Summery

A significant progress has recently been made in understanding and optimizing organic bulk heterojunction solar cells. The photocurrent and its major contributions from polaron pair dissociation and charge extraction, however, remained evasive from both, experimental and theoretical perspective. For instance, the widely used model to describe polaron pair dissociation, the Braun– Onsager model, has been shown theoretically and experimentally to not grasp the temperature and field dependence completely or correctly.
Within this proposal, we attempt to marry systematic experiments with parameter-free multiscalesimulations in order to determine the factors influencing the photocurrent and its contributions.
We plan to experimentally investigate mechanisms of the photocurrent generation, look at contributions of charge extraction and polaron pair dissociation, study field, temperature, and acceptor strength dependencies. The sample morphology will be studied as well. The active materials to be applied are the P3HT:PCBM reference system as well as a very promising alternative donor, PCPDTBT, and fullerene derivatives with a variation of the acceptor strength. At the same time parameter-free simulations will be performed in order to adapt the Braun–Onsager model as well as to understand whether the key parameters can be deduced from simulations.
The goal will therefore be to combine theoretical and experimental findings with the aim of a quantitative description of the photocurrent, and finally, formulation of appropriate structure-property processing relationships.