Merocyanine Dyes: Novel Materials for Organic Electronics and Photovoltaics

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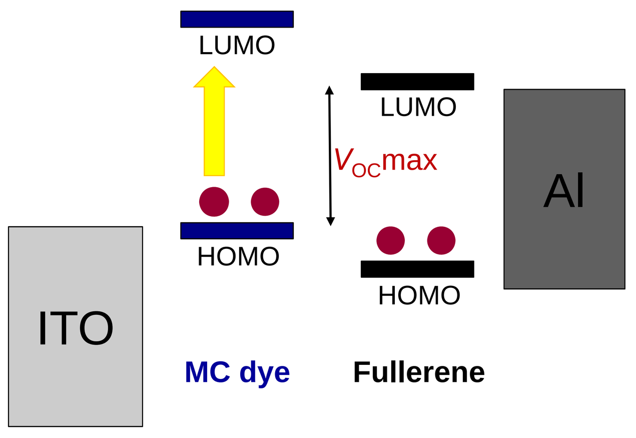
Introduction

Photovoltaic devices based on organic compounds bear the potential for large-scale and cost-effective power generation. Especially, the investigation of organic small molecules electronic materials for organic photovoltaics and thin-film transistors (OTFTs) has attracted considerable interest due to the simple purification procedures of the compounds.

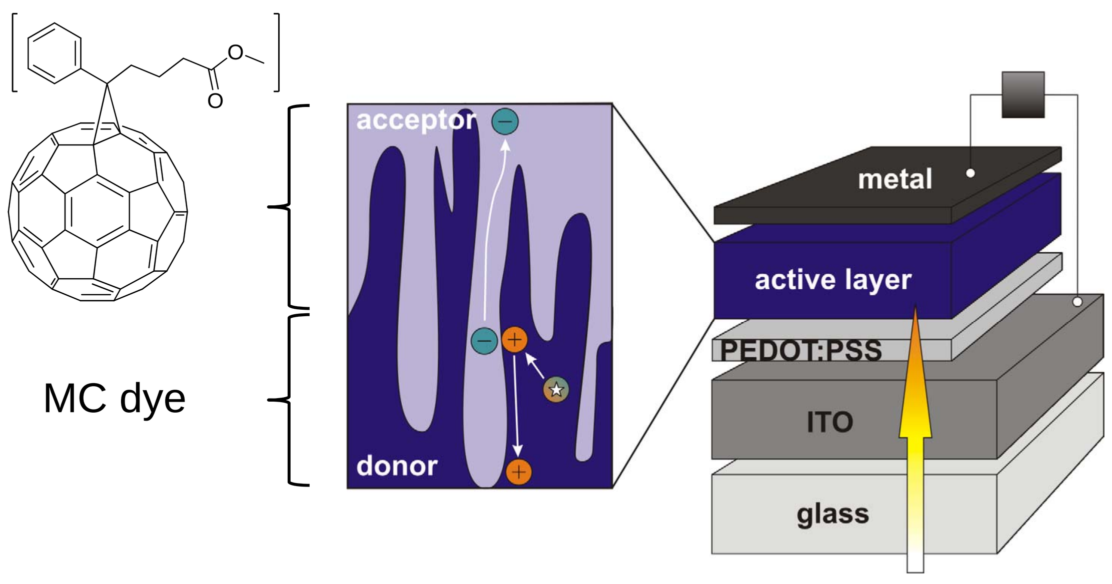
During the last years, we have developed a series of merocyanine (MC) dyes which showed power conversion efficiencies (η) of up to 6.1 % in BHJ solar cells combined with fullerene acceptor materials.[1] Furthermore, we have investigated OTFTs with MC compounds as p-type semiconductors, and reported the first high-performance OTFT based on a highly dipolar donor-acceptor (D-A) molecule.[2]

MC dye based BHJ solar cells

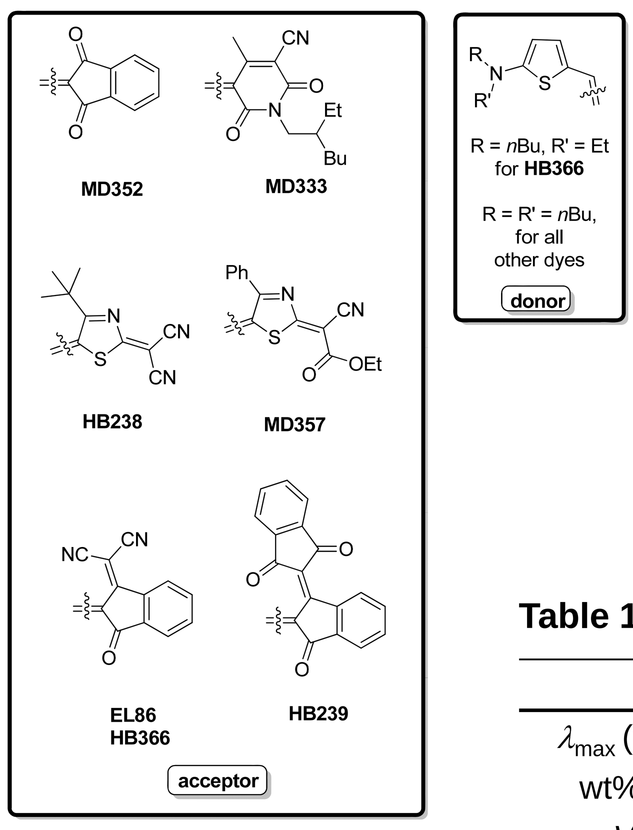


Fabrication methods:

- vacuum-deposition
- solution processing



Variation of the acceptor unit



H. Bürckstümmer *et al.*, *Angew. Chem. Int. Ed.* **2011**, *50*, 11628.

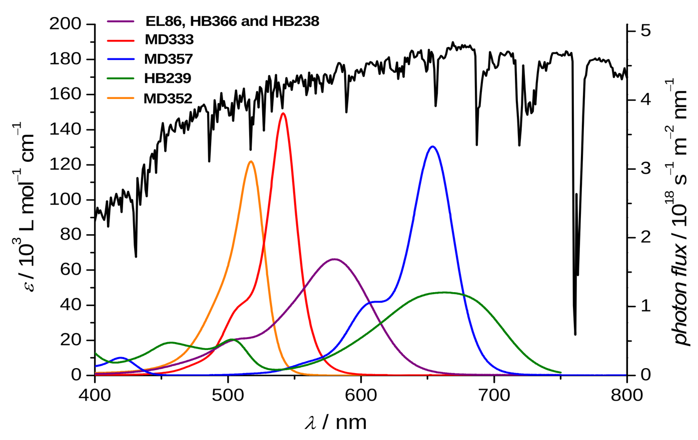


Figure 1. UV/Vis spectra of MC dyes in CH_2Cl_2 and solar photon flux at AM 1.5 conditions (black).

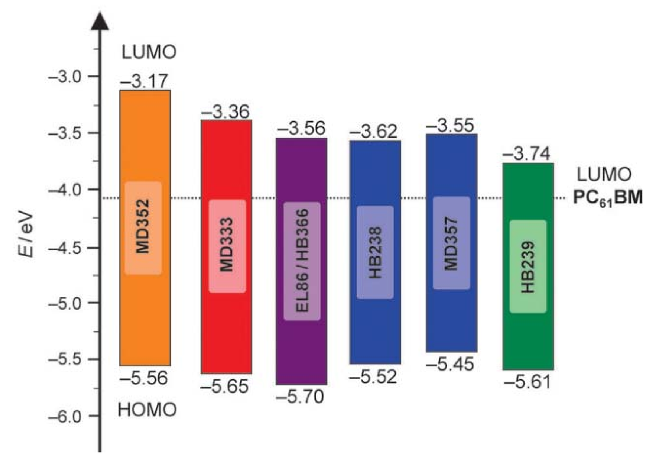


Figure 2. FMO levels, band gaps of dyes and their relative position to the LUMO of $PC_{61}BM$.

Table 1. Cell characteristics of chlorobenzene solution-cast solar cells.

	MD352	MD333	EL86	HB366	HB238	MD357	HB239
λ_{max} (film) / nm	532	556	595	595	682	689	700
wt% PCBM	70	70	60	55	75	70	75
V_{OC} / V	0.63	0.73	0.96	0.94	0.72	0.47	0.68
J_{SC} / mA cm^{-2}	2.9	4.0	5.8	8.3	4.5	4.0	4.0
FF	0.27	0.32	0.41	0.38	0.35	0.27	0.36
η / %	0.5	0.9	2.3	3.0	1.1	0.5	1.0

Best performance

Vacuum-processed BHJ solar cell:

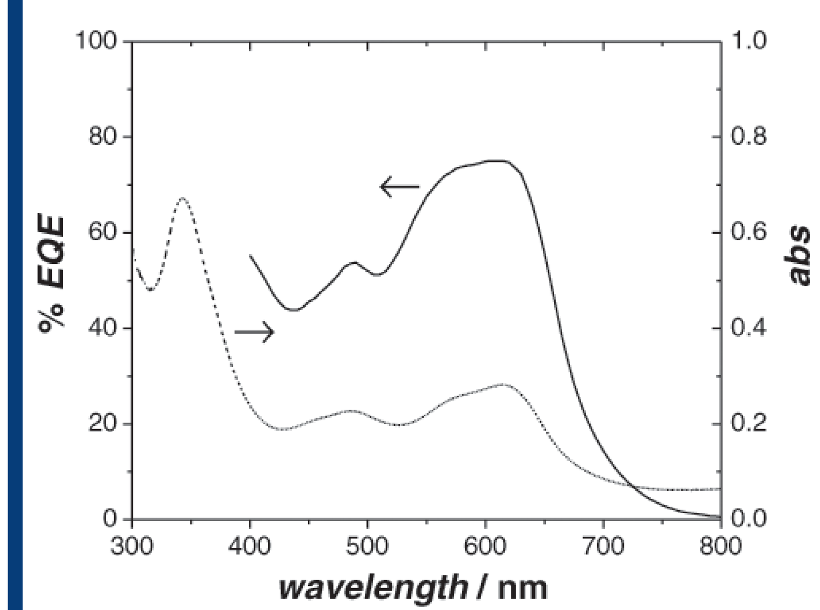
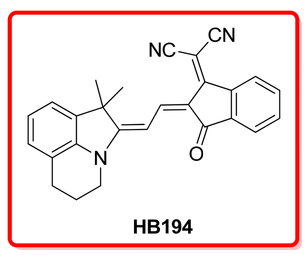


Figure 3. Absorption and EQE spectra of the investigated solar cell.

- active layer (55 nm):
  HB194 : C_{60} = 9 : 11
- exciton blocking layer (6 nm):
  Bphen
- hole-collecting contact layer (20 nm):
  MoO_3



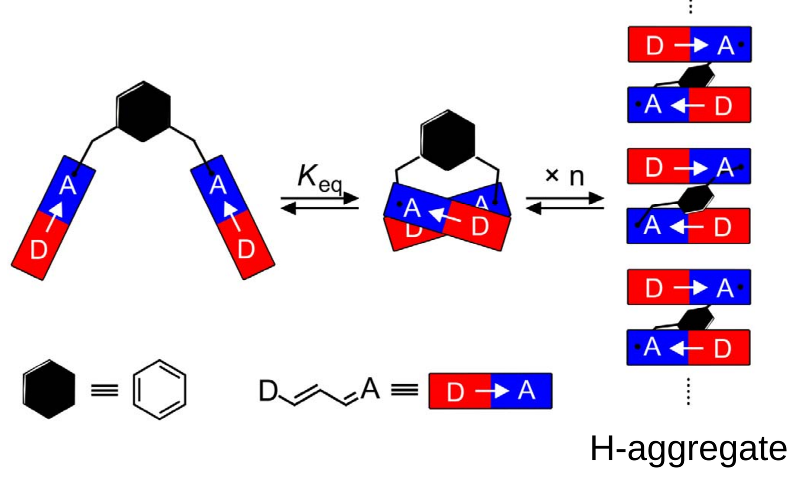
Solar cell characteristics

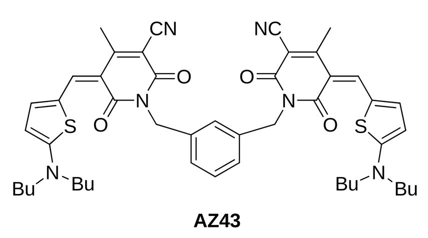
J_{SC} = 12.6 mA cm^{-2} V_{OC} = 0.96 V

FF = 0.47 η **= 6.1%**

V. Steinmann *et al.*, *Adv. Energy Mater.* **2011**, *1*, 888.

Effect of Aggregation





A. Zitzler-Kunkel *et al.*, *Chem. Sci.* **2013**, *4*, 2071.

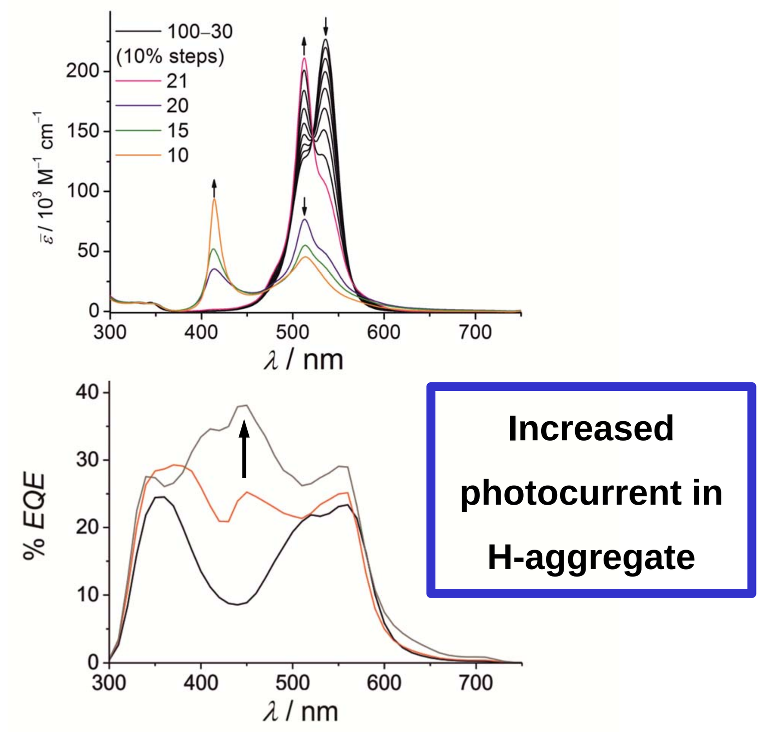
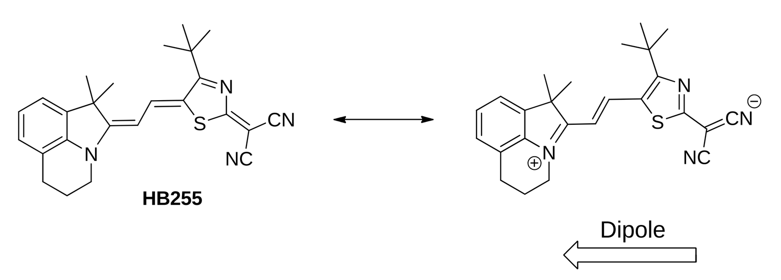
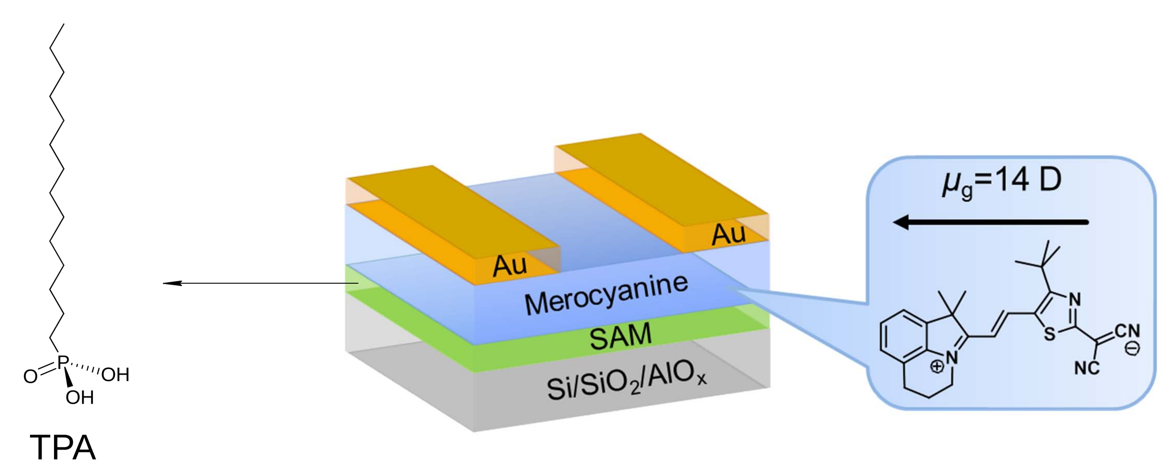


Figure 4. (a) Solvent dependent UV/Vis spectra of **AZ43** in THF/MCH mixtures starting in pure THF (grey) (b) *EQE* spectra of **AZ43**:PCBM (30:70) blends in dependence on the casting solvent mixture $CHCl_3$ (black), $CHCl_3$/toluene (red) and $CHCl_3$/*o*-xylene (grey).

High-Performance OTFT



First high performance OTFT based on a very dipolar D-A molecule



L. Huang *et al.*, *Adv. Mater.* **2012**, *24*, 5750.

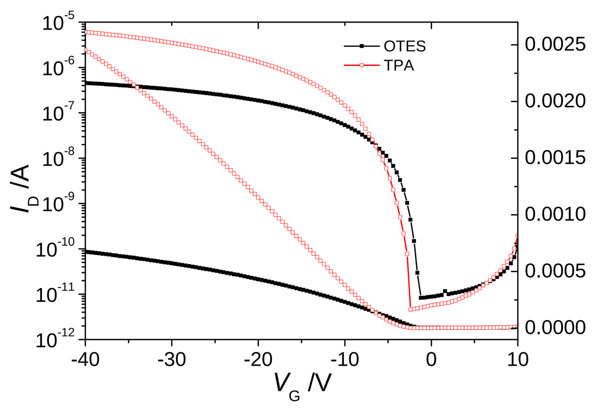


Figure 5. Transfer characteristics of the OTFT (V_D = –40 V).

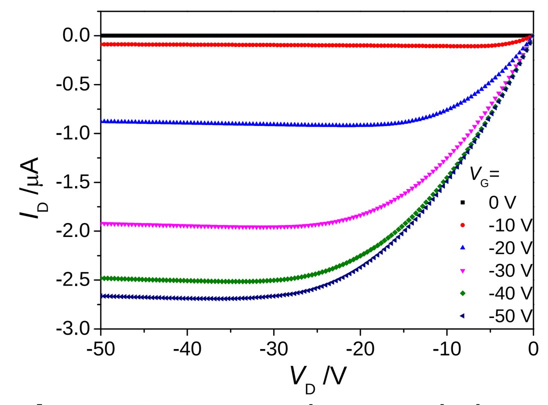


Figure 6. Output characteristics of the OTFT on TPA substrate.

Table 2. Transistor characteristics.

	TPA		
T_s / °C	μ / cm² V^{-1}s^{-1}	V_T / V	I_{on} / I_{off}
80	0.08 - 0.09	–5±1	10^6
100	0.16 - 0.17	–5±1	10^5
120	0.17 - 0.18	–5±1	10^6

Ordered crystalline films and antiparallel π-π-stacking
$\Rightarrow$ **hole mobilities of up to 0.18 cm² V^{-1} s^{-1}**

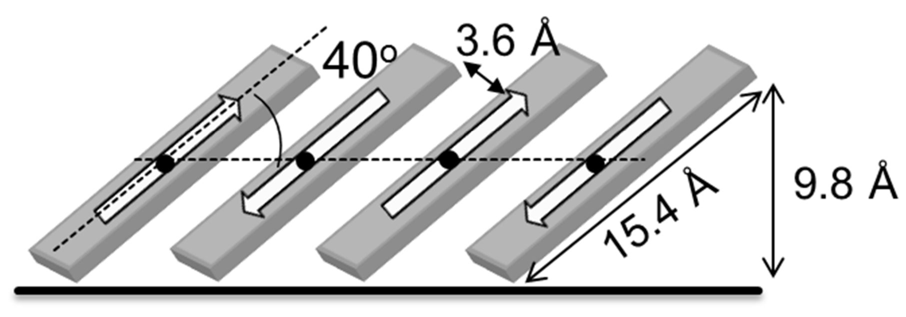


Figure 7. Packing model for thin- films of merocyanine **HB255** on TPA.

References: [1] a) N. M. Kronenberg, M. Deppisch, F. Würthner, H. W. A. Lademann, K. Deing, K. Meerholz, *Chem. Commun.* **2008**, 6489. b) H. Bürckstümmer, N. M. Kronenberg, M. Gsänger, M. Stolte, K. Meerholz, F. Würthner, *J. Mater. Chem.* **2010**, *20*, 240. c) N. M. Kronenberg, V. Steinmann, H. Bürckstümmer, J. Hwang, D. Hertel, F. Würthner, K. Meerholz, *Adv. Mater.* **2010**, *22*, 4193. d) H. Bürckstümmer, N. M. Kronenberg, K. Meerholz, F. Würthner, *Org. Lett.* **2010**, *12*, 3666. e) H. Bürckstümmer, E. V. Tulyakova, M. Deppisch, M. R. Lenze, N. M. Kronenberg, M. Gsänger, M. Stolte, K. Meerholz, F. Würthner, *Angew. Chem. Int. Ed.* **2011**, *50*, 11628. f) V. Steinmann, N. M. Kronenberg, M. R. Lenze, S. M. Graf, D. Hertel, K. Meerholz, H. Bürckstümmer, E. V. Tulyakova, F. Würthner, *Adv. Energy Mater.* **2011**, *1*, 888. g) A. Zitzler-Kunkel, M. R. Lenze, K. Meerholz, F. Würthner, *Chem. Sci.* **2013**, *4*, 2071. [2] L. Huang, M. Stolte, H. Bürckstümmer, F. Würthner, *Adv. Mater.* **2012**, *24*, 5750.