Optimum Experimental Design for Estimating Mobility Parameter in Organic Semiconductors

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Abstract: The transport of charge in semiconductors can be mathematically described by the Drift-Diffusion-Equation in a semi-classical way. The Scharfetter-Gummel scheme is widely used for spatially discretizing the continuity equation and yielding a constant current. The outer system is either solved by an iterative Gummel method or a Newton method with appropriate starting values. For organic semiconductors one may consider highly nonlinear mobilities like the ones used in the extended Gaussian disorder model. In this model the density of states is assumed to be Gaussian distributed and its stan- dard deviation is one of the mobility parameters which we like to estimate. Other parameters are the density of chargeable sites and the static mobility constant. Model extensions like including trapped states or injection barriers may contain additional parameters. With the software PARFIT - embedded in the VPLAN package - we estimate these parameters based on a Gauss-Newton algorithm with a globalization strategy. The derivatives are computed with internal numerical differentiation (IND) coupled with automatic differentiation. The applied infeasible path methods require techniques to keep the model evaluable.

The temperature and the length of a single organic material layer are suitable controls for which an optimal design is desired. We will discuss robust approaches like the worst-case or stochastically motivated ones. Results of our simulations and optimizations on test systems will be demonstrated.

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