Reduced Coulomb interaction in organic semiconductors: Tailoring the effective system permittivity

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Motivation
The impressive improvement in power conversion efficiency for organic solar cells over the last decade is mainly the result of three developments:
- Material design
- The Bulk-Heterojunction concept
- Morphology optimization

However, one aspect limiting the power conversion efficiency in the organic solar cell development has been ignored. This aspect is the enhanced Coulomb interaction in organic semiconductors as the result of their low permittivity ($\varepsilon_r \approx 3$).

The importance of the Coulomb interaction for OPV cell photocurrent extraction was substantiated by Marsh et al., even for the efficient P3HT:PCBM system.

Using transient optical absorption spectroscopy in dependence of an applied device reverse bias, an extended charge carrier lifetime was demonstrated. This indicates field assisted charge separation.

First OPV device
Realize a device structure which upon charge pair formation during charge transport forces part of the electric field through a high-$k$ structure

Device structure:
- High-SiO$_2$ Nanoparticles
- Under AM1.5 illumination

P3HT:PCBM $+$ SiO$_2$
$\chi = 2.34\%$

P3HT:PCBM
$\chi = 2.00\%$

Benefit for charge carrier transport
Consider the escape energy in an organic material for a test charge in the vicinity of a stationary charge (20 nm above an inorganic material).

Result:
The test charge escape energy at $d = 20$ nm to the stationary charge can be reduced by $\approx 30\%$

Concept
Increase the effective permittivity of the organic system, and in consequence reduce the Coulomb interaction in the organic semiconducotor.

Coulomb activation energy:
$$E_{\text{Coulomb}} = \frac{q^2}{4\pi\varepsilon_0\varepsilon_r}$$

Effective medium electric field simulation for point charges at $d = 4\,\text{Å}$, $1\,\text{Å}$ above inorganic interface

a) Low-$k$ organic and inorganic material.
- Strong field interaction between complementary charges.
b) Low-$k$ organic and high-$k$ inorganic material.
- Low field interaction between complementary charges, total field screening in the inorganic material.

Experimental verification
Considered is the photopumped free charge carrier density as a measure for efficient exciton separation in pentacene on substrates with varying permittivity.

Morphology effects are excluded by taking the ratio of photogenerated free charge carrier density / dark free charge carrier density into account:

This ratio represents a measure for the efficiency in exciton separation.

Benefits for pentacene with an increase in substrate permittivity

The experiment demonstrates a facilitated exciton separation in pentacene with an increase in substrate permittivity

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