Multiscale Modeling of Heterojunction Organic Photovoltaic Devices

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In this lecture, we present our most recent results in the modeling and simulation of heterojunction organic solar cells [2]. The proposed mathematical model is an extension of that introduced in [1] for planar heterojunction solar cells to treat arbitrary multi-dimensional morphologies. Our approach consists in describing diffusion and transport phenomena of excited states and charge carriers in a heterogeneous domain Ω of $\mathbb{R}^d$, $d = 1, 2, 3$, constituted by two non-overlapping subdomains Ω_i, $i = 1, 2$, using mass balance equations supplied with the Drift-Diffusion model for flux densities. Charge dissociation and recombination phenomena occurring in a thin region around the $(d-1)$-interface are lumped with a scale transition procedure into flux transmission conditions. This approach is twofold beneficial since it allows to account for the local dependence of dissociation on the orientation of the electric field and to reduce the computational effort compared to previous multi-dimensional models [5, 6]. The resulting system of fully coupled nonlinear PDEs/ODEs is faced with Rothe's method using a quasi-Newton technique for linearization, the Edge-Average Finite Element method studied in [7] for spatial discretization and adaptive BDF schemes for time advancement. Simulations are extensively discussed to validate the model against realistic data and results available in the literature. In the final part of the lecture, we show that the proposed model can be used also for investigating the behavior of different classes of devices, *e.g.* the photoactivated light harvesting capacitor proposed in [3] or the sensing substrate used for neuronal photostimulation in [4].

References

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