTWARE TOOL	TiberCAD (www.tiberlab.com)
3.4	TIME STEP	N/A: the steady state is simulated.
3.5	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION The full equations system (Poisson + drift-diffusion for charges + diffusion for excitons) is written in matrix form using finite-element methods (FEM) and then solved numerically using the Newton method (linearization of the system).
		MATERIAL RELATIONS The relations for the electron and hole mobilities, the exciton diffusion coefficients, the electron-hole recombination and generation rates, the exciton decay rates, the charge-exciton quenching rates, and the exciton-exciton quenching rates are parameterized.
		MATERIAL Each layer of the device is defined by its material composition (host + dye). Also traps can be introduced, leading to Schottky-Read-Hall (RSH) recombination. Each material is defined by its dielectric constant, HOMO and LUMO levels, electron and holes density of states, and its relations for the electron and hole mobilities, the exciton diffusion coefficients, the electron-hole recombination and generation rates, the exciton decay rates, the charge-exciton quenching rates, and the exciton-exciton quenching rates.
		COMPUTATIONAL BOUNDARY CONDITIONS Dirichlet boundary conditions are used to set the applied electric potential and the Fermi level of the metal contacts. Contacts are boundary models that allow a nonzero normal electrical current. At Ohmic or Schottky contacts one defines surface recombination velocities for electrons and holes. This imposes Robin-type boundary conditions for the continuity

			equations.
		ADDITIONAL SOLVER PARAMETERS	N/A
3.6	PUBLICATION	[

4 POST PROCESSING		
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	Luminance and current for the device as a function of the applied voltage and time (in case of degradation)
4.2	METHODOLOGIES	<p>From the solution of the equations system (Poisson + drift-diffusion for charges + diffusion for excitons) the following OLED properties are extracted with volume averaging :</p> <ol style="list-style-type: none"> 1. Current-voltage characteristics. 2. Luminescence-voltage characteristics. 3. Luminescence efficiency. 4. Colour balance. 5. Efficiency roll-off (decrease of efficiency with increasing current). 6. Emission profile. 7. Degradation rate (this process is faster than reaching the steady state). <p>These are the same properties that can be extracted from the mesoscopic Model 3, but the numerical efficiency of the continuum Model 4 is much greater.</p>
4.3	MARGIN OF ERROR	30%