

Investigations on Organic OPV materials with increased dielectric constant

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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.^{1,2} 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.

We will report on the design and preparation of new molecular OPV materials with increased dielectric constant.^{3,4} We will discuss the experimental details and challenges with respect to an accurate determination of the dielectric constant of molecular PV materials.⁵ We will report recent results regarding detailed computational investigations on photoinduced charge transfer at a molecular donor-acceptor interface.^{6,7} Finally, we may report on the performance of new fullerene-based electron extraction layers in hybrid perovskite solar cells.

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