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Titel des Beitrags: Impact of Phosphorescent Sensitizers and Morphology on the Photovoltaic Performance in Organic Solar Cells

Abstract: Phosphorescent sensitizers (PSs) are considered as a promising alternative for increasing the internal quantum efficiency (IQE) in organic solar cells (OSCs). By converting short-lifetime singlet into long-living triplet excitons, enhanced exciton diffusion and dissociation have been reported previously. However, only a limited increase in the OSC performance has been achieved. In this work, the interplay of the PS with both singlet and triplet excitons within organic blends is examined using kinetic Monte Carlo simulations including a comprehensive model of excitonic processes. Different morphologies of the conventional P3HT:PCBM solar cell are simulated, and the excitonic properties and their influence on the photovoltaic performance under doping are studied. The use of phosphorescent sensitization ensures high intersystem crossing and enlarges the diffusion length. An increase in the IQE of 34% is observed for a bilayer OSC. The increasing decay of triplets in proximity to the PS due to a strong spin-orbit coupling limits the IQE. Unlike expected, triplet-triplet annihilation does not provide a significant loss of excitons. A doped planar-mixed molecular heterojunction outperforms an undoped bulk-heterojunction OSC due to the enhanced exciton diffusion. A further study of optimal PS parameters predicts an increase in the IQE within bilayer solar cells by about 100%.

Stichworte:
kinetic Monte Carlo morphology organic solar cells phosphorescent sensitizer triplet dynamics