Physics-based Model: Continuum Electromagnetics – Optical (RoMM 4.6.3)

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	To perform optical simulations in order to optimize the optical performance of organic electronic devices (OPVs for maximal light absorption, OLED for maximal light extraction). To propose light management strategies and to generate input for linked electrical simulations.
1.2	MATERIAL	Simulated device for OPVs consists of front transparent contact (glass+ITO), HTL (PEDOT:PSS), active layer (P3HT:PCBM, PCDTBT:PCBM, etc), ETL (TiO2), back contact (Ag), embedded plasmonic metallic nanoparticles (Ag and Au). Input in the simulations are parameters for the dielectric functions of the raw materials according to a Drude-Lorentz model (obtained by spectroscopic ellipsometry)
1.3	GEOMETRY	For the active layer in mesoscale: up to ~ 100x100x100 nm^3 domains containing the bulk heterojunction to extract the effective complex permittivity. For the device in macroscale: all device layers including contacts and possible embedded plasmonic/photonic nanostructures to improve light management.
1.4	TIME LAPSE	N/A
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Incoming light
1.6	PUBLICATION ON THIS DATA	*E. Lidorikis et al, J. Appl. Phys. 101, 054304 (2007); I. Vangelidis et all, submitted.*

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum model – Electromagnetism - Optics	
2.1	MODEL ENTITY	Finite volumes	
2.2	MODEL PHYSICS/	**Equation**	PE: Maxwell's equations describing propagation of

	CHEMISTRY EQUATION PE		electromagnetic waves $\nabla \cdot \mathbf{D} = 0$ $\nabla \cdot \mathbf{B} = 0$ $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$ $\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}$
		Physical quantities	E - electric field D - electric flux density H - magnetic field B - magnetic flux density
2.3	MATERIALS RELATIONS	**Relation**	MR: $\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} = \varepsilon \mathbf{E}$, $\mathbf{B} = \mu \mathbf{H}$ (μ=μ_0 for the optical frequencies of interest). ε describes material properties and directly determines the complex refractive index of layers.
		Physical quantities/ descriptors for each MR	E - electric field P – material polarization D - electric flux density H - magnetic field B - magnetic flux density ε – permittivity (material property) µ- permeability (material property)
2.4	SIMULATED INPUT	The active blend microstructures obtained from the CGMD simulations	

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	Finite-difference time domain (FDTD)	
3.2	SOFTWARE TOOL	(a) in-house, (b) MEEP	
3.3	TIME STEP	0.01-0.1 fs	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}$ $\nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}_0}{\partial t} + \sum_{m=1}^{M} \frac{\partial \mathbf{P}_m}{\partial t}$ Material polarization is taken into account by intraband $\mathbf{P}_0$ (Drude model) and several interband $\mathbf{P}_m$ (Lorentz oscillator model) transitions, described by the following polarization equations:

			$\frac{\partial^2 \mathbf{P}_0}{\partial t^2} + \frac{1}{\tau}\frac{\partial \mathbf{P}_0}{\partial t} = \varepsilon_0 \omega_p^2 \mathbf{E}$ $\frac{\partial^2 \mathbf{P}_m}{\partial t^2} + \gamma_m \frac{\partial \mathbf{P}_m}{\partial t} + \omega_m^2 \mathbf{P} = \varepsilon_0 \sigma_m^2 \mathbf{E}$ For the Drude model: τ – free electron relaxation time ω_p – plasma frequency For the Lorentz model: γ_m - decay rate of the m'th Lorentz oscillator ω_m – resonance frequency of the m'th Lorenzt oscillator σ_m – coupling strength of the m'th Lorentz oscillator. All above differential equations are solved concurrently on a computational grid with finite differences. Resultant material dielectric function for each material $\varepsilon(\omega) = \varepsilon_0 \left(\varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\tau^{-1}} + \sum_{m=1}^{M} \frac{\sigma_m^2}{\omega_m^2 - \omega^2 - i\omega\gamma_m} \right)$ where the material parameters are adjusted in order to reproduce the experimental dielectric functions
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**	Top and bottom of the device: perfectly matched layers (PML), absorbing boundary conditions (ABC). Lateral sides of the device: Periodic boundary conditions (PBC), symmetry boundary conditions (SBC). Sources: OPV calculations: broadband incoming plane wave OLED calculations: point dipole sources distributed within the active	
3.6	**ADDITIONAL SOLVER PARAMETERS**	• Mesh grid 0.5-2 nm	

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT**	For the active layer in mesoscale we get the effective dielectric function (homogenization) of the bulk mixture (donor-acceptor), which is defined as the effective dielectric of a homogenized medium which reproduces the identical same transmission and reflection amplitudes and phases. The averaging volume is up to 100x100x100 nm^3. The homogenized dielectric is used as input (new MR) in the continuum optical modelling of the full device (larger finite volumes) in the macroscale. In the OPV device modelling in the macroscale we get the spectral absorption in each point of the device, including active layer and parasitic absorption (losses) in the barrier layers and contacts. Integrating the spectral absorption over

		frequency we get the exciton generation rate spatial distribution, to be used as input in the continuum electrical modelling of the device (drift-diffusion). In the OLED device modelling we get the radiative flux exiting the structure which yields the enhanced extraction efficiency and possible Purcell enhancement.
4.2	**METHODOLOGIES**	For the active layer in mesoscale we extract the complex reflection and transmission amplitudes r(ω) and t(ω) from the FDTD simulation of a representative cell (say 50x50x50 nm^3) of donor and acceptor blend (blend geometry input by the CGMD simulations) and invert them to get the effective index ñ (ω) according to (JAP 101, 054304 (2007)): $2\cos(\tilde{n}(\omega)\omega a/c) = t(\omega) + t(\omega)^{-1} - r(\omega)^2/t(\omega)$ In the device calculations for OPVs we get the absorption in each point in the active by $A(\boldsymbol{r},\lambda) = \left(\frac{1}{2}\right)\boldsymbol{E}(\boldsymbol{r},\lambda)\cdot\boldsymbol{J}^*(\boldsymbol{r},\lambda)$, where $\boldsymbol{J} = \partial\boldsymbol{P_0}/\partial t + \sum\partial\boldsymbol{P}_m/\partial t$ (all frequency related quantities are obtained by Fourier transform of the corresponding time series). The exciton generation rate is obtained by $G(\boldsymbol{r}) = \left(\frac{e}{hc}\right)\int\lambda A(\boldsymbol{r},\lambda)S(\lambda)d\lambda$, where $S(\lambda)$ is the solar radiative flux. The exciton generation rate $G(\boldsymbol{r})$ is used as input in the electrical modeling (DD). The total exciton generation rate $J_G = \int\boldsymbol{G}(\boldsymbol{r})d\boldsymbol{r}$ is used as a figure of merit for the optical optimization of light management. *In the device calculations for OLEDs we calculate the time averaged radiative flux by Poynting's theorem* $\mathbf{S}(\mathbf{r},\lambda) = Re\left\{\left(\frac{1}{2}\right)\mathbf{E}(\mathbf{r},\lambda)\times\mathbf{H}^*(\mathbf{r},\lambda)\right\}$ *on suitably chosen monitor planes.*
4.3	**MARGIN OF ERROR**	Discretization errors, the grid size is tuned so that the numerical error remains below 1%.