Kinetic Monte Carlo simulation of the efficiency roll-off, emission color, and degradation of organic light-emitting diodes

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Reinder Coehoorn, Philips Research Nederland B.V. (Netherlands); **Harm van Eersel, Peter A. Bobbert, Rene A. J. Janssen,** Technische Univ. Eindhoven (Netherlands)

ABSTRACT

(invited talk)
The performance of Organic Light Emitting Diodes (OLEDs) is determined by a complex interplay of the charge transport and excitonic processes in the active layer stack. We have developed a three-dimensional kinetic Monte Carlo (kMC) OLED simulation method which includes all these processes in an integral manner. The method employs a physically transparent mechanistic approach, and is based on measurable parameters. All processes can be followed with molecular-scale spatial resolution and with sub-nanosecond time resolution, for any layer structure and any mixture of materials. In the talk, applications to the efficiency roll-off, emission color and lifetime of white and monochrome phosphorescent OLEDs [1,2] are demonstrated, and a comparison with experimental results is given. The simulations show to which extent the triplet-polaron quenching (TPQ) and triplet-triplet-annihilation (TTA) contribute to the roll-off, and how the microscopic parameters describing these processes can be deduced properly from dedicated experiments. Degradation is treated as a result of the (accelerated) conversion of emitter molecules to non-emissive sites upon a triplet-polaron quenching (TPQ) process. The degradation rate, and hence the device lifetime, is shown to depend on the emitter concentration and on the precise type of TPQ process. Results for both single-doped and co-doped OLEDs are presented, revealing that the kMC simulations enable efficient simulation-assisted layer stack development.
[1] H. van Eersel et al., Appl. Phys. Lett. 105, 143303 (2014).
[2] R. Coehoorn et al., Adv. Funct. Mater. (2015), publ. online (DOI: 10.1002/adfm.201402532)

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