

Experiments and modeling towards organic OPV materials with enhanced charge separating properties

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We have recently predicted that when the dielectric constant of organic semiconductors is increased from 2-4 to about 10, a dramatic increase in (maximal) power conversion efficiency of organic solar cells, based on these materials as active layer constituents, can be achieved.¹ Binding energies of initial excitons, of charge transfer excitons, and between charges in any type of recombination process are diminished with increasing electric permittivity of the medium.

In order to design and develop new molecular materials with higher dielectric constant, the next challenge is to make the connection between the dielectric constant, as a macroscopic property, and molecular structure.

One approach is to connect suitable substituents to known (opto)electronically functional molecular moieties. We report here on the design and preparation of molecules bearing substituents that are to enhance the dielectric properties without diminishing other crucial parameters (like charge carrier mobility, bandgap, stability, etc.).

Through a computational chemistry approach, we investigate the influence of molecular moieties on the relative energies of various charge separated states resulting from photo-induced charge transfer between molecular donors and acceptors. We report on a system in which the energies of the charge separated states are tuned to a favorable situation by proper placement of dipolar substituents.

1. L. J. A. Koster, S.E. Shaheen, J.C. Hummelen, Adv. Energy Mater. 2012, **2**, 1246.