Study of transient phenomena in phosphorescent and TADF OLEDs: a Monte Carlo simulation approach

Harm van Eersel,[1] Alice Furlan,[1] Siebe van Mensfoort,[1]
Peter Bobbert,[2] Reinder Coehoorn[2]
[1] Simbeyond B.V., P.O. Box 513, NL-5600 MB, The Netherlands
[2] Eindhoven University of Technology, P.O. Box 513,
NL-5600 MB Eindhoven, The Netherlands

From an extensive study, we have shown how molecular-scale kinetic Monte Carlo (kMC) simulations can be used to understand the device physics of a hybrid (phosphorescent red and green, fluorescent blue) white OLED stack.[1] The $J(V)$ characteristics and color point were surprisingly well reproduced, starting only from physical parameters obtained from experiment. More recently, we have shown how such simulations can be used to study the cause of roll-off in prototypical phosphorescent monochrome red and green devices,[2] how it can be used to understand the concentration-dependence of triplet-triplet annihilation in phosphorescent dyes,[3] and how roll-off and degradation can depend on different material parameters.[4] In this contribution, we show how kMC simulations can be used to study transient electroluminescence in OLEDs, to facilitate the study of quenching processes,[5] and to understand phenomena such as the sometimes observed overshoot in emission[6] and delayed emission[7] as function of the voltage, dye concentration and host material. The simulations include exciton quenching processes (exciton-polaron quenching, exciton-exciton annihilation), field-induced dissociation, Förster and Dexter transfer between dye molecules, and delayed fluorescence due to triplet-triplet annihilation. As an outlook, we show how these techniques can also be applied to 3.5th generation OLEDs containing both a thermally activated delayed fluorescence (TADF) sensitizer and a fluorescent guest.[8]

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