**Computational design of organic semiconductors for light emitting diodes and solar cells**

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Improving lifetimes and efficiencies of *blue* light-emitting diodes (LED) and *non-fullerene acceptor* (NFA) solar cells are clearly two major challenges in the field of organic semiconductors.

Towards solving the first challenge, we discuss a unicolored phosphor-sensitized fluorescence (UPSF) approach, with phosphorescent and fluorescent emitters tailored to preserve the initial color of phosphorescence [1]. Using UPSF, it is possible to design an efficient sky-blue UPSF OLED with radiative decay times in the submicrosecond regime and operational lifetimes of up to 320 hours (LT80, initial luminance of 1000 cd/m2).

To quantify the potential of the UPSF concept, we develop a multiscale model of a UPSF OLED [2]. We start from atomistic morphologies, parameterize the rates of all processes on the available experimental data, and solve the respective master equation with the help of the kinetic Monte Carlo algorithm. We expand the scope of experiment by studying the effect of the acceptor concentration as well as Förster and (parasitic) Dexter energy transfer from the donor to acceptor on the characteristics of the UPSF OLED. Our study shows that an appropriate material design can further improve efficiency by more than 30 % and at the same time achieve radiative decay times below 0.02 µs thus significantly extending OLED operational lifetime.

To address the second challenge, we study the role of long-range electrostatic interactions at the donor-acceptor interface. For a set of recently developed NFAs, we demonstrate that the electrostatic bias potential, present at this interface, can be directly related to the stabilization (or destabilization) of CT states as well as changes of the photovoltaic gap [3]. We also show that there is a correlation between quadrupole moments, charge separation efficiency, and CT-state energy, predicted by our model and experimentally measured for several donor NFA combinations [4.5]. The observed correlations allow us to formulate design rules for new NFA structures for higher performance solar cells.

**References**

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